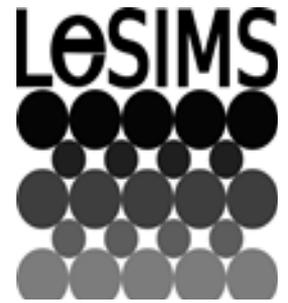




Ferhat ABBAS SETIF 1 University - Faculty Of Technology
Laboratory of Surfaces and Interfaces Studies of Solid Materials
(LESIMS)

- Materials and thin films synthesis characterizations and applications
- Soft Condensed Matter
- Magnetic Materials
- Semiconductor Materials
- Optoelectronic Materials
- Nanomaterials
- Functional Materials.
- Computational Materials Science

ICMS 2018 International Conference on Materials Science September 12-14, 2018



International Conference on Materials Science (ICMS2018)

Abstracts Book

11 September 2018

WELCOME MESSAGE

On behalf of the Scientific and Organizing Committees, we are pleased to extend you a very cordial welcome to the International Conference on Materials Science (ICMS2018) held at Ferhat ABBAS SETIF1 University. We would like to thank all the delegates for attending and for their efforts in making ICMS2018 a success. We are thankful to all our invited speakers for accepting our invitations and offering to share their knowledge with the ICMS2018 delegates.

This event *ICMS2018* has been planned to present up to date research and results in the field of emergent and functional materials. The Conference provides also an occasion for the delegates to share their findings and exchange advanced ideas and applications to establish a fruitful research and business relationship with each other. Indeed, it is a platform for the researchers to find global partners for future collaboration. ICMS2018 provides a productive platform with a motivating strength for material scientists, solid state physicists, chemists, engineers, technologists...The main conference topics consist of *Materials and thin films synthesis, characterizations and applications, Soft Condensed Matter, Magnetic Materials, Semiconductor Materials, Optoelectronic Materials, Nanomaterials, Functional Materials and Computational Materials Science*. We are immensely thankful to all the Responsibles of these topics, Profs. Amor AZIZI, Abdelkader BOURZAMI, Ahmed KHARMOUCHE, Nouredine BENOUEATTAS, Azeddine CHELOUCHE, Abdelkrim ROUMILI, Nouredine BOUAOUADJA, Abdelmadjid BOUHAMADOU, Ammar MOSBAH and Abdelghani MERDAS, for their efforts in evaluating the large number of submitted abstracts. We are especially grateful to our Colleagues, Profs. Kamel OUARI and Messaoud GUELLAL, for their efforts to design the different certificates. We are also very thankful to the Websmaster, Mr. Nassim BENACHOUR, for the effort and energy spend in managing the ICMS2018 Platform. Prof. Lahcene BENCHEIKH, my longtime friend, spared no effort to welcome our guests overseas and made sure everything went well, every day.

We hope you will enjoy the conference and will tremendously benefit from attending ICMS2018. Enjoy the Conference, enjoy SETIF and enjoy ALGERIA.

Prof. Ahmed KHARMOUCHE
ICMS2018 Conference Director



Prof. Dr. Ahmed KHARMOUCHE
Conference Director

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International Conference on Materials Science ICMS2018

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The Conference registration desk is located at the lobby/Salah KARMI Conference Room. All participants are kindly asked to go to the Registration Desks upon arrival. Access to the conference site will be only possible for registered participants. You are required to wear your name badge during the whole conference.

The ICMS 2018 Conference Registration desk will be open at the following times:

11 September Tuesday 14:00-17:00

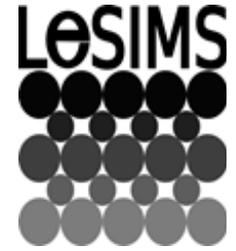
12 September Wednesday 7:30-17:00

13 September Thursday 7:30-15:00

CULTURAL PROGRAM

You are kindly invited to visit the archeological site of DJEMILA (CUICUL) on Friday morning, September 14th

**MATERIALS AND THIN FILMS SYNTHESIS,
CHARACTERIZATIONS AND APPLICATIONS**



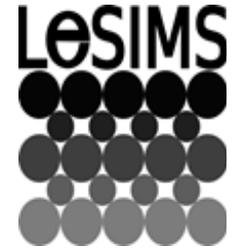
Effect of variation of operational parameters on the grapheme deposition

Mehdi Laoufi

Université de Chlef Laboratoire Eau et environnement, Algeria.

Abstract:

This work consists of modeling and simulating the deposition of graphene films by CVD (chemical vapor deposition) on a catalytic metal (Copper) which represents the result of a surface reaction and implying several gas phase reactions, and for the goal is to predict growth rates in order to obtain a uniform monolayer of graphene, we chose methane as carbonaceous source and the argon as an inert gas. Simulations were performed by using computer code FLUENT <6.3.26>, while trying to see the effects of the parameters such as: choice of precursor gases, the geometry of the reactor, models of calculation of the physicochemical properties, operating temperatures and pressures and essentially the mechanism and reactions retained. The results obtained (in the form of velocity fields, of isotherms, distribution of mass fractions of the components) show that the precise modeling of the hydrodynamics depends mainly on the composition and the flow rate of the mixture on the entry of the reactor, and the difference in the deposition rate is considered due to a change in the thickness of the boundary layer along the substrate.



Growth and characterisation of Czts single crystal

Safia Kerour

*Department of Electronics, Faculty of Technology, Ferhat Abbas University of Setif-1
Electrochemical and Materials Laboratory; Algeria*

Abstract:

In this work, we report the synthesis of $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) single crystal by cooling a molten stoichiometric of Cu, Zn, Sn and S elements. Weighed stoichiometric proportions were charged into a 200 mm length and 14mm diameter quartz tube sealed off under 5×10^{-6} Torr, placed in a horizontal furnace then heated up gradually. Secondary phases between Cu, Zn, Sn with S were formed by keeping the tube in below temperature range (200-700 °C) for 24-48h to reduce the vapor pressure and avoid any explosion in high temperature [1-3]. To ensure homogeneous mixing of the melt, the tube was kept at 1100 °C for 24-48 h. The furnace was then cooled down freely reaching room temperature. Removed from the quartz tube, the CZTS ingot was about 25 mm. The ingot chemical composition analyses determined by Energy Dispersive Spectroscopy (EDS) were found to be nearly stoichiometric. The crystal bulk structure was analyzed by using powder X-Ray Diffraction (XRD), the diffraction peaks indicate a remarkable crystalline nature with preferred orientations of (112) plan. We carried out the Raman measurements which indicate that crystal adopts a kesterite structure without secondary phases.



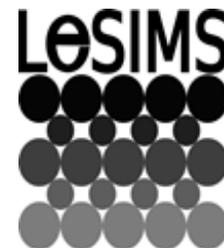
Elaboration and characterization of composites materials based on polypropylene/fumed silica nanoparticles: effect of surface treatment and compatibilizer agent

Lasmi Sofiane

Research unit of emerging materials, Ferhat Abbas Setif.1 University; Algeria

Abstract:

In the last years, inorganic nanoparticles filled polymer composites have received increasing research interests of materials scientists, because the filler/matrix interface in these composites might constitute a much greater area and hence influence the composites properties to a much greater extent at rather low filler concentration as compared to conventional micro-particulate composites [1, 2] in this study a composite material based on polypropylene and fumed silica nanoparticles were elaborated by melt compounding in an internal mixer, the effect of surface treatment of silica nanoparticles with the stearic acid (1Wt%, 2Wt%) and PP-graft-MAH as a compatibilizer (1Wt%, 2Wt%) on various properties of fumed SiO₂-filled polypropylene composites were studied. The mechanical properties of polypropylene matrix reinforced with silica nanoparticles were determined by tensile and impact test. The reaction of maleic anhydride groups with the hydroxyl groups on the surface of nanosilica was characterized by FTIR spectrum. The final nanocomposites result in a further improvement of mechanical properties because of silica agglomerate reduction and improving interface combination, even loading level being much lower than that of ordinary fillers in conventional composites.



Electrochemical study of self-assembled organic monolayers on a thin silver layer

Amira Madi

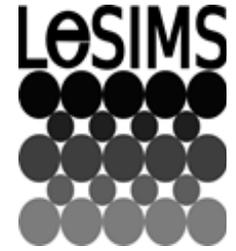
Ferhat Abbas University of Setif 1, Algeria

Abstract:

Nowadays, the construction of nano-structured materials is a technological approach in full swing. It is based on the design, creation and study of complex structures, consisting of simple elements of nano-metric size. These new materials are generally characterized by particular optical, electronic and chemical properties. The aim of the work is composed of two parts: the first is devoted to the study and the formation of a silver film on a copper support. Industrially these films are obtained from cyanide baths. The substance of the toxicity of these products, research on the formation of thin silver deposits is oriented to other non-toxic baths. The second aim is the study of the electrochemical properties of self-assembled octadecanethiol monolayer on silver deposit.

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Adhesion and corrosion of Ti, TiN and TiCrN films in a simulated physiological solution (SBF)

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¹*Département of mechanical engineering; Algeria*

²*University of Abderrahmane MIRA, faculty of Technology, Département of procedia engineering, Algeria*

³*Master of research was at the Centre of development of technical progress (CDTA); Algeria*

Abstract:

Ti, TiN, and TiCrN films have been deposited by magnetron sputtering on 316L stainless steel substrates to improve their surface properties. Electrochemical performances and adhesions of these deposits in a simulated physiological solution (SBF) were studied and compared. As a result, the TiCrN deposition has the lowest corrosion resistance in the SBF solution because of the presence of a high density of porosity in its structure. The TiN deposit has shown good resistance to corrosion, but its critical load (L_{c3-TiN}), corresponding to its removal from the substrate is relatively low and has a risk of delamination, which can limit its use. However, the Ti deposit has a high resistance to corrosion ($i_{corr}(Ti) = 0.57 \cdot 10^{-6} \text{ A.cm}^{-2}$ and $R_p(Ti) = 67.98 \text{ KW.cm}^2$). These parameters provide testimony to its strong passivation. The critical load (L_{c3-Ti}), the crack propagation resistance ($CPRs-Ti$) and the scratch hardness (HS_L-Ti) also testify to its high adhesion to the 316L substrate. Thus, the Ti deposit has proved to be the most favorable protective coating for 316L stainless steel in an SBF solution.



Elaboration and characterization of erbium electrodeposited on silicon nitride

Afaf Brik

Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE) 2 Bd Frantz Fanon, B.P.140 Alger-7 Merveilles, Algiers (Algeria), Tel & Fax: +213 21433511, Algeria.

Abstract:

In this work, we report on the electrochemical deposition of Er-doped silicon nanostructures grown in silicon rich SiN_x:H films (SRSN). Silicon nanocrystals have been produced by thermal annealing of SiN_x thin film obtained by low pressure chemical vapor deposition using a mixture between silane and ammonia. The applied doping process consists in a simple electrochemical deposition technique followed by a high temperature annealing step. The morphology, structural and chemical properties of the annealed Er-doped SRSN were studied using X-ray diffraction, scanning electron microscopy, and secondary ion mass spectrometry. Optoelectronic behaviors of the nanostructures were studied using micro-Raman and photoluminescence spectroscopies at room temperature. SIMS have revealed the distribution of the elements: Si, N, O, P, Cl et Er in the structures. Surface scanning electron microscopy (SEM) show Er concentration distribution in agglomerates around nanocrystalline particles. The characterization by photoluminescence of erbium doped based on heat treatment conditions show that oxidation at 900 ° C for an hour under O₂ followed by an annealing at 1000 ° C under N₂ for 2 hours allows having a best luminescence of erbium ions. The results presented in this paper indicate that erbium doped silicon rich silicon nitride affords promising applications in electronic and optical technologies.

Keywords: Erbium, Silicon nitride, electrochemistry, photoluminescence (PL).



Characterization and deposition of Sprayed cupric oxide (CuO) thin film and their sensing application

Meryem Lamri Zeggar
University Constantine 1; Algeria

Abstract:

Recently cupric oxide (CuO) thin films have attracted much interest as a promising material for photovoltaic, monoxide and dioxide sensor gas and photocatalysis applications [1-3]. The present work deals with CuO thin films deposition by a simple and easy technique such as ultrasonic spray pyrolysis, and the investigation of the influence of deposition parameters on films structural, optical and electrical properties. A set of CuO thin films were deposited at different substrates with temperatures in the large of 280-350°C using a precursor solution formed with the dissolution of copper salt in distilled water. The structural proprieties were characterized by mean X-ray diffraction (XRD). The optical properties were studied by mean of UV-visible and near-infrared spectroscopy. The conductivity was measured by the electrical D.C transport. XRD studies demonstrated the formation of pure CuO films. The optical transmittance spectra show a high absorption in the visible region. The electrical conductivity rise with an increase of substrates temperature. We have reported the dynamic sensing behaviour of the CuO sensor towards methanol gas. The sensor was tested at operation temperature equal to 50°C and for methanol concentrations of 300 ppm. The fabricated CuO based sensor exhibit high sensor response and low operation temperature which are very promising agreements for industrial applications.



Synthesis And Characterization of New Composite Films (ITO/PBTh-MnO₂) and their Luminescence Properties

Ahmed Bahloul, H. Zouaoui, D. Abdi

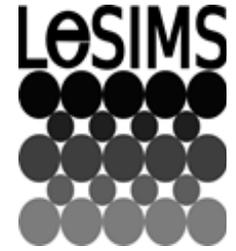
Université Mohamed El Bachir El Ibrahimi Faculté des sciences et de la technologie; Algeria

Abstract:

Polythiophenes constitute a particularly important class of conjugated polymers, which has been extensively studied for the relation between the geometrical structure and the optic and electronic properties. They are, furthermore, chemically and thermally stable materials, and are very attractive for exploitation of their physical properties [1]. The observation of photocurrents from polythiophene-modified metal electrodes has been reported by several groups of investigators [2, 3]. In this work, a composite thin film containing polybithiophene (PBTh) and manganese dioxide (MnO₂) on indium tin oxide (ITO) glass substrates was prepared by electro-polymerization of bithiophene in the presence of MnO₂ nanoparticles. The films ITO/PBTh-MnO₂ are characterized by AFM and SEM, the analyses show an increase in roughness and the incorporated MnO₂ particles are of size in the range of 50 nm. As a result, the optical gap is shifted by the incorporation of MnO₂ nanoparticles from 2.23 eV for ITO/PBTh to 2.03 eV for ITO/PBTh-MnO₂. The photocurrent measurements indicate that the ITO/PBTh-MnO₂ films show a value that is three times higher than that of polybithiophene substrate, so that such a composite can be used as a new active material in solar cells.

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Fabrication of A2024-T3/Al₂O₃ and A2024-T3/Ti₃SiC₂ Surface Composites By Friction Stir Processing

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¹Laboratoire des aeronefs; Algeria

²Centre de Recherches et Technologies Industrielles, CRTI, Cheraga, Algiers, Algeria.;
Algeria

Abstract:

Herein we present the fabrication of metal matrix composites (MMC) through Friction Stir Processing (FSP). The latter is one of new methods of fabricating surface composites through stirring process of a soft materials as aluminium alloys, magnesium and copper. MAX phases are new Nano laminated ternary ceramics, which combines some of best metals and ceramics properties, this later make them good enhancement phases for MMC. In this work, new A2024-T3 composites reinforced with Al₂O₃ and Ti₃SiC₂ hard phases are used to investigate their effect on microstructure, hardness and tribological properties. A ball-on-disc tribometer under dry sliding conditions, at room temperature, were used to study the wear and friction properties of these new composites. Scanning Electron Microscopy were used to analyse and determine the wear mechanisms occurring in the worn surfaces under different applied normal loads.



Thermal insulating behaviors of polypropylene/spanish broom flour composites

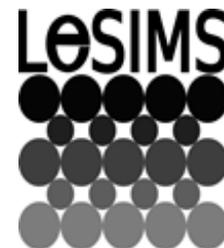
Zouaoui Nouar Fairouz, Nauar Yacine, Nekkaa Soraya

Laboratoire de Physico-chimie des Hauts Polymères, Département de Génie des Procédés, Faculté de Technologie, Université Ferhat ABBAS - Sétif1; Algeria

Abstract: The present work reviews current research on the field of green composites. The effect of chemical treatment on thermal and thermophysical properties of Polypropylene/Spanish Broom flour composites has been investigated. Polypropylene (PP) is a non-polar matrix; therefore it has a poor adhesion towards polar SB flour. Because an emphasis was put on evaluating the effects of modification, two chemical treatments like sodium hydroxide and silane were performed in order to reduce the hydrophilic behavior of SB flour, and to improve the interfacial adhesion PP-SB. The thermophysical study was performed according to ISO 22007 on transient plane source (TPS 2500S) Hot Disk. The heating powers were 11, 19 and 23 mW for a measurement time of 10 seconds. The thermal conductivity of the flour-reinforced composites increased after every treatment due to improved interfacial interactions. However, for flour ratio low than 20 wt%, we note a decrease of thermal conductivity of composites (i.e., under 19 mW: from 0.2668 W/m.K for neat PP to 0.2699 W/m.K for PP/10 wt% Untreated SB, 0.2562 W/m.K for PP/10 wt% SB-NaOH, and 0.2293 W/m.K for PP/10 wt% SB-VTMS, respectively). For an SB content of 20 wt%, the thermal conductivity values of all PP/SB composites are almost identical to those of neat PP, but beyond 20 wt%, there is a significant increase in thermal conductivity, and this is reflected in a lowering of the total temperature increases.

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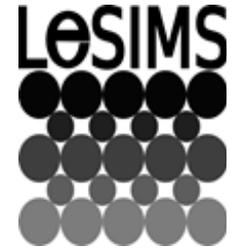
Physical properties of SnS thin films grown by ultrasonic spray

Imane Bouhaf Kherkhachi, Abdallah Attaf, Hanane Saidi, Zidane Hebboul

Physic Laboratory of Thin Films and Applications LPCMA, University of Biskra, Algeria; Algeria

Abstract:

Tin sulfide thin films (SnS) have been deposited by ultrasonic spray on glass substrate at 300°C. The influence of flow rate (25-60ml/h) in the crystal structure and optical properties was determined by X-ray diffraction and UV spectroscopy visible. *X-ray diffraction studies indicate that films have a hexagonal structure with peaks corresponding to SnS₂ hexagonal phase with preferential from (001) plane and other peaks of minimum intensity corresponding to SnS and Sn₂S₃ phases.* The grain size, lattice constants and strain in films were calculated. The studies on the optical properties show that the direct band gap value ranged from 2.57 to 3.86 eV and the films deposited at solution flow rate 60 ml/h show low optical transmittance (36%).



Properties of Ni:ZnO thin films deposited by pneumatic spray pyrolysis

Labidi Herissi

Larbi Tebessi University - Tebessa, Algeria; Algeria

Abstract:

Thin Ni:ZnO films were prepared onto glass substrates by pneumatic spray pyrolysis technique from zinc acetate dihydrate and nickel chloride hexahydrate solutions dissolved in distilled water. Solution concentration, substrate temperature and nozzle-substrate distance were kept constant during all deposition process at 0.05 mol/l, 350 °C and 30 cm respectively. Effect of nickel content on the structural, optical and electrical properties of as-prepared films was investigated by X-ray diffraction, UV–Vis-NIR spectrophotometer and four-point probe technique. The results indicate that the deposited films are homogeneous surface, good Transparency (60-70%), well adherent to the substrates and present surface roughness [1]. With increasing the Ni concentration in the solution of precursor sources, the both grain size, Urbach energy, and electrical conductivity of the films deposited are increasing although these films have optical energy gap almost constant ($E_g=3.3$ eV) that indicated the presence of the hexagonal phase of ZnO [2]



Synthesizing of hydroxyapatite powder for thin films applications

Selma Attabi¹, Majda Mokhtari², Hicham Elmsellem³, Abed Elaziz Himour¹

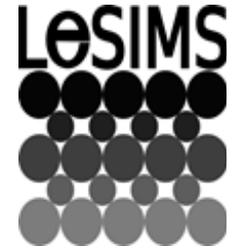
¹University of Badji Mokhtar, BP 233 RP, Annaba, Algeria; Algeria

²University of Echahid Hamma Lakhdar, El-Oued; Algeria

³University of Mohammed Premier, B.P. 717, 60000 Oujda, Morocco

Abstract:

Hydroxyapatite, with chemical formula $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, is a calcium phosphate compound regrouped with bioactive ceramics. Thanks to its best properties of biocompatibility, ostéoconduction, ostéoinduction, and of thermal stability, this mineral material was used intensively as thin film, especially on titanium alloys, in the fabrication of functional biomaterials[1]. THydroxyapatite (HAP) has better physicochemical properties thanks to its molar ratio Ca/P which is always fixed at 1,67 [2]. However, obtaining these good characteristics depends directly on the control of this molar ratio and thus on the control of synthesizing method of this material's powder. The pulverulent substance based on hydroxyapatite can be obtained by various methods. In this work, we study the elaboration of HAP powder by the method of double decomposition "in aqueous phase", which is very much used by industries thanks to its facility and its moderate cost. Thereafter, the powder was characterized by diffraction of x-rays, a thermal analysis TGA-DSC, and Fourier transform infrared spectroscopy to examine its characteristics. Results show that the chosen method of elaboration produces a powder with good properties that can be used in the synthesizing of thin films.



Wetting behavior of Ti_2AlC/Ti_3AlC_2 composites with Cu and Al fillers during tungsten inert gas (TIG)-brazing

Nabil Chiker¹, Abdessabour Benomar¹, Adel Haddad¹, Youcef Hadji¹, Mohamed Hadji¹, Mohamed Benamar²

¹Laboratoire des Aeronefs, University of Blida 1; Algeria

²Laboratoire de physique fondamentale et appliquée, University of Blida 1; Algeria

Abstract: Nanolaminated ternary ceramics with the general formula $M_{n+1}AX_n$ ($n= 1, 2$ or 3) have recently been defined as MAX phases, where M is a transition metal, A is a group IIIA-VIA element and X is C or N [1]. Ti_2AlC and Ti_3AlC_2 are fascinating members of this series and are renowned for their superior properties, i.e., low density, good thermal and electrical conductivity, self-lubrication, high thermal stability and excellent mechanical properties under irradiation. Similar to most other ceramics, large Ti_2AlC or Ti_3AlC_2 ceramics are difficult to synthesis due to their narrow phase range in the Ti-Al-C ternary phase diagram [2]. A common approach to this problem is to join the ceramics, by which the manufacture of large, complex, multifunctional ceramic components can be realized [3]. Therefore, studies on the joining of Ti_2AlC are significant in promoting the ceramic's applications. In recent years, a few studies have focused on the joining of MAX phases. The purpose of our work is to report, for the first time, on the development of our initial attempts to TIG-braze Ti_2AlC/Ti_3AlC_2 (TAC) composite with Cu and Al. The microstructures of the interfaces were investigated by scanning electron microscopy and energy dispersive spectrometry. Intensive interactions including dissolution and diffusion simultaneously occurred within the TAC at the TAC /Al interface during TIG-Brazing. The interfacial region between the TAC and Al filler is comprised of an interaction layer zone and a modified Aluminum zone. When the TAC comes into contact with the Al molten filler during TIG-brazing, it starts decomposing into $TiC_x + Al_{Liquide} + Al_{gas}$, and simultaneously, a deep penetration of the molten Al into the TAC occurred to form a mixture of two intermetallic [$TiAl_2$, $TiAl$] and TiC phase. The phases that most likely form when TAC is joined with Cu filler material are Cu in which some Al is dissolved, TiC_x and $Ti(CuAl)_2$. No cracks were observed during TIG joining of TAC with Al or Cu brazing filler materials.

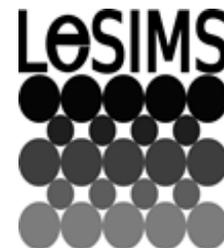
Keywords : MAX phases, Ceramics, TIG, dissolution

References:

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[3] Y.M. He, J. Zhang, C.F. Liu, Y. Sun, Mater. Sci. Eng. A 527 (2010) 2819–2825.



Heterogeneous UV-Fenton catalytic degradation of synthetic dye with MgCuFe-CO₃

Zoubir Manaa

Ferhat Abbas Setif University, Algeria.

Abstract: This work aims to optimize layered double hydroxide composition and its derivatives containing two transition metals which have an important effect in heterogeneous Fenton oxidation; iron and copper, synthesized by a classical method co-precipitation followed by calcination to produce the mixed oxides. The use of experimental design of mixture is to optimize the LDH ratio component. The material has been characterized by different methods such as, XRD, SEM, ATG/ATD, Particle size distribution and UV-DRS. The degradation of the synthetic dye patent blue V was investigated by studying the different effects of parameters; pH, dye initial concentration, H₂O₂ dose and photocatalyst loading. The catalytic reaction showed a good performance of oxidation of the dye in a wide range of pH especially in natural pH. The catalyst saves its activity after several reutilizations demonstrating its stability and its promising long-term application in the treatment of wastewater.

Keywords: heterogeneous Fenton-like, layered double hydroxide, degradation, synthetic dye, catalyst stability.

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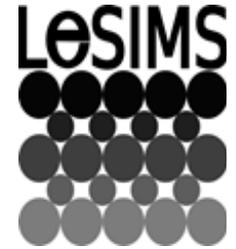
Structural and Optical properties of cuprous oxide Cu₂O Thin Film

Lakhdari Deloulla

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Abstract:

Polycrystalline Cu₂O layers have been prepared by cathodic reduction of an alkaline cupric sulfate solution on transparent conducting glass (FTO). X-ray diffraction (XRD) study revealed the formation of single cubic Cu₂O films. The nanocrystallite size is about 28 nm. The as-deposited films thickness was estimated at approximately 6 μm. The effect of pH solution on the structure is studied. Scanning electron microscopy image shows the pyramid structure of Cu₂O thin film deposited at -0.555V versus Ag/AgCl. The band gap of the film was estimated from transmittance spectra to be about 2.34eV.



Structural, Surface morphology and electrical properties of evaporated Permalloy Ni₈₀Fe₂₀ /Si (100) thin films

Ounissa CHERRAD

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Abstract: In the present paper, we have studied the effect of the thickness on the structural, surface morphology and electrical properties of Permalloy (Py) thin films Ni₈₀Fe₂₀ (Py). For then, a series of Py thin films samples were successfully evaporated on Si (100) substrates. Thereafter, we have opted for few characterizations in order to refine our study. In this context, we found that the growth interval of the thickness lies between 110 nm and 505 nm. XRD spectra analysis reveal that our samples were polycrystalline and principally growth within <111> and <200> textures. Lattice parameters for Py/Si (100) samples were found to be very close to that of bulk NiFe “Py” ($a_{\text{bulk}} = 3.5385$). As thickness of our samples increase from 110 to 505 nm, we found that grain size obtained from Scherrer formula expend in an abrupt manner from about 56 Å to 134 Å. Visualization of our samples surface was carrying out using an atomic Force Microscopy “AFM”. Our samples behave relatively smooth with little surface roughness. Consequently, the RMS factor values were a somewhat weak that change in the range from 1.324nm to 0.201nm. A good relationship was established between RMS factors, thicknesses and resistivity values. This last have reached their highest value of about 94.33μΩ.cm when thickness enlarges to about 505Å. As thickness rise, Py samples become little more resistive and rough. Indeed, this is was our ambition to refining this work and get more discussions about the influence of thickness evolution on surface morphology and electrical properties of Ni₈₀Fe₂₀ Py samples.

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Effect of Mn doping on the structural and optical properties of ZnO thin films

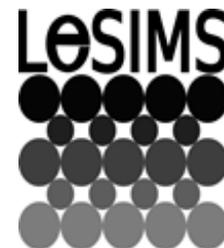
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Abstract: In this work, we have studied the influence of Mn doping on the structural, morphological, optical and photoluminescence (PL) properties of ZnO thin films. ZnO thin films with different concentrations of Manganese (0, 2 and 4 mol.%) were prepared by the sol-gel spin coating process and synthesized on glass substrates. By using an X-ray diffractometer (XRD) (Bruker 8 Advance) with Cu- α radiation having a wavelength $\lambda=1.5406 \text{ \AA}$, the structural properties of the films were characterised. To evaluate the band gap, the optical transmission spectra were measured by an ultraviolet-visible (UV-vis) spectrophotometer (UV-3101 PC-Shimadzu) in the spectral range 300-800 nm. Photoluminescence (PL) measurements were recorded using a spectrofluorimeter (Perkin Elmer LS 50B) with the excitation wavelength of 325 nm.

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Electrocrystallisation of Nickel-Raney electrode material for the production of hydrogen by alkaline water electrolysis

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Abstract: In this work we report the preparation of Nickel Raney coating providing high catalytic activity towards the hydrogen evolution reaction (HER) [1] by leaching electrodeposited zinc-nickel alloys. The electrodeposition process was carried out in a citrate-based bath at room temperature under potentiostatic regime. The ZnNi alloys coated at -1.3 V vs. SCE onto copper and low-carbon steel sheets sized 1x2 cm² contained 18 wt% Ni. The XRD study revealed the presence of the main peaks corresponding to γ -phase structure [2]. The as-deposited coatings showed excellent corrosion resistance in 3.5 wt% NaCl solution. The surface morphology studied by scanning electron microscopy (SEM) before and after leaching in 5M KOH revealed the dissolution of the superficial amount of zinc in the surface of the deposits, leading to an increased active surface area. Such electrode materials have become increasingly requested in the production of hydrogen [3] by alkaline water electrolysis.

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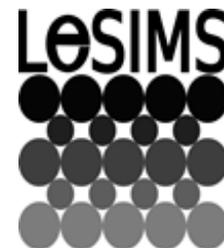
Current transport mechanism of Cd doped TiO₂ films based on MOS device

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Abstract:

Cd doped TiO₂ thin films were deposited onto n-type Si (100) substrates by the sol-gel dip-coating method. The samples treated at temperatures ranging from 600 to 1000°C for 2h. The effect of annealing temperature on the structural, morphological and electrical properties was studied by X ray diffraction (XRD), Atomic force microscopy (AFM) and Current-Voltage (I-V) characteristics. XRD analyzes shows that the crystalline phase of Cd:TiO₂ thin films comprised only the anatase phases and the crystallinity was enhanced by increasing the annealing temperature. From AFM micrographs, the films are dense and continuous, the surface is well covered with a relatively large grains and pinholes free. The Al/Cd:TiO₂/n-Si diode was formed by using Cd:TiO₂ film deposited at 1000°C, the different electrical parameters of such as ideality factor (n), series resistance (R_s) and saturation current (I_s) were calculated from (I-V) characteristics at room temperature. The obtained results show that the prepared Cd:TiO₂ films can be used for semiconductor device applications



Effect of the Masse Loading on the Oxygen Reduction Reaction Kinetics of the Nanocrystalline $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ Perovskite in Alcaline Medium

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Abstract: The oxygen reduction reaction (ORR) has been studied at length due to its great importance in energy conversion and storage devices, and extended to alkaline fuel cells[1], electrolyzers [2], and metal-air batteries[3]. Alternative non-precious metal oxides with comparable ORR activity to Pt-based catalysts are highly desirable for the development of fuel cells. In this regard, oxides with perovskite structure (ABO_3) have received wide attention due to their high activity and stability when used in alkaline media[4]. Recently, considerable attention has been paid to strontium doped-perovskite materials, e.g. $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (LSMO) as cathode catalysts. These materials are broadly established as ORR/OER bifunctional electrode materials. The particle size and microstructure are significant for the electrodes' performance[4,5]. As one of the most frequently used oxygen electrode of alkaline[5] and oxide[6] fuel cells, $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ (LSMO) perovskite oxide has proved promising catalytic properties[6]. Although this perovskite oxide, mentioned above, has provided interesting electrocatalytic properties in fuel cells, the literature however reports, to the best of our knowledge, few studies about the effect of the preparation method using low temperature synthesis during a short heating time (1h) on the properties of LSMO perovskite as an oxygen electrode. In this work, a Pechini route has been successfully used to synthesize homogeneous nanometric $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ powder with high purity. The influence of mass-loading on the ORR kinetics of this perovskite in 1M NaOH medium was examined.

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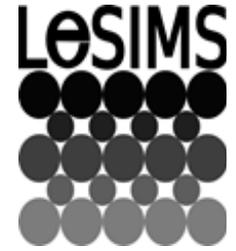


Comparative study on the influence of ZnO incorporation on the morphological properties of HDPE / ZnO and PVA / ZnO nanocomposites

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Abstract:

Filler-based materials dispersed in polymeric, metallic or ceramic matrices have many advantages over traditional materials. The objective of this work is a comparative study on the influence of ZnO incorporation on the morphological properties of HDPE / ZnO and PVA / ZnO nanocomposites. The preparation of the PVA-based mixtures was carried out by solvation in water, with different percentages of ZnO, namely 0.05 and 0.1 g, a temperature of 90 ° C., and intense stirring for 1 hour. The films were baked at 40 ° C for 72 hours. That based on HDPE is carried out by melt in a plastograph at a temperature of 200 ° C, with the use of several rates of treated and untreated filler. Two characterization methods were used to study the rheological behavior of the HDPE / ZnO and PVA / ZnO nanocomposites including scanning electron microscopy and X-ray diffraction.



Deposition of hybrid organic-inorganic perovskite films at low temperature

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Abstract:

In this work, we report methylammonium lead triiodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) thin films prepared by two-step deposition process (spin and Dip-coating). This study deals with the realization of perovskite thin films and the investigation of speed centrifugation effect on the films properties. The analysis by X-ray diffraction confirmed the formation of tetragonal perovskite structure with the apparition of secondary phases. Furthermore, the UV- Visible spectroscopy analysis showed that the deposited $\text{CH}_3\text{NH}_3\text{PbI}_3$ films have a high absorption coefficient greater than 10^4 cm^{-2} in the visible range and optimal direct gap energy equal to 1.5 eV which is suitable for photovoltaic application. The electrical characterization shows that perovskite thin film has high resistivity value which refers to the porosity of the film.



Current density effect on the morphology and structural properties of nanocrystalline Co-Ni thin films: Rietveld Analysis.

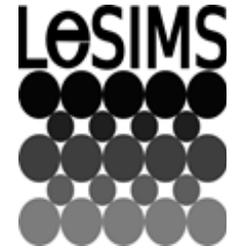
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Abstract:

Nanocrystalline Co-Ni thin films were synthesized by electrodeposition, at different current densities ($J = 1, 2, 3$ and 4 A/dm^2), on Cu substrate from chloride-sulfate aqueous bath containing thiourea as additive agent. A study of the surface morphology of as plated deposits was accomplished by Scanning Electron Microscopy (SEM) technique. The SEM micrographs exhibit a rough and compact surface with a cauliflower-like appearance at lower current densities and a smoother surface with the rise of the current density. The evolution of crystalline phases of the obtained thin films was followed by X-ray diffraction (XRD) technique through the Rietveld refinement of the XRD patterns using MAUD software. For the Co-Ni thin film obtained at $J = 1 \text{ A/dm}^2$, the obtained results reveal the formation of FCC and HCP structures: FCC (Cu), FCC Co(Ni), HCP (Co), HCP Co(Ni) and HCP/FCC Co(S). The Rietveld refinement of the XRD patterns ($J = 2, 3$ and 4 A/dm^2) shows the absence of FCC (Cu) peaks and the formation of several FCC and HCP (Co) based structures. The rise of the current density accompanies an increase in the nucleation rate and causes a decrease of the crystallite size down to the nanometer scale. The root-mean square strain of different structures increases with increasing applied current density.



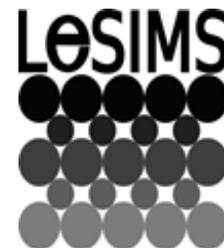
Effect of annealing time on recrystallization superplastic alloys Al-Li (8090)

Afef Derrouiche

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Abstract:

Aluminum alloys, especially lithium aluminum alloys (Al-Li), are important materials in the automotive and aerospace industries. Also these alloys exhibit superplastic behavior [1]. This one is closely related to a structure with fine grains and equiaxes obtained by static recrystallization (before the deformation) or dynamic recrystallization (during the first stages of the superplastic deformation). Studies have shown that the material has resistance to static recrystallization [2, 3]. We are interested in the influence of annealing on the recrystallization of AL-Li alloy designated by 8090. The material presents a microstructural evolution; three states are observed and correspond to the restoration, the recrystallization and the enlargement of the grains. This may explain the mechanism of recrystallization of this alloy since the precipitation process controls static recrystallization. We took into consideration the role of two parameters such as time and annealing temperature. Experimental results obtained by different characterization and observation techniques used such as X-ray diffraction, optical microscopy and scanning electron microscopy (SEM), and microhardness.



Effect of layered double hydroxides reinforcement on the curing characterisation of styrene butadiene rubber (SBR) nanocomposites

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Abstract : The utilization of organo-modified clays in polymer-clay nanocomposites by the Toyota Research Group of Japan ushered, in a new era in the field of polymer reinforcement, since it was demonstrated that a large increase in the strength and modulus of the composite is possible without decrease in the impact resistance, which is usually observed with polymers filled with silica, calcium carbonate and other inorganic fillers in the micron range [1–3]. Several publications in the field of polymer-clay nanocomposites highlight the research work carried out till date using both plastic and elastomeric matrices [4–9]. The objective of this work is the preparation of sulfur-crosslinked SBR membranes and the incorporation of layered double hydroxides (LDH), in order to improve interfacial interaction and reinforcement between the LDH-SBR nanocomposite. The goal is to develop efficient membranes for the fractionation of organic mixtures by pervaporation. We also proceeded to the characterization of these membranes by Fourier transform infrared spectroscopy (FTIR) and by examination of the surface morphology by scanning electron microscopy (SEM). In addition, swelling tests were carried out to estimate the crosslink density and to assess the qualities of these membranes in terms of pervaporation sorption.

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Structural and optical characterization of nano-Structured TiO₂ Dope Hg thin films obtained by Sol-Gel method

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Abstract:

The structural and optical properties of Hg-doped TiO₂ thin films, deposited on glass and silicon substrates by sol-gel method. The films were examined in the temperature range (400 to 550), as well as at different holding times. We calculated the refractive index (n) and the optical gap from the measured transmission spectra as a function of the annealing temperature and the holding time. The calculated values of the index (n) and gap (E_g) are in the order of (1.63-2.5) and (3.35-2.36) respectively. The transmission coefficient varies from (50 to 95)% with annealing and holding temperature. In the case of xerogel of TiO₂ doped with Hg aged for 3 months at room temperature, we observed the formation of the anatase structure, along the plane (101) in contrast to that of undoped one. Moreover, the thin films annealing between 400 and 550 ° C and different times, show the formation of anatase and brookite structure. The calculated grains are in order of 8.04 to 15.65 nm thin films doped as function of temperature and holding time.



Effect of Al₂O₃ doping on the properties of electrodeposited zinc alloy coatings

Diafi Malika

Abstract:

In this work an experimental study Zn- Al₂O₃ composite coatings was conducted. For this, the influence of the concentration of Al₂O₃ is the principal object in order to improve the corrosion resistance of the deposit, which has been made by electroplating on steel substrates previously treated, have been studied by several characterization methods, as the X-ray diffraction, measurement of micro hardness and scanning electron microscopy (SEM), protection against corrosion properties studied in a solution of 3 % NaCl in the potentiodynamic polarization measurements (Tafel), electrochemical impedance spectroscopy (EIS) to the potential of corrosion free. The parameters that characterize the corrosion behavior can be determined from the plots and Nyquist plots. Trends of increasing the charge transfer resistance and the decrease of capacitance values. XRD and SEM results and identify any coatings Zn-Al₂O₃ alloy composition have similar phase (simple cubic γ -phase structure) and the addition of Ni in the zinc matrix increases the micro-hardness, and we note the maximum hardness is obtained for 0.2M Al₂O₃.



Structural and microstructural properties of Al-doped ZnO thin films deposited on silicon substrate by sol gel method

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Abstract:

We have deposited aluminium-doped zinc oxide (ZnO: Al) thin films via dip-coating technique onto silicon substrate (111). Then we have characterized them by X-ray diffraction, scanning electron microscopy (SEM), atomic force microscopy (AFM). It is found that all the thin films are polycrystalline and it have a preferential c-axis orientation along the (0 0 2) plane. SEM and AFM have provided the information on morphology of these films where the size grain and average surface roughness (rms) depend on the number of layers. All the results will be discussed and correlated.

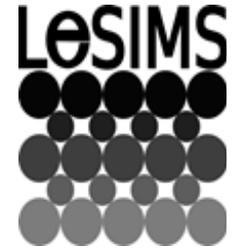


Characterization of ZnO thin films obtained by sputtering

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Abstract:

This work is to improve knowledge of the relationship between the ZnO thin film sputtering deposition process and the optomechanical properties of the resulting films. This knowledge can be used to improve the properties of deposited thin films and reduce the effort required to optimize these properties in the future.



Air pressure influence on properties of Indium oxide (In₂O₃) nanostructured thin films grown by an ultrasonic spray CVD process

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Abstract:

Indium oxide nanostructured thin films are successfully deposited by ultrasonic spray technique on glass substrates at 400°C. Air Pressure influence on the properties of these films is then studied using several techniques, as well as XRD, SEM UV-visible and four-point probe. The XRD analysis shows that the films are polycrystalline with body-centered cubic structure, and the preferred growth orientation change from the (222) to (400) plane with the increase of the air pressure. We attribute this change to the energy increasing of the arriving particles to the surface substrate. Surface morphology of the films changes with increasing of air Pressure. The optical transmittance of these films improves with increasing of air pressure. This improvement is related to the decrease of the films thickness and/or improvement in the crystalline state of the films. The optical band gap is found to decrease from 3.90 to 3.78 eV. The electrical resistivity decreases from 75 Ω cm to 12.3 10⁻³ Ω cm.



3D ordered mesoporous Fe-KIT-6 catalysts for methylcyclopentane (MCP)

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Abstract: The ring-opening selectivity of naphthenic compounds is one of the most viable methods for producing transportation fuels high octane / cetane from crude oil. The ring opening of MCP has been the subject of our work on new catalysts (Fe, Ni, and Zn) supported on the mesoporous framework KIT-6 with Ia3d cubic symmetric in an effort to substitute the precious metals. The catalysts were tested at temperatures between 200 and 500 ° C under H₂ for 4 h at 500°C. These catalysts were synthesized by different methods of preparations and characterized by XRD, N₂ adsorption/desorption isotherms, FT-IR, and EPR spectroscopy. The isolated Fe⁺³ ions in tetrahedral coordination and / or octahedral in Mesoporous materials Fe / KIT-6 synthesized by the self assembly method (S + I-) and the grafting method, promote the ring opening reaction of MCP (with the exclusive formation of n-H₂) . The active sites, tetrahedrally coordinated Fe and isolated atomic Fe sites were responsible for the endocyclic C-C bond rupture between substituted secondary-tertiary carbon atoms. At high temperature, the reaction favors the selectivity to cracking and the enlargement of cycle. This result can be attributed to thermodynamic phenomena because aromatization is favored at high temperatures. This catalyst contained a similar behavior with platinum based catalysts. Our work has made it possible to note that the new catalysts based on oxides supported on the frame KIT-6 may be considered as substituting for precious metals.

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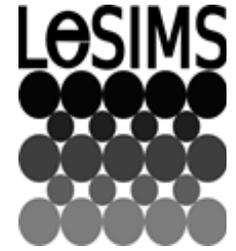
Synthesis of FeTiO₃/rGO composites for remediation of Methylene bleu: kinetics study under different artificial visible light intensity

Mohamed Khalil Guediri

Génie des procédés, option: Génie chimique; Algeria

Abstract:

The new rGO-FeTiO₃ composites with various graphene contents were synthesized successfully using a hydrothermal method that simultaneously reduced graphene oxide and allows the deposition of FeTiO₃ particles on graphene sheets. The prepared photocatalysts were characterized by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and UV-Vis diffuse reflectance spectroscopy. The obtained rGO/FeTiO₃ composites showed greatly improved photocatalytic performance for the degradation of Methylene blue (MB) compared to FeTiO₃ under visible irradiation ($\lambda < 420$ nm) that which could be related to the photosensitizer role of graphene in the rGO/FeTiO₃ composites as well as the formation of p-n heterojunctions between FeTiO₃ particles and rGO sheets. The highest photocatalytic activity in MB degradation reaction was observed for rGO/FeTiO₃ composite with 20 wt % graphene. The photocatalytic activity attributed to the synergistic effect of several factors such as extended absorption range in the visible light spectrum, intimate contact between graphene and FeTiO₃ particles and Shift in the Fermi level and decreases the band-gap potential of the semiconductor.



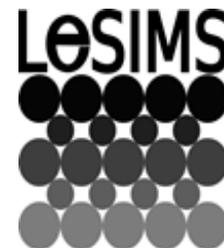
Chemical deposition of $\text{Cu}_2\text{ZnSnS}_4/\text{ZnS}$ hetero-junction using pneumatic spray pyrolysis

Fatima Zohra Boutebakh

Université des frères mentouri Constantine 1, Algeria.

Abstract:

In this reported work, we have realized CZTS/ZnS hetero-junction using an economical and sample technique such as spray pyrolysis. The phase formation of the thin films formed the hetero-junction were confirmed by X-Ray-Diffraction, the UV spectra revealed a strong absorption of CZTS thin films as ideal absorber for thin film solar cells, whereas the ZnS and FTO layers show high transmission values. The electrical properties of the realized hetero-junction were studied using current voltage measurement. The I-V measurement show high rectification behavior with a rectification ratio (RR) greater than 10, and high ideality factor and series resistance which can be explained by the presence of interface state between buffer/CZTS and CZTS/Mo interfaces.



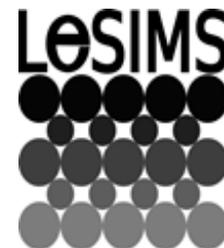
Infrared emissivity and microstructural properties of silica-based glass with different hematite quantities

Abdelaziz Gahmousse

Optique et Mécanique de Précision; UFA-Setif1, Algeria

Abstract:

High emissivity coatings are widely used in many cases where heat transfers through electromagnetic radiation that arises due to the temperature of a body. Extensive theoretical and experimental efforts have been made to synthesize and investigate high emissivity coatings. The emissivity can be improved through various or combined mechanisms. The emissivity here is characterized to describe the surface radiative property which involves the transfer of heat by electromagnetic radiation arising due to the temperature of a body. The surface emissivity, which is the efficiency of the surface for transmitting the radiant energy generated in the surface into its surroundings. The latter depends on the temperature (but the relationship between emissivity and temperature is not definite, depending on material nature, surface parameters and wavelength), composition, surface roughness, coating thickness, wavelength, and physical parameters of the surface. The characterization of emissivity is still a topical problem. For this purpose, silica-based glasses powders with different concentrations of Fe_2O_3 have been prepared, pressed, melted, crushed then deposited as a coating on ceramic tiles, in order to characterize their emissivity, reflectance spectra were measured from 0.8-2.5 μm , from the latter we could extract the emissivity spectra at room temperature for the same spectral range. X-ray diffraction analysis were measured to examine the effect of the iron oxide concentration on the crystallization phase of the glass matrix. To study and determinate, the surface morphology, microstructure, glass coating thickness and coating adhesion with the ceramic, micrographs was taken using and Scanning Electronic Microscope (SEM). Reflectance (Emissivity) spectra showed that the higher the Fe_2O_3 concentration the lower the reflectance goes the higher goes the emissivity in the IR spectra, where the XRD patterns showed that the crystallization phases (peaks) appears from a high concentration of Fe_2O_3 concentration. Finally, the SEM images showed that layer thickness varies in the same sample surface and from a sample to another, and a quite good adherence between glass coating and ceramic support.



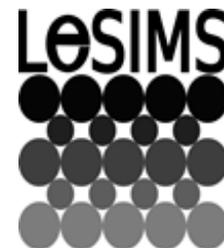
Elaboration and characterization of copper oxide (CuO) thin films deposited by the spray pyrolysis method

Youcef Bellal

Thin films development and applications unit 19000 Setif, Research Center in Industrial Technologies (CRTI) P.O.Box 64, Cheraga 16014 Algiers, Algeria.

Abstract:

In this work, a copper oxide thin films were deposited by a simple and inexpensive technique (spray pyrolysis) on substrates in ordinary glass at a fixed temperature $T=500^{\circ}\text{C}$. $\text{Cu}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ was used as a basis of copper and dissolved in two different solvents (Water, Methanol) to give solutions S_1 and S_2 respectively with a concentration $C_{S1} = C_{S2} = 0.5\text{M}$. The spray pyrolysis deposition made at different volumes 15, 30 and 45 ml of S_1 or S_2 on the glass substrates. The structural, morphological and optical properties of thin films of CuO were studied by X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-vis spectrophotometry. The X-ray diffraction patterns confirm the presence of the polycrystalline phase of CuO as monoclinic crystal structure with preferential orientation along (110), (002), (111) and (020). Their optical band gaps ranged from 3.95 to 4.02eV for thin films made with S_1 , and from 1.6 to 1.95eV for thin films made with S_2 with a high absorbency in the visible region, which is in agreement with the values of the literature.



Chemical synthesis and characterization of nickel oxide as semiconductor thin film and doping agent of titanium dioxide

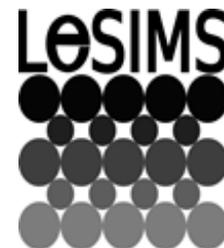
Antar Bouhank

Research Center in Industrial Technologies CRTI

Laboratory of Chemical Process Engineering (LCPE), Faculty of technology Ferhat ABBAS Setif-1 University, Algeria.

Abstract:

Nickel oxide (NiO) is a p-type semiconductor [1], is an important material because of its large direct optical gap between 3.6 and 4.0 eV [2], of its chemical stability and magnetic device[3], and easy to deposit in thin film by several chemical techniques. However, it used as a dopant of titanium dioxide. NiO thin films were deposited by spray pyrolysis on ordinary glass substrates heated to a fixed temperature of 500 °C, from a nickel nitrate hexahydrate as a precursor dissolved in distilled water. Titanium dioxide is doped with deferent percentage of NiO, this latter was elaborate with the sol-gel method. The both type of thin film, were characterized by several techniques, Such as X-ray diffraction, scanning electron microscopy, optical absorption, Atomic force microscopy and Raman spectroscopy.



Improvement of the hardness and wear resistance of chromium nitride by adding of the Zirconium

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Abstract: CrN has been the extensively studied and often used in different applications such as wear resistant films on cutting tools, mechanical and tribological devices due its low friction coefficient, high surface micro-hardness and high toughness, as compared with other nitrides transition metal such as diamond like and TiN films [1]. But, CrN still shows inadequate properties for many applications such as high speed machining [2]. For this cause, Cr-Me-N system with the addition of other transition elements into chromium nitrides was discovered by several investigators. The addition of transition metals and the formation of new solid solutions such as Cr-Ta-N, Cr-Ti -N and Cr-Zr-N [2-3] enriched obviously the hardness and wear resistance of CrN coatings. In this study Cr-Zr-N films were synthesized by RF reactive magnetron by co-sputtering of chromium and zirconium in a total working pressure (Ar+ N₂). The structures, morphology, mechanical and tribological properties of Cr-Zr-N films were characterized. The Cr-Zr-N films exhibit only a tow-phase microstructure, containing CrN and Cr₂N phase, as evidenced by X-ray diffraction. The results reveal that the mechanical properties are largely improved.

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Synthesizing of hydroxyapatite powder for thin films applications

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Abstract: Hydroxyapatite, with chemical formula $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, is a calcium phosphate compound regrouped with bioactive ceramics. Thanks to its best properties of biocompatibility, ostéoconduction, ostéoinduction, and of thermal stability, this mineral material was used intensively as thin film, especially on titanium alloys, in the fabrication of functional biomaterials[1]. THydroxyapatite (HAP) has better physicochemical properties thanks to its molar ratio Ca/P which is always fixed at 1,67 [2]. However, obtaining these good characteristics depends directly on the control of this molar ratio and thus on the control of synthesizing method of this material's powder. The pulverulent substance based on hydroxyapatite can be obtained by various methods. In this work, we study the elaboration of HAP powder by the method of double decomposition "in aqueous phase", which is very much used by industries thanks to its facility and its moderate cost. hereafter, the powder was characterized by diffraction of x-rays, a thermal analysis TGA-DSC, and Fourier transform infrared spectroscopy to examine its characteristics. Results show that the chosen method of elaboration produces a powder with good properties that can be used in the synthesizing of thin films.

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- [2] Daihua He, Ping Liu, Xinkuan Liu, Fengcang Ma, Xiaohong Chen, Wei Li, Jiandi Du, Pu Wang, Jun Zhao, *Journal of Alloys and Compounds*, 672(2016) 336-343.



One-step electrodeposition and characterization of Cu_2O nano-crystalline thin films for photovoltaic application

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Energetic and Solid-State Electrochemistry Laboratory, Department of Processes Engineering, Ferhat Abbas-Setif1 University, Setif, 19000, Algeria.

Abstract:

In this study, nano-sized cuprous oxide thin films were successfully synthesized by electrodeposition from a low-cost lactic acid -based aqueous solution. Cyclic voltammetry (CV) was used to investigate the deposition process and evaluate the effect of applied potential on the properties of the deposits. The XRD measurements indicated that the coatings structure was crystalline and contained the main diffraction peaks of Cu_2O [1] without need for additional heat treatment. The surface morphology investigation using field-emission scanning electron microscopy (FESEM) and atomic force microscopy (AFM) revealed that the Cu_2O thin films were around $6\mu\text{m}$ thick and composed of Desert Rose-like clusters of nanosized grains. The optical properties measurements including absorption in UV-Vis spectrum range, Tauc and Mott-Schottky plots [2] showed that the as-synthesized products were p-type [3] and photoactive with a direct band gap of 2.1-2.4 eV, depending on the deposition potential.



Elaboration and characterization of nickel phosphorus composite coatings to study the phenomenon of corrosion

Ahlam Belgroune, Linda Aissani, Mourad Zaabat, Farid Lakmine, Nassima Bouaziz
LB O.Bouaghi University; Algeria

Abstract:

Electro-deposition is an electrochemical method of metal film deposition on a solid surface contained an electrolyte [1], which was introduced by the Russian chemist Kistiakowsky in the early twentieth century [2]. This process is very used in industry for many types of applications [3, 4]. In this work, the nickel phosphorus coatings are elaborated on a steel substrate X52 by the electro-deposition method by varying the applied current and they are characterized by (X-ray diffraction, EDX and the micro-hardness) to study the corrosion phenomena. The aim of this study is to find the optimal conditions that allow obtaining the better coatings that are more effective against the corrosion when they are submitted to an aggressive environment (3.5%NaCl). For this we use the technique of polarization as a method for characterization and evaluation of corrosion. The results obtained by the stationary electrochemical method showed that the nickel phosphorus coating obtained at $I = 0.10$ presents a good corrosion resistance in the 3.5 % NaCl environment.



Frictional and wear behaviour of heat-treated and duplex-coated 35NCD6 steel

Soheib Mokhtara, Mosbah Zidani, Lahcene Mebarki

Affiliation

Abstract:

The aim of this study is to compare the frictional and wear behaviour of 35NCD6 steel in three different states: as received, heat-treated, and duplex coated by Cr/CrN multilayer. The samples of the second state were maintained at 850 °C for 15 min, and then they were quenched in oil. After that, they were tempered at 180 °C. The samples in the third state were surface coated in two steps. Firstly, a thin layer of chromium (about 200 μm) was electrodeposited using a plating bath consisting of chromic acid (250 g/L) and sulphuric acid (2.5 g/L) at about 57°C. Then, the electroplated samples were gas nitrated in NH₃+N₂ atmosphere at 750°C for 6 hours. Characterization of frictional behaviour of the three different types of samples was performed using a ball-on-disk tribometer, then, the sliding wear track was analysed using an optical microscopy. The results showed that friction coefficient at constant sliding velocity and normal load of the duplex-coated 35NCD6 steel was the lowest (0.272 compared to 0.387 and 0.359 for asreceived and heat-treated steels respectively). It showed also that the sliding wear track of duplexcoated steel was less profound than that in as received and heat-treated steel specimens, which means better wear resistance. The main cause of these results may be the high hardness of the chromium nitride layer formed at the surface of the duplex-coated steel specimens as confirmed by many researchers [1-3].



Influence of growth time and temperature on the morphology of ZnO nanorods via electrodeposition and sol-gel method

Fayssal Ynineb

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Abstract:

In this study, we investigate the effect of temperature and growth time on ZnO morphology. ZnO nanorods can be synthesized via electrodeposition and sol-gel method using zinc acetate and hexamethylenetetramine (HMT) or 2-methoxyethanol (MEA) as precursor and glass slide or FTO as a substrate. In samples deposited by sol-gel, growth time and growth temperature are fixed but in electrodeposited samples, the growth time varied from 15-60 min. The substrates with ZnO nanorods growth by sol-gel technique are annealed at different temperatures which are varied from 240 °C to 300 °C. Obtained films were characterized by means of scanning electron microscopy (SEM) and X-ray diffraction (XRD). The result indicates that different temperature and growth time produces nanorods with different size, diameter, growth density and orientation. Structural characterization shows a preferred c-axis (002) oriented growth. Scanning Electron Microscopy (SEM) images reveals uniformly distributed hexagonal ZnO nanorods. The best aligned ZnO nanorods obtained is that grown at 60 min via electrodeposition and that annealed at 280 °C via sol-gel method.



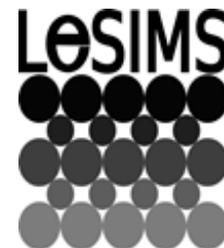
Characterization of galena surfaces and potassium isoamyl xanthate (KIAX) synthesized adsorption

Asma Nouioua, Zohir Nedjar

Laboratory of Molecular Chemistry and the Environment, Department of Industrial Chemistry, Faculty of Science and Technology, University of Mohamed Khider , 07000 Biskra, Algeria.

Abstract:

Separation of minerals from ores is a very important industrial process. The commonly applied separation method is flotation, which ensures the required relation between the hydrophobic and hydrophilic properties on the surface of the mineral particles. Much of the research was focused on the action of hydrophobic xanthate type surfactants on sulfide minerals. Different possibilities have been suggested in literature to explain how xanthates can render hydrophobic the surface of minerals [1–6] The effect of sulfite interaction with galena on the mechanism of potassium isoamyl xanthate (KIAX) synthesized adsorption onto galena surfaces has been studied in situ using electrochemical potential; FTIR spectra and SEM have been used to identify the mechanism of interaction between sulfite and galena surfaces. Activated galena with copper sulfate (10⁻⁴ M) has been investigated at pH 9.12 and potassium isoamyl xanthate (3x10⁻³ M) concentration. Oxidised galena surfaces have relatively low concentration of adsorbed xanthate and high potential ($E_{opt} = -89$ mV); adsorbed colloidal (Pb-IAX, 1,123.08 cm⁻¹) is found even at high xanthate concentration, colloidal lead oxide/hydroxide particles have been imaged after 10⁻⁴ M lead sulfate addition at pH 9.12. The behavior of this system is consistent with ion exchange between xanthate and hydroxide followed by oxidation to dixanthogen (X₂, 1,273.56 cm⁻¹) and diffusion of this species across the surface.



Investigating nanoparticles formation in PECVD using OES characterization

Fermi Youcef

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Abstract:

Nanoparticles formation in PECVD discharge is investigated using in situ Optical Emission spectroscopy characterization. Thin films have been deposited from pure HMDSO in Low Frequency reactor for different pressure and power discharge. results showed a relevant relation between some species (SiH, CO and CHO) [1-3] appearances and nanoparticles Formation. In this paper OES spectra were analysed to detect the presence of nanoparticles in plasma. SiH intensity increases were nanoparticles are formed upon the surface of samples. Also, Silicon molecules tend to band with hydrogen to form SiH, like it is shown in Fig. 1.



Influence of EDTA additive on the electrodeposited Zn-Ni thin films

Hayette Faïd

Université Bordj Bou Arréridj; Algeria

Abstract:

Several studies of electrodeposited iron group thin films (Fe, Co and Ni and their alloys) have been carried out because of their potential applications in computer read/write heads [1], microelectromechanical system (MEMS) [2], and ultralarge scale integration (ULSI) devices [3]. Additionally, the presence of zinc in nickel alloys is known to improve the corrosion resistance in comparison with pure Zn [4, 5]. These structures are obtained by physical technique in vacuum environment. Electrochemical deposition is an interesting alternative method for the synthesis of these nanostructures. It offers the advantages of low synthesis temperature and low cost in comparison with other deposition techniques. In addition, the structure and growth mode are controlled by easy regulation of the potential and choice of solution chemistry. In this work, the Zn–Ni alloys thin films were electrodeposited on steel substrates at different deposition potentials from a sulphate at pH 3.8 and the effects of adding EDTA to the bath on the electrochemical deposition, corrosion resistance, chemical composition and physical properties of the deposits were investigated. The structural and morphological properties have been investigated by X-ray diffraction (XRD), scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDAX). Results show that grain size increases with increase of EDTA concentration, and no change in phase structure. Corrosion resistance results show that deposits obtained from bath with low content of additive exhibits better corrosion resistance.



Effect of Mn substitution on structural properties of BSCCO ceramics superconductors.

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Physics Departement, Constantine 1 University; Algeria

Abstract:

The mechanism of high temperature superconductivity in cuprate superconductors has been a prominent issue in condensed matter physics since its first discovery in 1986[1]. BSCCO system, was discovered by Maeda et al, has three different phases with regard to its chemical compositions, be referred to as the Bi-2201, Bi2212 and the Bi-2223 phase depending on the number of layers in each superconducting block (n) [2-3]. $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi-2212) phase is considered to be one of the most promising high temperature superconductors (HTS) for practical applications under low temperature and high magnetic field conditions, due to its excellent properties, such as a high irreversibility field of nearly 100 T and large in field current capacity exceeding $266 \text{ A}\cdot\text{mm}^{-2}$ up to 45 T [4]. The study is focused on the effect of replacement of Cu by Mn. The samples $\text{Bi}_2\text{Sr}_2\text{CaCu}_{2-x}\text{Mn}_x\text{O}_{8+d}$ ($x = 0.0, 0.01, 0.02,$ and 0.03) have been successfully prepared by solid state reaction. The X-ray diffraction patterns (XRD) of all samples show that Bi-2212 phase is the major one, and main peaks corresponded to the (00ℓ) diffractions confirming that the crystallographic c-axis is perpendicular to the surface. SEM micrographs showed that samples are composed of well-stacked and oriented grains. The incorporation of the doping atoms into the grains is confirmed by qualitative energy dispersive X ray analysis (EDX).



Surface modification of activated carbon and application in water treatment to removal dyes and metals

Amel Belayachi

Université Oran1 Ahmed Benbella; Algeria

Abstract:

The commercial activated carbon of Merck was treated with KOH (10%), H₂SO₄ (96%) and K₂CO₃ (30%) and the commercial activated carbon of Riedel de Haen with NaOH (2N), citric acid (1M) and ammonium oxalate (10%) at different temperatures and time of impregnation and adsorption tests were performed on nickel and methylene blue by treated and untreated activated carbon of Merck and blue bemacid E-TL by treated and untreated activated carbon of Riedel de Haen for coal. Activated carbon treated with a higher percentage of the disposal after the adsorption tests compared untreated coal were characterized for their surface chemistry by infrared spectroscopy, X-ray diffraction and their structures and pH_{zpc} and porous morphology by scanning electron microscopy (SEM), iodine index and the specific surface area by the methylene blue method. Activated carbon from Merck and Riedel de Haen were treated compared to untreated for adsorption of nickel, methylene blue and blue bemacid, experiments and studied in a batch system as a function of pH of the solution, time contacting and the dose of the adsorbent. Adsorption isotherms were studied at room temperature on each of the adsorbents, the experimental data obtained and reproduced by simulating the equations of Langmuir isotherms, Freundlich and Temkin their linear model. The typical Langmuir adsorption monolayer is one that best matches the experimental adsorption isotherms with improvement rates 82, 12 and 25% for nickel, methylene blue and blue bemacid respectively. The pseudo second order model better represents the adsorption of nickel by Merck activated carbon treated with H₂SO₄ and methylene blue with coal treated with KOH and untreated blue adsorption with activated charcoal bemacid HR NaOH treated and untreated.

Keywords: activated carbon, surface modification, adsorption, heavy metals

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Treatment of aluminum alloy by laser excimer

Baziz Leila

Abstract:

The technology laser occupies an importance place in the industry and more exactly in the field of materials (cutting, welding, cleaning...), then the objective of this study is the characterization of the effects of the radiations by laser excimer on samples of industrial aluminum, and its consequences on the morphology and the microhardness. In this aim the analysis of irradiated samples is realized by scanning electron microscopy (SEM). Microhardness measurements were carried out on surface irradiated using a Vicker's pyramidal diamond indenters.



Annealing treatment effect on the structural, morphological and optical properties of erbium doped nanostructured ZnO films deposited by sol gel

Walid Allag

Laboratory of photonic systems and nonlinear optics, Institute of Optics and Precision Mechanics Farhat Abbas University, Sétif, Algeria.

Abstract:

We have deposited rare earth (erbium) doped zinc oxide (ZnO: Er) thin films on ITO glass substrates using sol gel “dip coating” process. Thin films were annealed at 400°C and 500°C for 60 min and tried to observe the effect of annealing temperature on structural, morphological and optical properties of EZO films. The morphological, structural and optical properties were studied by Atomic force Microscopy (AFM), X-ray Diffraction techniques (XRD) and UV–visible spectrophotometer. The deposited films were found to be well crystallized with hexagonal wurtzite structure having a preferential growth orientation along the ZnO (002) plane. The AFM images show that the roughness of the films has increased from 16 to 27 nm with an increase in the annealing temperature (400°C to 500°C). A red-shift was observed in the band gap of EZO films with increasing annealing temperature, the red shift of the band gap in the ZnO: Er films treated at high temperature was observed as the crystallinity of the films became better. The optical transmittance of rare earth element (Er) doped ZnO thin films were increased when increasing annealing temperature. The Er doped ZnO thin films showed high transparency (>85) in the visible region (400-700 nm). Rare earth elements (RE) (Er), which are a hot topic to study for its optical emission due to their intra 4f-4f shell transitions, doping into the ZnO can achieve photoluminescence properties of ZnO.



Layer number effect on SnO₂ thin film prepared by dip-coating technique

Djedjiga Haouanoh

Université M'hamed Bougara Boumerdes; Algeria

Abstract:

SnO₂ is a wide direct band gap n-type semiconductor possessing much importance in various fields of science and technology, it belongs to the important family of transparent oxide films that combine low electrical resistance with high optical transparency in the visible range. In this work the effect of layer number; was investigated on the structural, optical and electrical properties of tin oxide thin films prepared by a sol gel-dip coating process, onto glass substrate using starting material SnO₂ and ethanol solution. Deposited films are characterized by XRD diffraction, AFM and UV-Visible. X-Ray diffraction patterns confirm the formation of SnO₂ tetragonal cassiterite structure with preferred growth orientation (110). The crystallite size varied between 2.55nm to 3.422nm. AFM images show that the smooth surfaces and roughness decreases with increasing of layer number (1697nm -0.515nm). While UV-Visible showed that higher transmittance in the infrared and visible ranges (75-96%). The band gap decreases with increasing layer number.



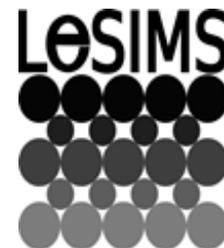
Synthesis and crystal structure determination of tin(ii) oxalate

Khaoula Kerbouche

University of 20 aout 1955 Skikda; Algeria

Abstract:

The objective of this work is the synthesis and the characterization of new hybrid material, tin(II) oxalate, which has been prepared using hydrothermal method which is simple and very effective. Its crystal structure has been solved from single-crystal diffraction data. The symmetry is monoclinic, space group $C2/c$ (No.15), cell dimensions $a=10.3696(3)$ Å, $b=5.5042(2)$ Å, $c=8.2312(3)$ Å, $\beta=125.092(2)^\circ$ and $Z=4$. The characterization of new compound, tin(II) oxalate with formula SnC_2O_4 , by X-ray single crystal shows that this compound has a three dimensional structure constitute of tin polyhedrons SnO_6 , with the lone pair of electrons presumably occupying one apex, linked together by oxalate groups. The resulting framework displays ellipsoidal holes parallel to c-axis.

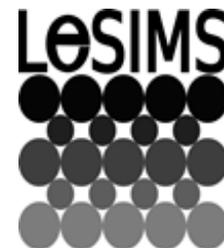


Sequential deposition of Cu/In/Se₂ thin films

Benchouk Kheireddine, Benameur Khedidja
LPCMME-Université Oran1 BP 1524 Oran El Mnaouer; Algeria.

Abstract:

The chalcopyrite layer of CuInSe₂ was synthesized by thermal evaporation under secondary vacuum at 10⁻⁵ mbar. Indeed, sequential Cu / In / Se₂ deposits were made on glass substrates whose thickness and deposition rate were calculated to have the stoichiometry of our layers. Then an in-situ annealing by secondary vacuum infrared lamp was carried out to synthesize our layers. The DRX characterization gives us information on the chalcopyrite structure and gives us an average grain size of 19 nm. The morphological examinations SEM and AFM show us the good homogeneity of our layers. The EDX characterizations show us the good stoichiometry of our deposits. At the end the visible UV gave us a good absorption coefficient and a gap of 0.98 eV. All of its results confirm that our compound is a very good candidate to be used as an absorbing layer in a photovoltaic structure.



Synthesis and characterization of n-ZnO/p-NiO heterostructure

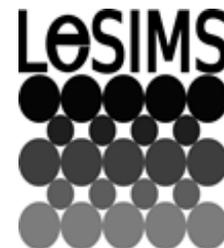
Abdelouahab Noua

Abstract:

In this study, ZnO/NiO heterostructure thin films were prepared by sol-gel dip-coating method. first, NiO thin films were deposited onto clean glass substrates, NiO precursor solution and preparation method was mentioned in[1]. Second, ZnO thin films were deposited on the prepared NiO thin films and the obtained ZnO/NiO thin films were annealed at 550 °C for 2h. The structural, optical and morphological properties of the ZnO/NiO thin films were investigated using: X-ray diffraction (XRD), UV-Vis spectrophotometer and atomic force microscopy. The most important results come from the XRD spectrum; it can be clearly to observe the peaks of NiO and ZnO with dominant (002) peak belonging to ZnO. Also a good optical transmittance of the films within the visible and near infrared region was found to be more than 75%.

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Electrocatalytic effect of polybithiophene films containing transition metal nanoparticles

Lila Lamiri

Research centre industrial CRTI, Algeria.

Abstract:

A new composite material based on poly(bithiophene) (PBT) film containing palladium (Pd) particles has been synthesized by electrochemical method using a two-step procedure. First, PBT film was deposited on indium tin oxide (ITO) substrate by oxidation of the monomer bithiophene dissolved in acetonitrile (CH_3CN) containing lithium perchlorate (LiClO_4) as supporting salt. Then, the incorporation of Pd particles on the PBT film was performed by the immersion of the modified electrode in a Pd solution. The obtained electrode (PBT-Pd/ITO) was characterized by cyclic voltammetry (CV), UV-visible and SEM. Results demonstrate that the proposed PBT-Pd nanocomposite act as good catalysts for the oxidation of ascorbic acid in 0.01 M phosphate buffer solution.



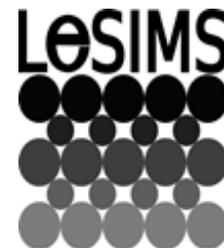
Effect of Plating Parameters on Electrodeposited Ni-Fe Thin Films using Experimental Design Strategies

Adila Talbi

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Abstract:

Experimental design strategy through the fractional factorial design (FFD) and response surface methodology has been used for the statistical analysis of the electrodeposited Fe-Ni binary alloys. A series of 16 experiments obtained from 2^{5-1} (FFD) was successfully prepared via electrodeposition method. The main and interaction effects of several electroplating variables, including Fe/Ni molar ratio (Fe/Ni), current density (I), pH of plating solution, deposition time (t) and stirring rate (stir) on the chemical composition and the coatings hardness were evaluated. The structural changes effect on the deposits mechanical properties (hardness) have been established on the basis of XRD analysis. The obtained statistical results show that all the factors exhibit an important effect on the studied properties with different contributions. Hence, the deposit prepared under the following optimum conditions: Fe/Ni=0.2, I=30 mA/cm², pH=3.5, t=39 min, stirr =500 rpm can be considered to have the best suitable mechanical properties.



XRD characterization of iron oxide nanoparticles

Grabsi Imen Imen

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Algeria*

Abstract:

Nowadays, the nanotechnology has been used in many applications includes ferrofluids, catalysts, biological and chemical water pollution and so on [1, 2]. The main task of this study is to elaborate the nano-particles of iron oxide by the sol-gel method, which has already proved to be an effective and economical way of fabrication. The samples have been characterized by the X-ray diffraction (XRD) using $\text{CuK}\alpha$ radiation of copper ($\lambda_{\text{CuK}\alpha} = 1.5418 \text{ \AA}$) and identification of the existing phases was carried out with the help of JCPD-ICDD data file [3]. The analysis of the XRD patterns was presented in the Figure, show that the majorities of the identified peaks assimilate to the hematite ($\alpha\text{-Fe}_2\text{O}_3$) phase, besides of the grain size of the nano-particles was determinated according to Scherer's law.

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Optical characterisation of SiO₂-ZrO₂ hybrid coatings, deposited on soda lime glass substrate through sol gel rout using nanoparticles of silica and zirconia

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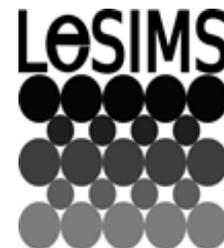
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ABSTRACT

The external face of glass plays a key role in vision; it provides information on the environment, the visibility of objects through the glass depends essentially on the quality of the surface condition of the external face [1]. In Sahara, North Africa, the external face is exposed to aggressive condition. Lead to a decrease of optical property of solar panels, solar mirrors, or every type of glazings [2]. The protection of glass surface is possible, by deposition of coating; sol gel coating can increase the strength of glass, by the filling of micro flaw, and increase of its K_{IC} [3]. The strength of soda lime glass could be increased with SiO₂, ZrO₂, SiO₂-ZrO₂, AL₂O₃. The coating leads to a remarkable increase in strength which can be attributed to a clamping of the defects. [4, 5, 6] In the present work, different SiO₂-ZrO₂ sol gel coating were deposited on soda lime glass substrate, through sol gel rout, using Methyltriethoxysilane (MTES) and Tetraethylorthosilicate (TEOS) with a SiO₂, and ZrO₂ colloidal suspensions. Transparent layers were obtained, with a thickness between 0.65 and 1.3 μm. the optical transmission of the deposited layers depends on the ZrO₂ molar ratio. The transmission varies from 88.5% to 93%, with 30% and 10% ZrO₂ respectively. The addition of ZrO₂ increases the refractive index, which varies from 1.42 to 1.57 for 10 and 30% ZrO₂ respectively. The nano silica particle slightly increases the refractive index. In the second step, the substrates were eroded and coated with one and two layers of composition 0.9SiO₂ - 0.1ZrO₂. In general, the coating reduces the roughness caused by sanding. For example, the roughness Ra of eroded substrate by 200 g of sand, decrease from 100 to 25 nm, and the total roughness drops from more than 6 to less than 0.5 micrometer. The transmission has been significantly improved compared to the sandblasted state. For example for a mass of 200g of sand, it goes from it goes from 81 to more than 89%.

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Growth and characterisation of czts single crystal

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Abstract:

In this work, we report the synthesis of $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) single crystal by cooling a molten stoichiometric of Cu, Zn, Sn and S elements. Weighed stoichiometric proportions were charged into a 200 mm length and 14mm diameter quartz tube sealed off under 5×10^{-6} Torr, placed in a horizontal furnace then heated up gradually. Secondary phases between Cu, Zn, Sn with S were formed by keeping the tube in below temperature range (200-700 °C) for 24-48 h to reduce the vapor pressure and avoid any explosion in high temperature [1-3]. To ensure homogeneous mixing of the melt, the tube was kept at 1100 °C for 24-48 h. The furnace was then cooled down freely reaching room temperature. Removed from the quartz tube, the CZTS ingot was about 25 mm. The ingot chemical composition analyses determined by Energy Dispersive Spectroscopy (EDS) were found to be nearly stoichiometric. The crystal bulk structure was analyzed by using powder X-Ray Diffraction (XRD), the diffraction peaks indicate a remarkable crystalline nature with preferred orientations of (112) plan. Lattice parameters of $a = 5.416 \text{ \AA}$, $c = 10.837 \text{ \AA}$ are found. Crystal electrical proprieties are estimated using Hall Effect measurements at room temperature. The carrier concentration p, hole mobility μ_h and conductivity s are measured to be $\sim 10^{15} - 10^{17} \text{ cm}^{-3}$, 4.32-55.5 $\text{cm}^2/\text{V s}$, 2.18-13.5 $\text{W}^{-1} \text{ cm}^{-1}$, respectively.



Structural properties of cigs thin films grown by csvt technique

Lasladj Meryem^{1,2}, Abedesselam Bouloufa^{1,2}

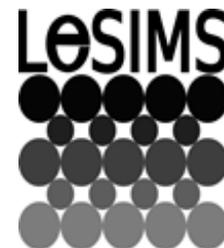
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UFAS1, Algeria

Abstract:

Polycrystalline thin-film chalcopyrite $\text{CuGa}_x\text{In}_{1-x}\text{Se}_2$ (CIGS) is currently used as an absorber layer for high efficiency photovoltaic (PV) solar cells. The efficiency of record laboratory polycrystalline thin-film solar cells based on CIGS has reached more than 22% [1]. The aim of this work is to analyze the surface morphology, phase structure and chemical composition of the $\text{CuGa}_{0.3}\text{In}_{0.7}\text{Se}_2$ and $\text{CuGa}_{0.2}\text{In}_{0.8}\text{S}_2$ thin films grown on glass substrate by close-spaced vapor transport low-cost technique with the deposition at short distances (CSV T) at various substrate temperatures (480 °C and 500 °C) [2-3]. The surface morphology is characterized by scanning electron microscopy (SEM) and revealed the good crystalline of layers. The cross-section with SEM was used to estimate the layers thicknesses and the quality of crystallites which are about 2 to 7 μm and confirm that the deposition was homogenous and successful. The energy dispersive spectroscopy (EDS) is performed to control the layers atomic composition, EDS measurements revealed that layers are quasi-stoichiometric, which represents one of the strong point of the CSV T technique. Structural analyses of the grown layers were performed by X-ray diffraction (XRD) and Raman spectroscopy, the layers exhibited highly crystalline chalcopyrite structure, with a preferential orientation in the (112) direction. No other secondary phases were detected in the films.



Cooper electrodeposition from non aqueous solution

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Abstract:

Nowadays copper is largely used in the electronic industry to manufacture semiconductor based products. This is related to the recent replacement of Al with Cu in microelectronic interconnections production, which increased the performances in terms of lower electrical resistance, higher thermal conductivity and lower cost [1, 2]. As a side effect, the need of developing economically affordable and reliable processes to plate copper having the required features became a priority. Copper electroplating is commercially carried out using aqueous solutions[3] due to the high solubility of the corresponding metal salts resulting in high conductivity of the electrolytes and consequent good throwing power. Nonetheless, some issues such as their toxicity, corrosivity ($\text{pH} \ll 1$) and environmental impact led to the investigation of less dangerous electrolytes, like ionic liquids [6]. The use of these novel solvents is a promising way to solve the cited issues. Among the air and water stable ionic liquids, glycerin-based electrolytes were used due to their moisture stability, low price, biodegradability and non-toxicity. The present work investigates for the first time the influence of the physical properties of glycerin on the deposition of copper on indium tin oxide (ITO)-coated conducting glass substrate, in particular the relation between chemistry, viscosity, conductivity of the solutions and the quality of the obtained Cu layer. The electrochemical study by cyclic voltammetry shows a difference in the deposition process of Cu from glycerin compared to the aqueous solution. On the other hand, the use of glycerin as solvent has reduced the cathodic peak current density which means that the deposition rate has been decreased. This decrease of rate deposition caused a remarkable change in the morphology of Cu deposits. X-ray diffraction (XRD) analysis confirms that the films are pure Cu and all samples have a cubic structure with a notable change in preferential orientation, crystallite size and lattice parameter.

Keywords: Cu, glycerin, electrodeposition, nanostructures, copper.

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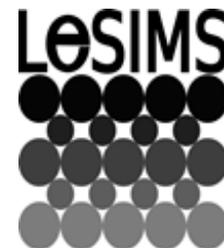
Synthesis of submicronic alumina powders from aluminum slag

Benkhelif Ahmed

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Abstract:

Alumina is a very hard material, unalterable by common chemical compounds. It melts at more than 2000 °C. The combination of a high thermal coefficient, a low thermal expansion and a high strength allows a good resistance to thermal shocks. All of these important properties make alumina a material suitable in a wide variety of application fields. It is used as a refractory material, for example for the coating of furnaces or as crucibles, and thermocouple protective tubes subjected to thermal shocks. Alumina also offers good electrical insulation at high temperature and good wear resistance, which allows it to be used as a tooling material. In Algeria, there are several national industries of aluminum transformation such as: ALGAL M'Sila, El Acher men Ramadhan El-EULMA ... Its transformation produces great quantities of aluminum slags very rich in alumina which also contain more or less quantities of other compounds (metal salts ...). In this work, we studied the extraction of alumina from aluminum slag provided by the local aluminum industry. This action will reduce the harmful effect of this slag on the health and on the environment and ensure the supply of the local ceramic industry with a locally produced alumina. The synthesis technique is based on leaching slags with sulfuric acid (H₂SO₄). The alumina is precipitated by complexation, in the form of Al³⁺ rich compounds. The precipitated powder was calcined at 1050 °C for 2 hours and characterized by X-ray fluorescence, X-ray diffraction and laser granulometric tests. The obtained results show that the produced alumina is of high purity (98.91%). The X-ray diffraction result shows clearly that the developed phase is mainly alpha alumina. The particle size distribution of the synthesized powder is relatively fine. It ranges from 50 nm to 20 µm while the mean particle size d₅₀ is equal to 440 nm.



Development of novel hybrid materials based on PPA/ZnO: Preparation, characterization and electrochemical studies.

Samia Daikh

Abstract:

An in-situ polymerization method has been employed to prepare nanocomposites PPA/ZnO doped HCl and PPA/ZnO doped (HCl-ZnCl₂). Structural characteristics were investigated by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), ultraviolet spectroscopy (UV), thermogravimetric analysis (TGA) and Transmission Electron Micrographs (TEM). TGA results showed that the decomposition of the HCl doped PANI/ZnO nanocomposites was less than that of nanocomposites PPA/ZnO doped (HCl-ZnCl₂). Conduction studies were done by using four-probe method. Electrical conductivity study shows an increase in the conductivity of the samples with the PPA/ZnO doped (HCl-ZnCl₂) to 0.081S.cm⁻¹. To further explore the advantages of these nanocomposites for real applications, we investigated the electrochemical properties of these samples electrodes, the nanocomposite PPA/ZnO (doped HCl-ZnCl₂) presented much higher electrochemical response to PPA/ZnO (doped HCl) and nanocomposites PPA/ZnO doped (ZnCl₂).



Improvement of the properties of the nanocomposite materials

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Abstract: A material does not appear just as chemical entity but as the harvest of a technology of elaboration which confers him a particular microstructure which is going to lead not only chemical but also physical, mechanical properties [1].The Not miscible mixtures of composite have limits of phase between both components, then it is necessary to add an agent compatibilisant to a not miscible mixture called the active material which lives specifically between both phases, by creating mutual actions to help improve the mixture of both materials[2]. The elaboration of graft copolymer was the most current method to form a copolymer of compatibility between two not miscible polymers but also the modification of the surface properties of Nanoclay is an essential stage for the manufacturing of nanocomposites polymer/clay a study in the case of the PP that of Pozsgay and al. They work with clays exchanged until 1 CEC and to study the influence of the rate of adsorption of alkylammonium of their clay on their mixtures [3]. Besides, several studies [4] - [7] which used the mixture to the state melted to know the stability of nanocomposites formed by other techniques. The working objective is to characterize the effect of the incorporation of compatibilisants and the (Org-MMT) on the mechanical and thermal behaviour of nanocomposite system. In this study of nanocomposites with polypropylene (PP) / high-density polyethylene (PEHD) / Montmorillonite organophile (Org-MMT) with various quantities (1 %, 3 % and 5 %) was prepared by insertion for the molten state. The main reason explaining the properties improved by nanocomposites are the strong interfacial interaction between the polymer matrix and the nanolayers of clay for it the addition of comptabilisants as the PP-g-MAH and PE-g-MAH in our polymeric blend has proved necessity. The organic modification of the montmorillonite was studied by Infrared spectroscopy (IRTF).

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Study of structural and optical properties of nanostructure Ni doped ZnO thin films prepared by sol-gel spin coating technique

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Abstract:

In this work the undoped thin films and doped ZnO with nickel concentrations were deposited on glass substrates by sol-gel spin coating. The doping concentrations of Ni are 0.2 and 5% (molar ratio). The structural and optical properties were characterized respectively by X-ray diffraction (XRD) and UV-Vis-IR spectrophotometer. The results show that all the thin films crystallized in the wurtzite hexagonal structure with a preferred orientation along [002] direction. The results also showed that the nickel molar ratio affect the crystalline parameters a and c. The obtained values of a and c parameters are in good agreement with those reported in the JCPDS card and with literature. We have found also that the crystallite size increases with the Ni concentration. The linear nature of the plot of $\ln T$ against $\ln(1-T)$ near the absorption edge confirmed that all prepared films are semiconducting material with a direct allowed transition. The energy band gap of the elaborated films varied between 3.06 and 3.40 eV as the nickel ratio concentration increased from 0.2 to 5% (molar ratio).



The structural and optical behaviour of copper oxide (CuO) nanostructures obtained by sol-gel method

Amir Moussaoui

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Abstract:

Since the absorption spectrum of CuO is well matched with the spectrum of the sunlight, it is considered to have potential applications in some optoelectronic devices such as solar cells etc [1]. In order to obtain better performance of CuO-based devices, it is necessary to deeply understand the effect of structural parameters of thin films such as thickness on the physical properties of CuO thin films. Copper oxide exists in two different crystalline phases viz; cuprite or cuprous oxide (Cu₂O) and tenorite or cupric oxide (CuO), CuO has a monoclinic structure and a band gap of 1.2–1.9 eV while Cu₂O has a cubic crystal structure and a band gap of 2.1–2.6 eV [2]. In this study, the CuO thin films with different thicknesses were prepared by a facile sol-gel: dip-coating method. The structural and the optical properties of the samples were analyzed by X-ray diffraction (XRD) and UV-Vis absorption spectra, respectively.



Low-temperature electrodeposition of zno nanostructured thin films

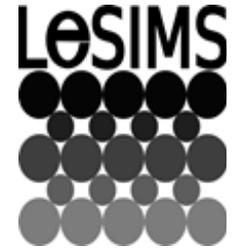
Rania Kara^{1,2}, Hala Hahmar, Rachid Siab², Amor Azizi¹

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Abstract:

Zinc oxide (ZnO) is a typical n-type semiconductor with a direct band gap of 3.2–3.3 eV. It is a nontoxic and abundant material of low fabrication cost. Because of its electrical, optical and acoustic properties, ZnO is promising for photovoltaic cells, transistors, piezoelectric transducers, catalysis and chemical sensors. Among the various techniques available for the preparation of ZnO thin films, the electrodeposition is an attractive technique for its simplicity and usefulness [1-3]. In this study, ZnO films were potentiostatically electrodeposited on FTO substrate at different applied potential from Zn (II) nitrate bath. The samples were characterized by Mott-Schottky (M-S), X-ray diffractions (XRD), Atomic Force Microscopy (AFM) and optical measurements (UV-Vis). The M-S measurements confirmed the n-type conductivity for ZnO thin films with a notable increase of the carrier density at high deposition potential. The XRD measurements revealed pure phase of ZnO hexagonal (wurtzite) structures. All the samples show a (002) preferential orientation and the crystallite size increased with increasing the deposition potential. The AFM images showed that the ZnO thin films obtained at high potential are more homogenous in appearance. The optical measurements show a strong transmittance in the visible region reach 80 % at high potential with direct band gap of 3.3 eV.



Photoacoustic spectroscopy analysis of xenon implanted CuInSe_2

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Abstract:

This paper presents the optical properties results obtained from the Photoacoustic Spectroscopy (PAS) analysis of the effect of xenon implantation into CuInSe_2 single crystals with the energy of 40 keV and a dose of $5 \cdot 10^{16}$ ions/cm². Photoacoustic spectroscopy is an important technique for the study of semiconductors. It is contactless and hence non-destructive, and consequently offers distinct advantages over many conventional techniques. The technique offers also the potential for depth profiling analysis. A new and generalized photoacoustic (PA) signal formula of a gas-coupled cell for multi-layer systems that takes into account the multiple reflections of light in all layers composed the sample has been derived. This relation allows the extraction of the absorption spectrum of the implanted layer from that of the bulk. The photoacoustic spectroscopy method yields direct information on absorption into non-radiating states of CuInSe_2 compound which are usually associated with band structure and defect-related energy loss mechanisms. The results revealed that xenon not only has created a new deep impurity level with an ionization energy of 223 meV, which agrees well with published data, but also affects the region close to the fundamental edge by creating a new shallow level at 17 meV.



Corrosion inhibition of carbon steel in 1M HCl solution by *Lamium Flexuosum* Ten extract

Mahfoud Hiba, Benahmed Merzoug, Morakchi Karima
Larbi Benmhidi Oum El Bouaghi University, Algeria

Abstract:

Methylene dichloride extract of *Lamium flexuosum* was investigated as corrosion inhibitors for carbon steel (CS) in 1.0 M HCl using weight loss and potentiodynamic polarization measurements, electrochemical impedance spectroscopy techniques. The effect of temperature on the corrosion behavior of CS was studied in the range of 293–323 K. The experimental results show that the extract is a good corrosion inhibitor and the protection efficiency increased with increasing concentration of the extract, but decreased with rise in temperature. The extract behaved as mixed-type corrosion inhibitor with highest inhibition at 900 ppm. The adsorption of the extract on the CS surface was found to follow the Freundlich isotherm, and the adsorption mode was found to be physisorption.



Development of a novel inorganic material and its adsorption performances for pharmaceutical micropollutants in wastewater: Equilibrium and kinetics studies

Rima Ghemit

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Abstract:

In this study, MgAlFe-CO₃ layered double hydroxide (LDH), with a Mg to (Al+Fe) molar ratio of 2 and Al to Fe molar ratio of 1:1, was successfully synthesized by coprecipitation method and its calcined product (MgAlFe-C) was obtained. The MgAlFe-CO₃ and the MgAlFe-C samples, were characterized by FTIR, XRD, TGA and BET. Batch sorption studies were conducted to investigate adsorption of Diclofenac (DIC) and Ibuprofen (IBU) from water onto both adsorbents [1,2]. The results show that MgAlFe-C can be used as an effective adsorbent and its sorption capacity is higher than that of MgAlFe-CO₃. The effects of various physicochemical parameters such as pH, contact time, effect of anions competitions and initial IBU/DIC concentration on the adsorption of IBU/DIC onto MgAlFe-C were investigated. Also, the regeneration study was done. The results show that adsorption processes can be well described by the pseudo-second-order kinetic model. The adsorption data are fitted well with the Langmuir isotherm equation. The maximum adsorption capacity is 484 mg/g for DIC and 129 mg/g for IBU. The thermodynamic parameters were calculated. The negative ΔG^0 and ΔH^0 indicate that the adsorption processes are spontaneous and exothermic in nature. Coexisting ions such as CO₃, Cl⁻ could compete with IBU/DIC anions. The adsorption of IBU/DIC on the adsorbent can be mainly attributed to the memory effect process. Regeneration study proves that calcined MgAlFe-C can potential material for the decontamination of pharmaceuticals micropollutants in wastewater.



PREPARATION AND CHARACTERIZATION OF NANOCOMPOSITE MEMBRANES BASED ON TITANIUM DIOXIDE

Affaf Tabbiche^{*1}, Leila Aouinti¹

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Abstract:

The design and preparation of hybrid membranes with matrix based on PVC (Polyvinyl chloride) have been studied for the separation of toluene-n-heptane mixtures by pervaporation. PVC was chosen as the starting organic matrix because it is an inexpensive polymer with a very high selectivity for aromatics. In order to improve that performance of pure PVC films, i.e with high selectivity and very low flux, nanocomposite membranes have been prepared by incorporating different percentages of TiO₂ (Titanium Dioxide) introduced as selective absorbent fillers for toluene. The transport properties of these membranes have been characterized by measurements of swelling rate and pervaporation of binary mixtures.

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Preparation and characterization of PbO_2 and SnO_2 electrodes and its effect on degradation azo Dye Wastewater

Zaim Keltoum

Abstract:

This work focuses on the feasibility of treating industrial wastewater containing azo dyes such as B-Scarlet by direct oxidation on Pt/PbO_2 and SnO_2 anodes. The Pt/PbO_2 electrode was synthesized by the anodic electrolytic deposition method and SnO_2 was prepared by the attack of the tin with nitric acid. The physicochemical characterization of the synthesized Pt/PbO_2 electrode proved that PbO_2 was deposited with two structures crystalline tetragonal and orthorhombic also the DRX spectrum of SnO_2 presents the structure cassiterite. The result SEM obviously shows that the surface of PbO_2 synthesized was homogeneous.

The removal of azo dye on different anodes such as Pt, Pt/PbO_2 and SnO_2 can be followed by UV-vis spectroscopy. The results obtained show that the electrode Pt/PbO_2 offers better oxidation of the dye than in SnO_2 and Pt.



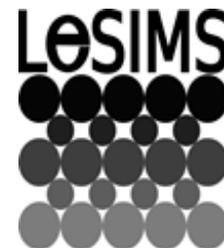
Environmental properties of composites based on polypropylene/poly(lactic acid) blend and copper modified nanoclay

Farida BOUZIDI

Ferhat Abbas University Setif-1, Algeria.

Abstract:

In this study, MMT-Cu²⁺ has been prepared via an ion exchange process. After its characterization to prove the effective intercalation of copper into the MMT, and the confirmation of its antibacterial activity, the modified nanoclay is used to formulate PP/MMT-Cu²⁺ composites, PLA/MMT-Cu²⁺ composites and (50/50) PP/PLA blend composites by varying the MMT-Cu²⁺ ratios. These materials were subjected to several investigations such as X-rays diffraction, antimicrobial activity and environmental tests. The characterization of the modified MMT by XRD analyses showed an increase in the basal space. An additional evidence of the presence of copper ions into the mineral is provided by the inhibitory activity against the bacterial growth revealed by the PLA composites. The incorporation of MMT-Cu²⁺ to the PLA and (50/50) PP/PLA blend accentuated their aptitude to water absorption and ensured an efficient antimicrobial activity over a satisfactorily long period of around six months.



Microstructure and physical properties of nanocrystalline Cu_2O thin films prepared by electrodeposition

Ibrahim Yaacoub Bouderbala, Abdelmadjid Herbadji, Loubna Mentar
Laboratoire de Chimie, Ingénierie, Moléculaire et Nanostructures, Université Ferhat Abbas - Sétif 1, Algeria.

Abstract:

Cuprous oxide (Cu_2O) is one of the few oxides that has a p-type conductivity [1] with a direct band gap of 2.1. Effectively, many researchers explored the cuprous oxide as a p-type semiconductor in junction for photovoltaic applications [2-4]. Electrochemical deposition is one of the most attractive methods for the synthesis of thin films of semiconductors oxides [5-7]. Researchers have fabricated Cu_2O films using various deposition methods [8-10]. Among the deposition techniques, electrochemical deposition is one of the most promising methods because the composition of a Cu_2O thin film can be easily controlled by varying the deposition parameters, such as the precursor concentration, pH, deposition potential, temperature etc. In this study, we have electrodeposited cuprous oxide (Cu_2O) thin films onto a fluorine-doped tin oxide (FTO)-coated conducting glass substrates from copper sulfate solution by applying different potentials that were characterized through different techniques. The Mott–Schottky plots and photocurrent measurements show that all the films present a p-type semiconductor character with a carrier density varying between $4.01 \times 10^{17} \text{ cm}^{-3}$ and $2.67 \times 10^{17} \text{ cm}^{-3}$. X-ray diffraction measurements indicate a single phase of cubic structure with good crystallization with an increase in crystallites size. The optical transmission spectra in the UV-Visible domains revealed that the calculated gap values varied from 2.26 to 2.33 eV.



Alginate modified montmorillonite as emerging porous microspheres for drug carrier

Rima Ghemit

Laboratory of Chemical Process Engineering, Department of Process Engineering, Faculty of technology, University of Ferhat Abbas, Setif, Algeria.

Abstract:

The scope of the present study was the preparation and characterization of Ibuprofen composite beads based on montmorillonite (MMt) and sodium alginate (Alg) as drug carriers [1,2]. After Ibuprofen (IBU) incorporation into MMt, the resulting hybrid was compounded with alginate, and IBU-MMt-Alg composite beads were obtained by ionotropic gelation technique. The structure and surface morphology of the hybrid and composite materials were established by means of X-ray diffraction (XRD), IR spectroscopy (FT-IR), thermal analysis (TG-DTA) and scanning electron microscopy (SEM). Diclofenac incorporation efficiency in Mt and in alginate beads was determined both by UV-Vis spectroscopy and thermal analysis and was found to be high. The hybrid and composite materials were tested in vitro in simulated intestinal fluid (pH=7.4, at 37°C) in order to establish if upon administering the beads at the site of the delivery of the drug is sustained. The in vitro drug release test results clearly suggested that MMt, and MMt along with Alg were able to control the release of Ibuprofen by making it sustained, without any burst effect, and by reducing the released amount and the release rate. The composite beads may be a promising drug delivery system.

Keywords: Montmorillonite, Alginate, composite material, Ibuprofen, Drug delivery.



Effect of Deposition Parameter on ZnO Thin Films Prepared by Dip-coating Method and Their Photocatalytic Activity

Toubane Mahdia

Mhamed Bougara University, Algeria

Abstract:

ZnO thin films were prepared by sol-gel dip coating method onto glass substrates. The effects of pre-heating temperature and layer number on structural, morphological and optical properties were investigated. Photocatalytic efficiency was also assessed. X-ray diffraction analysis indicates that all the films exhibit a Zincite-type structure with a different preferred grains orientation direction. The crystallites size..... The field emission scanning electron microscopy observations reveals nanorods for the samples preheated at 100°C and spherical grains morphology of the samples preheated at 200°C and 400°C. The length of ZnO nanorods increase with increasing number of layers whereas the diameters of grains decrease with increases of preheated temperature. A high optical transparency is observed for all ZnO thin films, ranging from 90 up to 96%. Methylene Blue (MB) dye photocatalytic degradation was found increases layer number reaching almost 94% after 10h under UV irradiation. The apparent reaction rate (K_{app}) obtained by Langmuir- Hinshelwood model show a small variation of K_{app} was recorded when varying the number of coats; $0.223h^{-1}$ - $0.226 h^{-1}$.

Keywords: ZnO Thin films, preheating temperature, layer number, photocatalytic activity



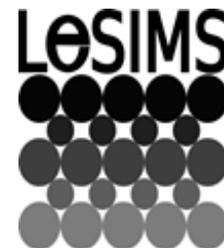
Synthesis of new materials for use as organic active layers characterization spectroscopy and cyclic voltammetry of z (2-phényl-3-(3,4-éthylènedioxythién-2-yl)- acrylonitrile

Mosbah Belaidi Salima

Laboratoire de chimie des matériaux de Constantine; Algeria

Abstract:

Organic P-conjugated oligomers and polymers constitute an important class of functional materials in organic electronics. They are used as active layers in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) or in organic solar-cells (OSC). In this latter application, efficient materials usable as p-conducting layer in bulk-heterojunction (BHJ) solar cells in association with fullerene derivatives as n-conducting materials are needed [1, 2] In fact, a material with a bandgap of 1.1 eV is able to absorb 77 % of the solar irradiation, however, semiconducting polymers or oligomers have bandgaps higher than 2 eV and can then harvest only 30 % of the solar photons. In the last few years, the scientists seek to synthesize organic molecules having gaps similar to those of metals. Recent studies showed that the family of the poly (thienylenevinylene) (PTV) presents a gap electronic E_g lower than that of polythiophen (Pt), 1.8 and 2.1eV respectively. Other work showed that the introduction of an acceptor group into the combined chain has an advantage in the control of this forbidden band. Indeed, the substitution of the electron-withdrawing cyano group in the double connection of the poly (thienylenevinylene) leads to a polymer with a great electronic affinity. We have synthesized monomers to study a class of soluble low band gap conjugated polymers based on heterocyclic units and cyano vinylenes. We report a sample study of one of this class of material, the poly Z (2-phényl-3-(3, 4-éthylènedioxythién-2-yl)- acrylonitrile. The poly Z (2-phényl-3-(3, 4-éthylènedioxythién-2-yl)- acrylonitrile film was synthesized electrochemically by anodic way in an electrolytic bath of Bu_4NPF_6 (0,2M)/ CH_2Cl_2 . The polymer formed on Pt or ITO electrode, either by cyclic voltammetry or by potentiostatic method, was characterized by spectroscopic methods NMR, IR, UV and fluorescence.



Physical and tribological proprieties of rf sputtered chromium aluminum nitrides coatings

Fellah Mamoun

Mechanical Engineering Department, ABBES Laghrour- Khenchela University P.O 1252, 40004, Algeria.

Abstract:

Super hard coatings have been applied to increase the lifetime and to improve the efficiency of machining tools for drilling, cutting, and molding. [1]. For this, physical vapor deposition (PVD) method is mostly applied. They have been reported to increase the abrasive wear resistance and to increase the economical benefits of coated materials. [2-4]. In the present study, a nanostructured Cr-Al-N thin film with different Al content (0 to 50 at.%) have been deposited using radio-frequency (R.F) reactive magnetron sputtering system on Si (100) wafer and XC100 steel substrate without heating. The structural evolution and morphological changes as a function of the Zr content were performed using XRD, (EDS, WDS), WPS, XPS, SEM, AFM, Nanoindentation, Scratch adhesion. The tribological performances were evaluated using a ball-on-disk type Oscillating tribometer. The tests were carried out under normal loads of 2, 4 and 6 N respectively, with an alumina ball (Al_2O_3) as a counter face. Different concentrations of Aluminium (Al) (0 – 50 at.%) were studied. The results show, that, with increasing Al content, the film structure changed with the coexistence of (Cr-N, Al-N) crystallographic orientation mixture. The films formed a (Cr, Al) N solid solution where Al atoms substitute Cr atoms, The crystallite size of the CrAlN system was reduced to 10.8 nm at 31.8 at.% Aluminium content. CrN Lattice parameter increased from 4.17 to 4.32 Å with the crystallite size refinement. Morphological studies of the films showed that the roughness continuously decreased with increasing zirconium content, exhibiting a value of 11.2 nm at 31.8 at.% Aluminium. The mechanical parameters (H, σ , E, H/E and H³/E²) were significantly improved in comparison to binary films, especially at 30 at. % Al. The friction and wear rate tends to decrease with increasing zirconium content, reaching the lowest value of $1.95 \times 10^{-2} \mu m^3/(N \cdot \mu m)$ at 31.8 at.% zirconium . The sliding wear rate and coefficient of friction were lower in the samples with 31.8 at.% zirconium content. The improved friction and wear resistance were attributed to the grain refinement strengthening mechanism at 31.8 at.% of zirconium.



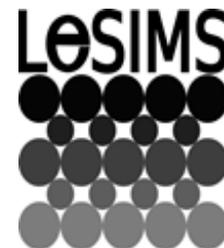
The influence of glycine on the formation of calcium carbonate polymorphs

Louiza Abidi

A. MIRA University of Bejaia, Algeria

Abstract:

Calcium carbonate is one of the most abundant minerals in nature, it is found at the level of limestones rocks, shells of molluscs, oceans, and bones of several animal species. Natural or precipitated CaCO_3 have been used as filler and pigments in the paper industry, foods, cosmetics and pharmaceutical. It can be found in three different allotropic forms, calcite, aragonite, vaterite the most thermodynamical stable polymorph is the Calcite, followed by Aragonite and Vaterite. In this work, we have studied the effect of glycine as an additive on the growth of calcium carbonate polymorphs. CaCO_3 were elaborated by mixing of two salts solutions CaCl_2 and NaCO_3 , in the presence and absence of glycine. The samples prepared are examined by X-ray diffraction and infrared spectroscopy for the identification of crystalline phases. In absence of glycine at 30°C , The Rietveld quantitative phase analysis shows that the volume fraction of calcite is 100%. In presence of glycine at 3°C , Large changes in phase proportions are observed, The Rietveld quantitative phase analysis shows that the volume fraction of calcite is 2% and the volume proportion of vaterite is 98%.



Mononuclear Ni (II) complex as antibacterial agent: synthesis, characterisation, and antimicrobial study

Guadouri Hana Amira, Ouari Kamel

UFAS1, Algeria

Abstract:

The synthesis of coordination complexes is presently of increased interest because of their potential application in catalysis [1], adsorption, storage, molecular recognition, fluorescence, sensors, magnetism, etc [2]. Moreover, they play an important role in the medical and pharmaceutical fields. They show potential applications and properties such as antibacterial, antifungal, anti-tumor [3-4] and anti-inflammatory [5] activities. In previous works, we reported the synthesis of new metal complex (Ni^{II}), as well as the characterization by IR, UV-Vis and electrochemical study. Further support for the structure was derived from elemental analysis. The antibacterial activities of the metal were investigated on gram positive *Staphylococcus aureus* (ATCC25923) and gram negative bacteria *Pseudomonas aeruginosa* (ATCC27853), by disc diffusion method.



Nanocomposites: preparation, characterization and application in the field of water treatment

Aichour Amina

Ferhat Abbas Sétif1 University, Algeria.

Abstract:

Novel hybrid gel beads with a well defined and controlled size formed by alginate biopolymer and activated carbon were prepared and characterized using the zero charge point to show the surface charge, elementary analysis, X-ray diffraction to define the crystallinity of beads, FTIR to identify the functional groups present on the surface since each group has a unique energy absorption, and surface area using BET method. Prepared composites were used effectively in the field of water treatment to remove many pollutants, in this study textile dyes were successfully eliminated by this composites using adsorption method in the batch system. Many parameters such as the effect of initial dyes concentrations, pH, temperature and composites mass were investigated. Desorption study was also investigated using distilled water to show the capacity for regeneration of this material. Results show that the model of kinetic of pseudo-second order and Langmuir isotherm model were much suitable to describe the adsorption process with a coefficient of correlation of 0.99. Regeneration study showed more than 90% desorption capacity.

Results show a potential regenerable material can be used with success in the elimination of textile dyes.



Mechanical characterization of Ni-Co alloy coatings electrodeposited at different bath temperatures

Mohamed Hamidouche

Unité de Recherche Matériaux Emergents; UFA-Sétif1, Algeria

Abstract: Ni-Co alloy coatings are important in engineering where they are used for many applications in various fields such as aeronautics, automotive, digital means of information storing and industry in general, this thanks to their good properties such as good resistance to wear and corrosion, electrocatalytic activity, magnetic properties and electrical and thermal conductivity. Researches on Ni-Co alloy electrolytic coatings has shown that their microstructure and properties are strongly depend on their cobalt content, which can be controlled by the experimental parameters such as bath composition, pH, current density, bath temperature...Etc. In the present work, the effect of bath temperature on electrodeposition mechanism, composition, and morphological, mechanical and tribological properties of nanocrystalline Ni-Co alloy coatings has been studied. Chronopotentiometric study shows that the reduction potential of Ni^{2+} and Co^{2+} ions is substantially reduced with increasing bath temperature which indicates that temperature is a kinetic factor that facilitates the electrodeposition of Ni-Co alloy. The analysis of elaborated coatings composition by XRF shows that bath temperature is strongly influenced the composition of deposits where it is noted that cobalt and nickel contents in coatings are varied with bath temperature variation. On the other hand, despite bath temperature variation but deposition mechanism of the Ni-Co alloy is still anomalous where cobalt concentration in coatings is still always higher than that in the bath. Observations of coatings surfaces by confocal microscope show that the surface morphology of deposits becomes rougher and irregular with the increase of bath temperature, which explains by the increase of the deposition rate with the increase of bath temperature. Micro-hardness of coatings is also varied with the variation of bath temperature and presents a maximum value in Ni-Co coatings which contain the highest cobalt content deposited at ambient temperature (25°C.). Non-lubricated pin-disk tribometric analyzes have shown that the friction coefficient of Ni-Co coatings is strongly influenced by the temperature of electrodeposition bath, this coefficient is substantially reduced with the increase of the cobalt content, it has also been found that coatings elaborated at the ambient temperature (25°C) have the lowest wear rate, this good wear resistance is attributed to their lower friction coefficient and higher hardness compared to coatings which deposited at higher bath temperatures.

Key words: Coating, Electrodeposition, Ni-Co, Temperature, Hardness, Wear.



Synthesis, spectral characterization and biological studies of new material

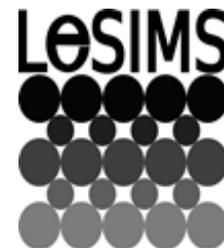
Benabid Wafa, Ouari Kamel

UFAS1, Algeria

Abstract: Materials are considered as a very important class of organic compounds. In the last years, some of these materials have been studied extensively and have received considerable attention because of their attractive chemical and physical properties [1]. The materials are Versatile for a wide range of applications, in catalysis, in photochromic industry, in magnetism and as fluorescent sensors for toxic metal ions [2-4]. Moreover, we can see that there in recent decade a continuing interest in study of these materials has been observed, due to a variety of applications in biochemical, analytical, industrial fields [5.6] and biological activities containing antibacterial, antifungal, antimalarial, anti-inflammatory, antiviral properties [7-9]. Our work focuses on the synthesis of a new material which has been characterized by elemental analysis, UV-Vis, IR, ^1H RMN and Cyclic Voltammetry (CV). Furthermore, the bio-efficacy of this material was tested *in vitro* against various strains of bacteria at different concentration levels to evaluate their utility potential antimicrobial agents.

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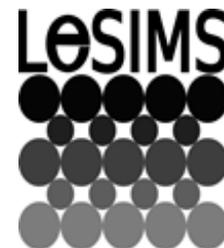
Comparison of two blowing agents for rigid polyurethane foams

Zahir BAKIRI, Saci NACEF

Laboratory of Chemical Process Engineering (LGPC) University of Setif-1, Setif, 19000, Algeria; Algeria

Abstract:

The polyurethanes (PUs) are polymers which contain the urethane group; this group is obtained from the reaction between an alcohol and an isocyanate. The PUs have been used in the manufacture of a plastic compound, very widespread use during the Second World War. Since these polymers are used in various fields of application of such elastomers, expanded systems, and wood coatings, adhesive... This work is located on the preparation of various polyurethane foams by polyaddition with the use of two blowing agents (cyclopentane, cyclohexane). These foams are prepared by the reaction between a polyol and isocyanate. From the experiments carried out on the various polyurethane formulations using two swelling agents, we found that the cyclopentane gives good thermal insulation because its density is low and their better mechanical properties. We also note that the molecular weight effect of the isocyanate is very important to the polymerization reaction.



Sol-gel synthesis, characterization and application of pyrochlor-type solid solutions $\text{Bi}_{1,5-x}\text{Pb}_x\text{Sb}_{1,5}\text{CuO}_{7-\delta}$ et $\text{Bi}_{1,5}\text{Sb}_{1,5}\text{Cu}_{1-x}\text{M}_x\text{O}_{7-\delta}$ (with $\text{M} = \text{Zn}, \text{Mn}$)

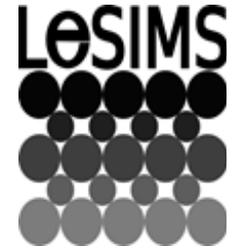
Imen Kadi Allah¹, Alaoui Chakib, Touati Wassila, Ahmed Bekka

Laboratoire de Chimie des Matériaux Inorganiques et Applications Faculté chimie – Université des Sciences et de la Technologie d'Oran « Mohamed Boudiaf », Oran, Algeria

Abstract:

This study is a contribution to the development of materials to access a wide variety of catalysts. Two solid solutions based on transition metal oxides of pyrochlors structure $\text{Bi}_{1,5-x}\text{Pb}_x\text{Sb}_{1,5}\text{CuO}_{7-\delta}$ and $\text{Bi}_{1,5}\text{Sb}_{1,5}\text{Cu}_{1-x}\text{M}_x\text{O}_{7-\delta}$ (with $\text{M} = \text{Zn}, \text{Mn}$) were synthesized by "sol-gel" route. The products obtained were characterized by X-ray diffraction, infrared spectroscopy, electron microscopy coupled to energy dispersive X-ray spectroscopy, differential, and thermogravimetric thermal analyses. They were finally applied as catalysts in phenol degradation. The phases obtained are all of pyrochlors type structure of great purity. The degradation products analyzed by liquid chromatography have demonstrated a powerful catalytic character of these oxides to degrade phenol

Keywords : Sol-gel, pyrochlors, solid solution, crystal structure, catalysis, degradation, phenol.



Investigation of multilayer thermal barrier coatings Y_2O_3 -Stabilized ZrO_2 And Ni-Cr-Al-Y Made by APS and HVOF thermal spraying.

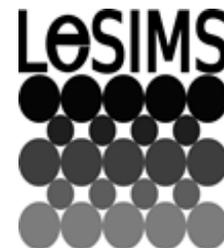
Lounes BELAID

Laboratory of Material Science and Engineering, USTHB, Babezzouar, Algeria.

Abstract:

Hastelloy X alloy is a nickel-based superalloy that has excellent corrosion resistance. Furthermore, it offers corrosion resistance at very high temperatures up to 1200 ° C. It has been widely used in the forming and welding industry. We found it in the gas turbine engines for combustion zone components such as transition ducts, combustor cans, spray bars and flame holders as well as in afterburners, tailpipes, and cabin heaters. However, this alloy has to be protected from thermal cycling [1]. TBC's or thermal barrier coatings are used to protect parts from heat, TBCs consist of a metal bond coat resistant to oxidation and hot corrosion and top coat (Ceramic material), an HVOF spray has been used to deposit the bond coat (NiCrAlY) and an APS has been used to deposit the top coat ((a)ZrO_x(b)Y₂O₃) on an HASTELLOY X and a stainless steel.

Metallographic microscope and Scanning Electron microscopy have been used to investigate the structure and the morphology of the powder and the substrate before and after thermal spraying. A microhardness tester has been used to realize a hardness profile on a lamellar sample [2, 3].



Synthesis of new bio-actives molecules. Study of their photophysical properties

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² *Laboratoire Synthèse et Catalyse (LSCT), Université Ibn Khaldoun de Tiaret, Algérie.*

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Abstract: In this present work, we propose the synthesis, spectroscopic and photophysical characterization of organic materials when exposed to a light. The theme is particularly aimed at the investigation of compounds with actives sites, heterocyclic rings as well as conjugate arms affecting them mixed properties of fluorescence and magnetism (ferromagnetic and diamagnetic materials). The interest allowed to bioactive materials continues to grow in recent decades given their easy process of preparation, their structural diversity as well as their ability to complex. After chemical characterization such as: UV-visible, Infrared (IR), NMR of C^{13} and proton H^1 as well as mass spectrometry (MS), physical properties (dipolar moment, fluorescence...) probabilities of application in nonlinear optics.

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Synthesis and characterizations of $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite thin films for solar cells applications

Sana Hariech, Jamal Bougdira, Mohamed Belmahi, Ilhem Menzri, Nadhir Attaf, Mohammed Salah Aida, Ghouti Medjahdi

Unit of research Materials Sciences, Faculty of Sciences, Department of Physics, Mentouri Brothers University, Constantine1-Algeria.

Abstract:

Our work has concentrated on the elaboration and characterizations of $\text{CH}_3\text{NH}_3\text{PbI}_3$, a type of organic-inorganic hybrid perovskite thin films. Indeed, we have adopted a chemical and simple deposition technique, such as the spin-coating, in order to deposit a series of these films. This series of samples was prepared on glass substrates by varying the rotation speed (1000 to 2000 rpm) and keeping the rotation time fixed (30 s). The obtained films were annealed in air at 70°C for 40 min. Also, our investigation is focused on the understanding and study of the effect of the rotation speed on the physical properties of the thin films to which it was referred. For this purpose, we used several characterization techniques which are: the X-rays diffraction (XRD), the optical microscopy, the UV-Visible spectrophotometry and the electrical characterization in the dark and under. The structural characterization reveals that the structure of the prepared perovskites films is tetragonal with preferential orientation in accordance with the plane (110). The optical characterization shows that these films have a fairly high absorbance in visible region and a direct band gap. The characterization $I(U)$ shows that all elaborated films have a ferroelectric hysteresis behavior in the dark which it become Ohmic under illumination. It can be suggested that these properties make this type of perovskites films perfectly suitable for their use as absorbents films in solar cells fabrication and in other photovoltaic and microelectronics applications.

Keywords: Thin films, Spin-coating, Perovskites materials, organic-inorganic hybrid materials, Structural properties, Optical properties and electrical properties.



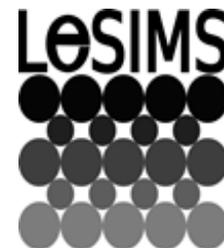
Study of crystallization of ZnO–Al₂O₃–SiO₂ glass containing B₂O₃

Amina GRABSI

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Abstract:

A glass in a ZnO-Al₂O₃-SiO₂ system was elaborated with adding an amount of B₂O₃ in the basic composition, this element (B₂O₃) is a value component used as a raw material of glass ceramic or frits for the purpose of reducing glass melting temperature, and acts as a glass network former [1-2]. The crystallization of this glass was investigated by DTA, after the heating treatments of different pieces of this same glass at 800°C for 2, 8 and 4 hours as holding time, the glass ceramics obtained were characterized by colorimetric analysis and the most white one was studied with XRD in order to identify the crystallin phases. In this work we can deduce the effect of the duration of heat treatment, and that of B₂O₃ according to the phases that appear in the glasses.



Comparative Study Of The Adsorption Of Fatty Acids On The Mineral Surfaces Of Calcite And Quartz

Belkacem Benaissa

Université Larbi Ben M'hidi-Oum El Bouaghi; Algeria

Abstract:

The salt minerals (carbonates, sulphates, fluorides, and phosphates) represent an important family, whose properties are homogeneous due to the presence of cations and anions, between which there are ionic bonds. The collectors most commonly used as surfactants for these minerals are the long chain fatty acids and their alkaline salts, in particular oleic acid and sodium oleate. The objective of this study is to compare the adsorption of various fatty acids on mineral surfaces of calcite and quartz by different analysis methods such as FTIR infrared spectroscopy, X-ray diffraction and UV-Visible spectrophotometry. On the basis of this study, the adsorption of fatty acids is quantitatively greater than that on quartz, which confirms the possibility of separation of calcite from quartz by a process based on the difference in hydrophobicity of the studied minerals. This hydrophobicity is favored by the preferred use of fatty acids that act as collectors. The method used is flotation which involves these collectors under well defined pH and concentration conditions. All fatty acids have the carboxyl function, which is frequently invoked as a means by which organic acids attach to carbonate mineral surfaces.



Annealing effect on the structural and optical properties of Fe-doped WO₃ thin films

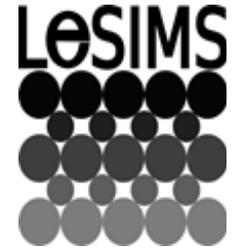
Elaid Ouadah

Laboratoire de Micro et de Nanophysique (LaMiN), ENP Oran Maurice AUDIN, BP 1523 El Mnaouer, 3100 Oran, Algeria

Abstract:

In this work 1% Fe-doped tungsten trioxide WO₃ thin films have been prepared on glass substrates heated to a fixed temperature of 350 °C, using the spray pyrolysis technique, from an aqueous solution based on ammonium tungstate (NH₄)₁₀.H₂(W₂O₇)₆ with 0.005M concentration. The films were annealed at 400 °C, 450 °C, 500 °C and 550 °C for 4 hours. We used X-ray diffraction (XRD), thickness measurement by stylus profilometer for structural characterizations and UV-Visible spectra in the wavelength range [190nm to 1100nm] for optical characterizations. The structural characterization of the WO₃ thin films by XRD shows that they crystallize in a monoclinic structure, with a space group P2/n. The lattice parameters of samples annealed at 400 °C for 4hours were: a=7.4017Å, b=7.5703Å, c=7.7323Å, β=91.44 °. The average grain size is of the order of 62 nm and the thickness varies between 271 and 351 nm. The UV-Visible transmission spectra confirm that it is possible to obtain good transparent WO₃ thin films, with a 72% and 81% of transmittance in the visible. From the transmittance spectra, we determined the indirect transition band gap value of 3.68 eV at 450 °C for 4 hours.

Keywords: WO₃ Thin films, Spray Pyrolysis, XRD, Spectrophotometry.



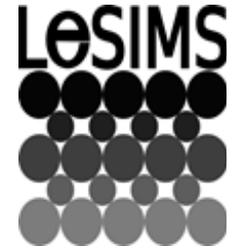
Morphological study of thin chromium layer deposited on glass substrate

Rebiha Labbani

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Abstract:

In this work, we studied the morphology of thin chromium layer by simulation and experimentally. We deposited the metallic layer, by means of thermal evaporation, on a glass substrate. We used the atomic force microscopy (AFM) method to analyze the topographical properties. By this imaging technique, we obtained several qualitative and quantitative results. For instance, we have computed the roughness and the Root Mean Square (RMS) of the films with a good accuracy. On the other hand, we obtained the topography, in two and three dimensions with a high resolution. The chromium layer was porous which was in agreement with the simulation result. We obtained very good geometrical forms that were not in agreement with literature. The disagreement was probably due to the surface state of the glass substrate.



Study of substrate effect on magnetic and structural properties of Co thin films deposited on Si (100), glass and GaAs

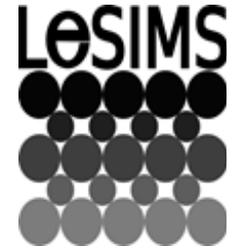
Massinissa Tinouche¹, Ahmed Kharmouche²

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²*Ferhat ABBAS Sétif1 University, Laboratory of Surfaces and Interfaces of Solid Materials (LESIMS), Sétif, Algeria*

Abstract:

The effect of substrate on the magnetic and structural properties of series of cobalt thin films deposited onto Si (100), Corning glass and GaAs substrates, is investigated. The samples were prepared using physical vapor deposition under vacuum. The thickness of the magnetic layer ranges from 19 to 250 nm. The static magnetic properties are studied using Physical Property Measurement System (P.P.M.S.) tools. The XRD spectra reveal a polycrystalline structure for all the films whatever is the substrate nature. The hysteresis loops infer that the easy axis of the magnetization lies in the films plane, the highest spontaneous magnetization (fig.1) being 1240 emu/cm^3 , measured for Co (74 nm)/Si(100) thin film. All these results will be discussed.



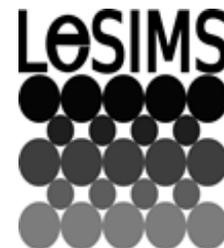
Investigation on subsurface damage and surface roughness in brittle materials

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Research Unit in Optics and Photonics (UROP), Centre for Development of Advanced Technologies (CDTA), University of Setif 1, Setif, Algeria

Abstract:

Thin film coatings, and materials is greatly influenced by imperfections such as surface and interface roughness and surface or subsurface damage (SSD). The deposit of thin films requires well polished substrate. In most cases, the grinding process is the first step of the brittle material machining, where SSD is produced. Therefore, the generated SSD depth in this step is very important and influences the time of succeeding operations and therefore the cost of optical components and their qualities. Moreover, during lapping and polishing, SSD must be removed in order to improve the quality of the thin film that will be deposited on the substrate. This study inspects and measures the SSD of brittle materials developed in lapping process through a bonded interface sectioning technique. A series of experiments is conducted to reveal the influence of lapping parameters on SSD depth and surface roughness. Results indicate that SSD depth and surface roughness are mostly sensitive to abrasive grain size. The ratio of SSD depth to surface roughness (peak to valley) is confirmed to be (2.92 ± 0.75) , which can predict the SSD depth of brittle materials lapped by different abrasive grain size with a rapid roughness measurement.



Thickness dependence of structural, electrical, and optical properties of In_2O_3 films

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Abstract: During the last decades, an increasing interest has been paid to the transparent conducting oxides (TCO) thin films due to their interesting properties such as large electrical conductivity and high optical transparency. Therefore, TCO thin films are considered as serious candidate for numerous applications namely: photovoltaic devices, transparent windows; liquid crystal displays (LCD), solar cell and gas sensors [1, 2]. Among these TCO films, indium oxide has been less studied by comparison to the commonly used zinc and tin oxides thin films. In this work, Films of In_2O_3 of various thicknesses were deposited onto glass substrates by the sol-gel spin-coating method and heated at 500°C for 1 hour. The structural, electrical and optical properties were studied with the respect to the In_2O_3 film thickness. The In_2O_3 XRD patterns of films showed that the In_2O_3 films exhibited a bixbyite structure with a lattice parameter of 10.1nm and the corresponding grain size increased with increasing film thickness. Indeed, it reached a value of 35nm for 105nm film thickness and it decreased at 120nm. In addition, the FTIR analysis revealed the presence of In-O bonding within In_2O_3 films indicating the formation of In_2O_3 bixbyite structure. On another hand, for 105nm film thickness, the Raman spectrum exhibited a sharp and intense peak around 590cm^{-1} characterizing of the In_2O_3 bixbyite structure. For the electrical properties, the measurement of In_2O_3 sheet resistance showed a clear variation with the film thickness, indeed, decreased from 22 to 0.1 when the film thickness increased from 65nm to 105nm. However, up to 120nm film thickness the increased and reached 10. Optical measurements of the transmission spectra showed that all the films have a transmittance greater than 90% in the visible-ultraviolet region with a band gap value that varies between 3.5 and 3.57 eV. The present results showed that the obtained thin films could be used as an optoelectronic material.

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Galvanostatic electrodeposition thin film of nickel with TiO₂ nanoparticles on copper substrate from nickel sulfate bath.

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Laboratoire des Matériaux Inorganiques · Faculté des Sciences · Université Mohamed boudiaf de M'sila

Abstract: The aim of this work was to produce and to characterize composite deposits of nickel titanium dioxide on copper substrate. These deposits are obtained from watts bath without additives [1]. Titanium dioxide is one of the most important oxides used in the engineering materials. The oxide is used in electrochemical deposition of a substrate within sufficient properties. Ni and Ni-TiO₂ films were galvanostatically deposited on copper substrate from nickel sulfate bath. The composite coatings of nickel incorporating TiO₂ nanoparticules were characterized by using electrochemical methodes such as open circuit potential (ocp) measurements, polarization curves and electrochemical impedances spectroscopy, the corrosion behavior of the nickel-TiO₂ coating was examined. The corrosion tests in an aggressive 3.5% NaCl solution indicate a reduced electrochemical activity and a high corrosion resistance in the case of composite deposits compared to the deposition of pure Ni, being confirmed the beneficial effect of the incorporation of TiO₂ into the Ni matrix. The best results are obtained for a concentration of 5 g / l of TiO₂. The results of the impedances are in agreement with the results of the currents of corrosion and the resistance of polarization which indicate the best resistance to corrosion in the case of the deposition of Ni obtained from the bath in the presence of 5 g / l TiO₂

Keys word : Corrosion, electrolytic codeposition, nickel composite

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Incorporation of sol gel prepared silica in thin film composite nanofiltration membrane

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Abstract: The concept of thin film nanocomposite is a new and recent method of introducing silica in the membrane morphology, as silica nanoparticles [1] or mesoporous silica [2]. This aimed at improving nanofiltration membrane capabilities such as permeability and antifouling. In the present work, a novel method to incorporate silica on a polyethersulfone (PES) membrane surface was successfully developed. An *in situ* hydrolysis/condensation of tetraethylorthosilicate (TEOS) precursor was carried out, followed by coating with thin film composite (TFC) via interfacial polymerization using trimesoylchloride TMC and Piperazine PIP, in order to immobilised the as-prepared silica. This modification Lead to a good rejection of salts $MgSO_4$ and Na_2SO_4 accompanied with proportionally high water flux.

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Elaboration and characterization of thin films of Cu on a silicon substrate prepared by electrodeposition process

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Abstract:

Copper thin films were elaborated by the electrodeposition on silicon substrates unknown type, then impossible deposition on black silicon; to their high resistivity. The prepared films were carried out under the chronoampérométrie and chronopotentiometry. Voltammetry was used initially in order to study the electrodeposition and growth model mechanism. Deposits were characterized by three techniques: the profilometer, the X-ray diffraction (XRD), the Hall Effect. The films have the Cu phase in the cubic system with a preferential growth orientation in the direction (111), (200), (220) and (311) located in diffractometer angles 42.9 °, 50.0 °, 73.8 °, and 89.6 °, respectively. The electrical analysis indicates reports of low resistivity copper to $10^{-9} \Omega \text{ cm}$. The results obtained were compared with other previous work.



Characterization of Silicon Surfaces Implanted with Arsenic Ions

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Abstract:

A series of {100} silicon samples were implanted with As⁺ ions at an energy of 100 keV, at room temperature, to a dose of $1.5 \times 10^{16} \text{As}^+ \text{cm}^{-2}$. To recover the radiation defects generated by ion implantation and to activate As atoms, annealing treatments were carried out. They were performed, under high vacuum, to a temperature of 900°C during 30min. The samples were analysed by different experimental techniques namely X-ray diffraction and electrical measurements. For as-implanted specimens, an increasing of the tensile strain was noticed in the Si layer. After the annealing treatment, a good recovery of defects was obtained. The electrical measurements were in agreement with X-ray analysis. We note that the obtained results were in agreement with literature.



Effect of deformation on the structural and mechanical properties of drawn copper wires

Fayçal Baira, Zidani Mosbah

Batna 2 University, Mohamed Khider Biskra University, Laboratoire de Génie Energétique et Matériaux, Faculté des Sciences et de la Technologie, Algeria

Abstract: The principle of wire drawing is based on the reduction of the section of the cylindrical pieces of the materials according to their plasticity by the forced passage of the latter in a sector. The aim of this work is to study the influence of the deformation level resulting from the wire drawing process at ENICAB of Biskra on the evolution of the microstructure, the texture and the mechanical properties of the copper wire destined for the transmission of electrical energy. The characterization methods used in this study to identify the evolution of microstructure and texture and also the mechanical properties of deformed wires are: electrons backscattered Diffraction (EBSD), X-ray diffraction, optical microscopy (MO) and electronics microscopy (MEB), the microhardness and the tensile test. Structural analysis by EBSD shows that the wire strongly deformed by wire drawing consists of two fibers $\langle 111 \rangle // DN$ (majority // to the drawing axis) and $\langle 001 \rangle // DN$ (minority // to the wire drawing axis) and also a decrease in the size of the grains which becomes more homogeneous after the elevation of the level of deformation. The study of the mechanical properties shows a significant increase in the hardness and the mechanical resistance as a function of the deformation [1-3].

Keys words: Wire Drawing, Mechanical properties, EBSD, Texture, Mechanical properties

References

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New polymer-metal composite materials poly[4-(pyrrol-1-methyl) benzoic acid] film-cobalt (0)

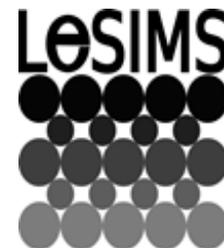
Nesrine Hakimi

Laboratoire de Croissance et Caractérisation de Nouveaux Semi-Conducteurs, Département de Génie des Procédés, Faculté de technologie, Université Sétif 1 (19000) Sétif Algérie.; Algeria

Abstract:

This work consists of the electrochemical development of new polymer-metal composite materials on a support of ITO, vitreous carbon and platinum and their physicochemical characterizations.

The polymer used and the poly [4- (pyrrol-1-methyl) benzoic acid] deposited on the surface of the electrode by electrochemical oxidation of the monomer in acetonitrile medium. The metal chosen is cobalt, it is deposited by two methods, one is the direct electrochemical reduction of the cobalt ions on the electrode modified by the polymer film and the other is the complexation-reduction of the cobalt ions for precipitating the metallic cobalt in the form of particles. The characterization of these materials was performed by electrochemical, spectroscopic and magnetic surface analysis techniques.



New material type carbon nano-spheres, preparation and characterization

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*Centre de recherche Scientifique et technique en analyses physico-chimique (CRAPC);
Algeria*

Abstract: The future development of material science hinges on the ability to control the synthesis of nanomaterials with distinctive morphologies and functional properties [1]. Carbon chemistry is an integral part of the recent revelations seen in nanotechnology for several reasons. These include its abundance and its ability to form many allotropes like diamond, graphite, nanotubes or graphene which exhibit different physical and chemical properties [2-3]. Carbon, the sixth element in the Periodic Table, is unique in the number and variety of ways in which it can bond, leading to a wide range of carbonaceous structures with quite different properties. Carbon has the ability to form long chains of interconnecting C–C bonds and can form covalent bonds with other elements, which are strong and stable. Carbon can have different hybrid orbitals sp , sp^2 , and sp^3 , which allow it to form pentagonal, hexagonal, and heptagonal carbon rings. These distinctive and diverse arrangements allow carbon to form an almost infinite number of compounds and build up to form various shaped carbon materials [4]. Among these materials are an intriguing set of spherical nanostructures called carbon spheres (CSs). The tunable diameter, structural architecture, surface functional groups, porosity and thermal stability of carbon spheres has attracted much attention from material scientists because of their potential applications in catalysis, as adsorbents, and in drug delivery, gas storage and as electrode materials. The aim of the present work is the elaboration of carbon spheres by non chemical vapor deposition method using organic compound as carbon source. The carbon spheres were characterized by several techniques such as XRD, TEM, Raman, TGA/DTG, FTIR and reflectance diffuse.

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Ag/Na ion-exchange effect on the optical and mechanical properties of soda-lime silicate glass

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Abstract:

The ion exchange process between glass and a molten salt bath is now well known. This technique, combined with thermal treatment, is received a good practical application such as gradient index rod, planar waveguides and fabrication of passive integrated optical devices. The common procedure for ion exchange method includes the immersion of glass into a molten silver metal salt such as AgNO_3 . Then, the Ag^+ ions from the molten salt replace monovalent ions such as Na^+ in the glass surface. In this work, we study the effect of the temperature and the immersion time on the optical and mechanical properties of the treated glass. The used molten salt bath is formed by a mixture of 95 mol% NaNO_3 and 5mol % AgNO_3 . The experimental conditions are fixed: Temperature ion exchange = 350°C , immersion time: from 5 min to 310 min. We have determined the optical, mechanical and structure of ion-exchanged glass. We have used Fourier transform infrared spectroscopy (FTIR), UV-Vis absorption spectroscopy and indentation. The found results showed that no surface Plasmon resonance (SPR) peak appears (peak of absorption) in the ion-exchanged sample. However, SPR peak appears at about 410 nm after annealing the ion-exchanged sample at 450°C , indicating that the thermal treatment favourite the formation of Ag nanoparticles in the glass surface.



Annealing temperature effect on structural and optical properties of Nickel oxide thin films

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Ecole Nationale Polytechnique d'Oran Maurice Audin (ENPO-MA); Algeria

Abstract:

The aim of this work is to study structural and optical properties of nickel oxide (NiO) thin films deposited onto glass substrates heated at 350°C by spray pyrolysis technique, using 0.1M aqueous solution of Nickel chloride $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ annealed at 400°C for 2 hours in air. The thickness measurements, structural and optical properties of the films were characterized using stylus profilometer, X-ray diffraction and UV-Vis spectrophotometer in the spectral rang 190 - 1100 nm respectively. Profilometer analysis revealed that the thin films thickness is about 610 nm. The X-ray diffraction (XRD) analysis indicates that the films have cubic polycrystalline structure with preferred orientation along (200) corresponding to $2\theta = 43.30^\circ$ and lattice parameter $a = 4.18$. Various microstructural properties have been calculated such as average particle size $D = 39$ nm, dislocation density $= 0.65 \times 10^{15}$ [lines/m²] and strain $\epsilon = 9.02 \times 10^{-4}$. From the optical studies it is found that, the maximum transmittance of nearly equal to (75%) in near- infrared and the band gap is about 3.20 eV.



Photoelectrochemical Characterization of (P3T+6T) Composite Film Doped with TiO₂ Nanoparticles

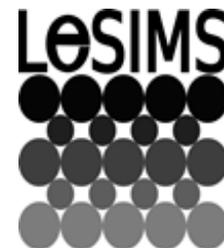
Leila Hasniou

Centre de recherche scientifique et technique en analyses physico-chimiques, BP 384, Bou-Ismaïl CP 42004, Tipaza; Algeria

Abstract:

In recent years, the composite materials have attracted interest as inorganic semiconducting nanoparticles owing to their small size and novel properties and the conjugated polymers for their attributes as easily processed semiconductor materials with a great potential in optoelectronic applications [1, 2]. The composites are usually prepared in the form of bilayers of conducting polymer/semiconductor. In the present work, a composite material was electrochemically synthesized. This composite material was containing the monomers (terthiophene, sexithiophene) and semiconductor (TiO₂) particles, films obtained from (3T+6T) and titanium dioxide (TiO₂) at a platinum electrode or ITO glass electrodes (SOLEMS). The so obtained films were characterized using cyclic voltamperometry (CV), impedance spectroscopy measurement (SIE), EDX, SEM to study their electrochemical properties. These modified electrodes can be used in various applications, such as light emitting diodes (LEDs) and photovoltaic cells.

Keywords: electrosynthesis, composite materials, polyterthiophene, sexithiophene, titanium dioxide (TiO₂).



Study of the annealing effect on the structural and optical properties of Bi_2O_3 thin films

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Abstract:

In this work, the annealing effect on structural and optical properties of bismuth trioxide thin films was investigated. The Bi_2O_3 Thin films were prepared by spray pyrolysis method, from aqueous $\text{Bi}(\text{NO}_3)_3$ solution onto glass substrates heated at 350°C . The samples were annealed at 450°C for 2 hours in a programmable tube furnace. X-rays Diffraction (XRD), spectrophotometry techniques and thickness measurement by stylus profilometer were used to characterize the thin films. The XRD results show that the as-prepared bismuth oxide films are polycrystalline, with mixed phases of monoclinic Bi_2O_3 , cubic $\delta\text{-Bi}_2\text{O}_3$ and tetragonal $\text{Bi}_2\text{O}_{2.33}$. After annealing the diffraction peaks intensity increases, only cubic $\delta\text{-Bi}_2\text{O}_3$ phase is obtained, and one peak of tetragonal $\beta\text{-Bi}_2\text{O}_3$ appears. Profilometer analysis reveal that the thin films thickness and profile roughness parameters increase after annealing which mean that thin films became less smooth. The specrophotometry measurements carried out in the spectral range (190-1100) nm; show that after annealing, the thin films absorbance increases, and percent transmittance decreases from 65% to 45%. The optical studies show the increase in direct and indirect energy of optical band gap from 3.97 eV to 4.31 eV and 3.76 eV to 3.79 eV respectively after annealing, this results indicate that the indirect transition are controlling the optical response of the films.



Optical and structural properties of Al and Mn co-doped ZnO thin Films Prepared by Sol-Gel method

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Laboratory of Active Components and Materials, Faculty of Exact Science and science of nature and life, Larbi Ben M'Hidi University, Oum El Bouaghi; Algeria

Abstract:

ZnO is a promising n-type semiconductor material with a wide band gap (3.37eV), a high excitation binding energy (60 meV), a high optical transparency in the visible region, a low cost and a non-toxicity [1,2]. These properties give ZnO a widely uses in various applications, such as, gas sensors [3], magnetic materials [4], and photo catalysis[5]. In this study we are interested in Aluminum (Al) and Manganese (Mn) co-doped ZnO (AMZO) thin films which were successfully synthesized into glass substrates by the dip-coating sol-gel method. Al concentration in the films was varied from 1% to 5%. The structural, morphological and optical properties of the resultant films were characterized by X-ray diffraction (XRD), Atomic force microscopy (AFM), and UV-VIS spectroscopy. XRD pattern described that the films were polycrystalline having the hexagonal structure and a preferred orientation along (100) for undoped ZnO thin films, further AMZO thin films show a shifted preferred orientation to (002) direction, without any Mn or Al related phases. The AMZO thin films doped with 5% Al showed a highest value of transmission, All films exhibited a dense homogenous microstructures, with a reduced grain sizes for AMZO thin films doped with 5% Al as evaluated by AFM microscopy.

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Structural and optical properties of (Sn, Mn) co-doped ZnO thin films by spray pyrolysis

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Abstract:

Sn and Mn co-doped ZnO thin films have been successfully prepared on glass substrates temperature at 350°C by spray pyrolysis method. Structural and optical properties of pure and co-doped ZnO thin films are studied in detail. The deposited films were characterized by X-ray diffraction (XRDBruker à rayons X D2 PHASER) to determine structural properties and the Optical properties of the deposited films were obtained using transmittance measurements in the wavelength range [200–2500 nm] using an UV (Ultra-Violet) Visible JASCO type V-570 double beam spectrophotometer. XRD patterns showed a successful growth with high quality polycrystalline films on glass substrates. The predominant orientation of the films is (002) at dopant concentrations. Incorporation of Sn and Mn to the ZnO crystal structure decreased the crystallite size and increased residual stress of the thin films. All films were highly transparent in the visible region with average transmittance of 79 %. Increasing doping concentrations increased the optical bandgap, from 3.12 to 3.21.



The atmosphere annealing effect on the properties of electrodeposited CuInSe₂ thin films

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Abstract:

Polycrystalline chalcopyrite CuInSe₂ (CIS) thin films were deposited by the electrodeposition technique onto ITO coated glass substrates. The used bath solution is formed by dissolution of CuCl₂, InCl₃, and SeO₂ salts in de-ionized water. Two samples (noted CIS1 and CIS2) were synthesized under the same experimental conditions. The CIS1 and the CIS2 thin films have been annealed at 300°C during 30 min respectively under the air atmosphere and the argon and neon gaseous mixture atmosphere. In this work, the influence of the atmosphere annealing on CuInSe₂ films properties was examined using X-ray diffraction, optical transmittance and the Raman spectroscopy. The X-ray diffraction investigation indicated that, the both films exhibits the tetragonal CuInSe₂ chalcopyrite structure, with preferred orientation along [112] direction. The obtained values of the lattice parameters are in good agreement with those reported in the JCPDS card and with literature data. The films show the direct allowed band gap and their energy band gap values were 1.25 and 1.08 eV. The observed Raman modes in the films match well with those reported for single crystal CuInSe₂; all Raman spectra show the A₁ mode at 127 cm⁻¹ confirming the chalcopyrite crystalline quality of these films.

Keywords: Photovoltaic, Thin Films, CuInSe₂, Electrodeposition.



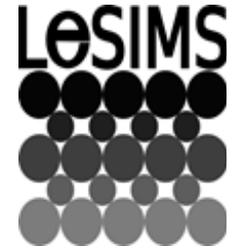
Effect of a thin iron film as an interlayer on the formation of nickel silicides

Ahlem Kolli

University of Setif; Algeria

Abstract:

The effect of Fe alloying element on the formation of nickel silicides has been investigated. Nickel allied with iron on a Si substrate leads to the formation of NiSi_2 at low temperature according to the results of some authors.^{1,2} In this work, we studied the effect of a thin Fe interlayer with the nickel ($\text{Ni}(25\text{nm})/\text{Fe}(2\text{nm})/\text{Ni}(25\text{nm})/\text{Si}$) on the formation sequence of nickel silicides. Ni and Fe thin films were deposited on Si(100) substrate by evaporation and treated thermally at different temperatures. Ex situ X-ray diffraction (XRD) results show that adding iron as an interlayer delayed Ni consumption up to 300°C compared to the reference system $\text{Ni}(50\text{nm})/\text{Si}(100)$ and suppressed the formation of Ni-rich phases. The formation of NiSi appears directly at 300°C and persists up to 700°C . Furthermore, the formation of the polycrystalline NiSi_2 phase is initiated at a temperature that is more than 700°C . The high formation temperature of the NiSi_2 phase in the presence of Fe can be attributed to the formation of FeSi_2 at 500°C . AFM analysis shows that the Rms roughness of the samples increase with the annealing temperature of 1.73 nm at 300°C up to 10.67 nm at 900°C . The measurement of sheet resistance R_s and magnetic proprieties of nickel silicides with the presence of thin iron interlayer film has been studied also.



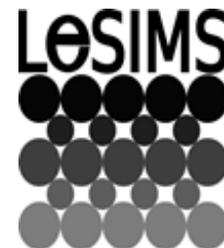
Quantitative analysis of high chromium cast irons by the Rietveld method

Boulassel Fatma Zohra

Mohamed Seddik Ben Yahia University; Algeria

Abstract:

Grinding balls or crushing mills are elements used in cement industry. They require a high wear resistance under the action of abrasive products in the transformation of rock into fine particles smaller than a millimeter. To satisfy the mechanical and technological requirements, these balls are made of high chromium cast irons (10 to 13% chromium). The quantitative analysis of the phases containing these balls by the Rietveld method is an accurate and very important method to select their appropriate composition. The characterization techniques used in this work are the DRX and the SEM.



Preparation and characterization of the Zn(O,S) thin film buffer layer for Cu(In, Ga)Se₂ solar cells

Hanane Houadsi

Université Larbi Ben M'hidi Oum El Bouaghi; Algeria

Abstract: Solar energy is arguably the cleanest and most reliable form of renewable energy available, and transforming it into electrical power represents one of the most attractive research fields. Thin films are among the most important processes for the construction of photovoltaic solar cells. A thin layer of CdS or Zn(O,S) is used as the buffer layer. The requirements of this intermediate layer are to be n-type and widely spaced. Its role can be summed up in the formation of a heterojunction with the absorbent layer which is p-type with a narrower gap [1]. We use in this work Zn(O,S). A choice that could be justified by the numerous advantages that Zn(O,S) may offer. First, and from an environmental point of view, it's considered to be non-toxic [2]. Second, its wide gap allows higher energy photons to be transmitted which increases the absorption of light at the level of the absorbing layer [1]. We represent in this work our methodology in creating and using thin films of Zn(O,S). In a nutshell, the thin layers were deposited using the sol-gel method associated with dip-coating on glass substrates, a straightforward method which is distinguished by its ease of application and low costs. The transmittance of the films was measured using a UV-Visible spectrophotometer and the optical gap was determined. The structural properties, as well as the morphology of the films, were determined and analysed by X-ray diffraction (XRD), and by atomic microscopy (AFM) respectively. The results we obtained show that the deposited films have good physical properties.

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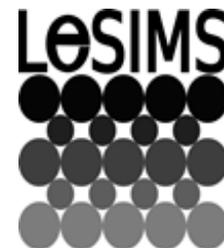
Electrodeposition of In_2Se_3 thin film from citrates electrolyte. Structural, morphological and optical studies.

DILMI Oualid

Energetic and Solid State Electrochemistry Laboratory, Ferhat Abbas-Setif 1 University, Setif 19000, Algeria

Abstract:

In_2Se_3 is a photoactive binary compound; it has received great interest in recent years for applications in photovoltaic and photoelectrochemical devices [1-3]. In this work, In_2Se_3 thin film was synthesized by electrodeposition using voltammetry and chronoamperometry methods from an aqueous solution containing InCl_3 and SeO_2 in acid medium (pH=4.2) with sodium citrates as complexing agent at ambient temperature, the structural characterization of elaborate films was performed by X-Rays Diffraction (XRD) and RAMAN spectroscopy, The morphological one was carried out by the Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM), the UV-VISIBLE spectroscopy was used to investigate its optical proprieties, whereas the Mott-Schottky measurement was used also to study its semiconducting proprieties. The results shown that; The obtained phase of as-deposited In_2Se_3 is the rhombohedral β -phase, as-deposited In_2Se_3 is photoactive thin film with an energy gap of about 1.6 eV and blogs to N semiconductor type.



Effect of Heat treatment on FTIR and Raman spectroscopy of Tin oxide thin films

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Abstract:

The effect of heat treatment on structural morphological and vibrational properties of APCVD SnO₂ thin films deposited on glass substrates has been investigated. Structural, morphological and chemical characteristics of the SnO₂ thin film surface have been determined by means of X-ray diffraction (XRD), SEM Fourier Transform Infrared (FTIR) techniques. All the diffraction peaks of the characteristic XRD patterns show rutile structure of SnO₂ which is in good agreement with the standard JCPDS card No. 77-0452. SEM analysis show polycrystalline films. The FTIR spectrum displays principal bands at 411, 518 and 770cm⁻¹ with shift of peaks due to annealing. In addition to the “classical” modes observed in the rutile structure, two other regions shown Raman activity for Tin oxide thin films. The Raman bands in the low-frequency region are attributed to acoustic modes.



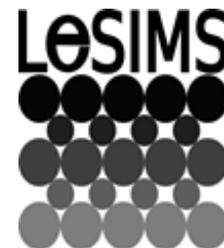
Electrodeposition and characterization of Ni-W as cathode for hydrogen release from alkaline medium

ASSELI Rabah

Energetic and Solid State Electrochemistry Laboratory, Ferhat Abbas-Setif 1 University, Setif 19000, Algeria

Abstract:

Objective of this work is to study the electrodeposition conditions of Ni and Ni-W alloy owing to its catalytic capabilities in electrolysis of water in alkaline medium for hydrogen production at low temperatures [1] which is of increasingly considered a clean and promising source of energy, Electrochemical measurements by cyclic voltammetry and chronoamperometry, morphological and structural analysis by SEM and EDX were exploited. The synthesis of Nickel-Tungsten alloys has been made possible by the modification of the watt bath. The electrodeposited alloys are characterized by a remarkable stability in corrosive medium (NaCl 3.5%), the W element is an improving corrosion resistance factor, tungsten preferentially migrates on the surface to form tungsten oxides [2] the Ni-W alloy is an excellent catalytic cathode to produce hydrogen by electrolysis in an alkaline medium KOH (25%). It has been found that these properties are closely related to the synthesis conditions: applied potential, temperature, pH and electrolyte composition.



Décontamination d'un champ d'exercices militaires par un procédé électrochimique

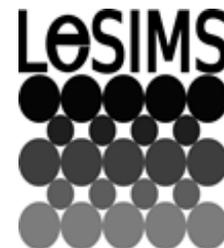
Karima Kada

Ecole militaire polytechnique; Algeria

Abstract: Electro-mediation is a promising technique that is generating increasing interest, applicable in situ for the decontamination of soils, or low permeability sediments, which can be polluted by a wide variety of organic or inorganic substances, such as heavy metals, or molecules. Based on aromatic nuclei potentially dangerous for humans and the environment. It is based on the galvanostatic application of a low density electric current in a contaminated soil or sediment matrix. [1,2,3] In this work, the electrokinetic remediation phenomenon was tested to remove lead ions ($[Pb^{2+}] = 200 \text{ mg / kg}$) from an artificial soil. The experimental study was performed in a Plexiglas cell (volume = 1987.5 cm^3), consisting of three compartments: anodic, cathodic, and the central compartment which containing the specimen, separated by a tissue. Sulfuric acid H_2SO_4 (0.1N) was used as a study medium. The imposed current is 100 mA, for duration of 240 hours (10 days). The results obtained showed a substantial decrease in the concentration of Pb^{2+} ions in the soil, with an elimination rate of $\sim 42\%$.

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CZTS Thin Films Synthesis Using One-Step Electrodeposition Process: Structural and Optical characterization

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Mentouri Brothers Constantine University, Algeria

Abstract:

In the last years, quaternary kesterite copper zinc tin sulfide $\text{Cu}_2\text{ZnSnS}_4$ (noted CZTS) is becoming one of the most promising semiconductor materials for thin film solar cells applications. This is due to its high absorption coefficient, reasonable work function and suitable band gap (1.5 eV). In this work, CZTS thin films were deposited by electrodeposition technique onto ITO coated glass substrates. The deposition was carried out at room temperature, during 50 min, without stirring and the applied potential was fixed at -7.5 V. The x-ray diffraction (XRD) and the optical transmission were used, respectively for analyzing the crystalline structure and the optical properties of the elaborated films. The x-ray diffraction results indicate that the films exhibit a kesterite phase $\text{Cu}_2\text{ZnSnS}_4$ with a highly preferred [112] orientation, resulting in the improvement of crystalline quality. The optical study shows that the transmission of the layer is less than 20 % in the visible range and the optical absorption coefficient is greater than 10^{+5} cm^{-1} . The CZTS obtained films can be used as an absorbing layer for thin film solar cells fabrication.

Key words: Electrodeposition, CZTS, Thin Film.



Synthesis, characterization, crystal structure and Hirshfeld surface analysis of new copper complex

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Abstract:

Azo compounds are very important in the fields of dyes, pigments and advanced materials. Azo dyes are synthetic colours that contain an azo group, as part of the structure. They are characterized by the azo linkage (-N=N-). We are involved in the color generation mechanism of azo pigments typically characterized by the chromophore of the azo group to synthesize new copper complex with $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$. Metal complexes with azo ligands show interesting chemical and physical properties and are of interest as new materials, for example in bioinorganic and coordination chemistry, as well as in biological systems which can lead to the development of new products with specific properties. In this work the structure of the title molecule, $\text{Cu}_2(\text{C}_{17}\text{H}_{13}\text{N}_2\text{O}_2)_4$, is reported. The dinuclear Cu^{II} complex consists of two inversion related asymmetric units, in which the Cu^{II} atoms are each coordinated by two *N,O*-bidentate phenylazo-naphtholate ligands. The two N atoms and two O atoms around the Cu atom are trans to each other with an O2—Cu—N1 bond angle of $86.83(7)^\circ$ and O2—Cu—N3 angle of $96.06(7)^\circ$. The inversion related asymmetric units are linked by one bridging O atom [O2i; symmetry code: (i) $x + 1, -y, -z + 2$] with O2i—Cu—O4 and O2—Cu—O2i angles of $104.51(6)$ and $81.69(5)^\circ$, respectively, to form a distorted square pyramidal geometry. In the crystal, molecules are linked *via* weak C—H \cdots O hydrogen bonds forming a layer.

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Synthesis, characterization of polyaniline and its application for adsorption of salicylic acid

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Abstract:

Polyaniline (PANI) is one of the most interesting polymers because of its easy preparation, high electrical conductivity, environmental stability, a wide range of applications in plastic batteries and more recently for adsorption removal of pollutants. In this study, polyaniline material was synthesized by in situ chemical polymerization method using ammonium peroxydisulfate (APS) as an oxidant, and characterized by SEM, XRD, FTIR, and TGA techniques. The synthesized PANI has been utilized as the adsorbent for the removal of salicylic acid (SA) from aqueous solution by the adsorption technique. The SEM of PANI shows aggregated particles with no uniform size. The XRD shows the peaks at $2\theta = 9.1^\circ$, 15.7° , 20.7° and 25.3° which are characteristic of PANI [1]. The FTIR spectrum of PANI shows the presence of characteristic absorption bands at 1555 cm^{-1} (C=C stretching vibration of the quinoid ring), 1476 cm^{-1} (stretching vibration of C=C of the benzenoid ring) and 1288 cm^{-1} (C-N stretching vibration) [2]. The DTA curve for the PANI shows three weight losses at 105°C , 286°C and 520°C corresponding on the TGA curves to three step decompositions. The first step of 9% ranging from room temperature to approximately 140°C corresponds to the loss of physisorbed and interlayer water. The second weight loss of 11% corresponds to the removal of dopant molecule and oligomer [3], whereas the third mass loss of about 30% is attributed to the thermal decomposition and degradation of the PANI chains. The maximum experimental adsorption capacity of adsorption of salicylic acid (SA) was 393,5 mg/g. Attempts were made to fit the isothermal data using Langmuir and Freundlich equations. The experimental results have demonstrated that the equilibrium data is fitted well by a Freundlich isotherm equation. These results show that the prepared PANI is excellent adsorbent in the removal SA from aqueous solutions.



Effect of Nitrogen rate on the formation and the crystallization of Titanium Nitride layer deposited on MgO Substrate

Bachir Eddine MESSAID^{1,2}, Claire Le Paven², RazikaZair Talaighil^{1,3}, Ratiba Benzerga², Laurent Le Gendre², Florent Marlec², Faycal Bensouici¹

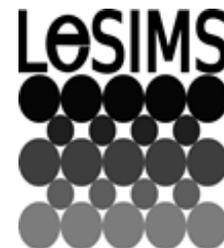
¹Advanced materials by Sol-Gel, Research unit of materials processes and environment (URMPE), University M'hamed Bougara of Boumerdes 35000, Algeria

²FunMAT team, Electronics and Telecommunications Institute of Rennes (IETR), University of Rennes, France

³Institute of Electrical & Electronic Engineering, University M'hamed Bougara of Boumerdes, 35000, Algeria

Abstract:

In this study, a Titanium Nitride TiN was deposited by active radio-frequency (RF) magnetron sputtering on a monocrystalline substrate "magnesium oxide MgO"[1,2], the layers is deposited with the creation of plasma, the amount of nitrogen introduced in the chamber of deposition which presents an essential factor to have a stoichiometric layer, for this purpose, three levels of nitrogen were used $N\% = 30\%, 50\%, 100\%$, the X-ray diffractions of TiN deposited at 50%, show the presence of two peaks (200) and (400), also four peaks separated by 90° in Phiscan, this peaks show an epitaxial growth of the TiN layer deposited on MgO, the stoichiometry of TiN is shown by EDX analyzes with a 0.94 Ti / N ratio, the increase in the amount of N₂ up to 100% clearly results a decrease of cristallization of TiN, however, the deposition at an atmosphere of 30% N₂ shows an additional peak at about 44° , which corresponds to Ti₂N, and a Ti / N ration of 1.12. Morphologically, a high surface density with similar morphologies observed by using a 30% and 50% of N₂, however, a less homogeneous surface that contains relatively large bumps is observed with a pure atmosphere of N₂. According to the variation of the nitrogen levels, a deposit of TiN on MgO in an atmosphere of 50% of N₂ has an epitaxial and stoichiometric layer.



Removal by adsorption of phosphate on synthesized and encapsulated Zn-Al-LDH (layered double hydroxide)

Elhachmi Mounira

University of Saad Dahleb Blida1

Abstract:

In this study, we are interested in the shaping of an anionic adsorbent: (Zn-Al-LDH layered double hydroxide) integrated in an alginate gel to produce a composite material, which can be used in reactors dynamic, for the removal of phosphates. The HDL prepared by the coprecipitation method is characterized by the technique of XRD and infra-red spectroscopy FTIR. The experimental results show that the adsorbed quantity of the phosphates increased from 0.66 to 62.35 mg by g of LDH with the increase of flow from 0.015 to 0.05 l.h⁻¹ and the decrease of diameter from 4 to 1 mm. The height of the bed hardly influenced this quantity. In the case of the HDL-encapsulating beads, the conditions applied allow an almost total phosphates removal at the column outlet, then the concentration increases to return to the initial concentration (saturation of the adsorbent). The results are interesting, since mathematical modeling by the Thomas model shows globally a good description of the experimental values.



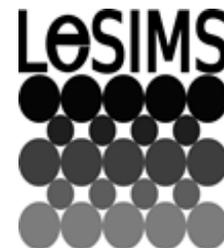
CuO sol-gel thin films for optoelectronic applications: effects of annealing and thickness on physical properties

Chahinez Djidjeli

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Abstract:

In this work, copper(II) oxide (CuO) thin films are synthesized on glass substrates using different number of coatings (2, 5, 10 and 15) by sol-gel dip-coating technique. The effects of thickness and annealing temperature on structural, morphological, optical and electrical properties are investigated using X-rays diffraction (XRD), atomic force microscopy (AFM), UV-Vis-NIR spectroscopy and I-V measurements. To prepare the solution, anhydrous Copper(II)-chloride, ethanol and triton X were used as precursor, solvent and stabilizer agent respectively. The results showed that all films are well crystallized in CuO monoclinic structure. AFM images showed that the morphology of films is affected by the thickness and temperature annealing. UV-Vis-NIR optical spectra revealed that optical transmittance decreases with increasing film's thickness. The (I-V) measurement of the realized ITO / CuO-p / SnO₂-n junction provided short-circuit current density of 0.05 (μ A) and open circuit voltage of 0.005 (V).



Preparation And Properties Of NiO Doped Copperthin Films Prepared By Spraypyrolysis

Rafia BARIR

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Faculty of Mathematics and Material Sciences, University of Ouargla; Algeria

Abstract: In the present work, undoped nickel oxide (NiO) and doped copper thin films were deposited on 500°C heated glass substrates using spray pyrolysis at (0-5wt%) range of dopant, we were obtained by decomposition of nickel nitrate hexahydrate in double distilled water [1-2]. Effect of 0-5 wt. % copper doping on structural, , optical and electrical properties of NiO thin films was studied. XRD indicates that the 0-5 wt. % copper doped NiO thin films have polycrystalline nature with cubic structure and (111) plane as preferential orientation. Crystallite size of the films changes, from 37.1 to 11.7nm, with the Cu doping level. Ni-O bonds vibrations modes in the product of films were confirmed by FT-IR analysis. Transparency of the films was decreased from 64-35% with increasing Cu doping was observed with an increase in the band gap energy values, from 3.62 to 3.95eV, after doping. All the films are deposited p-type semiconductor showing an increase in their conductivity, from 2.33 to $5.91 \times 10^{-2} \Omega^{-1} \cdot \text{cm}^{-1}$, with Cu increasing.

Keywords: NiO thin films; spray pyrolysis; X-ray diffraction.

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Synthesis and characterization of multilayered CuO-Cu₂O/ZnO thin films

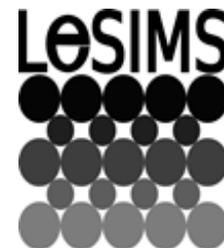
Elhadj Benrezgua Benrezgua Ibrahim
Mohamed Boudiaf University Msila, Algeria

Abstract: In the present work, multilayered CuO-Cu₂O/ZnO thin films have been deposited layer by layer onto glass substrates by sol-gel spin coating method. Zinc acetate dihydrate, copper chloride dihydrate, Ethanol and monoethanolamine (MEA) were used as a precursors, solvent and stabilizer respectively. For both solutions, the molar ratio of MEA to metal ions was maintained at 1.0 and a concentration of metal ions is 0.6 mol.L⁻¹. The structural information of different metal oxides and their crystallite size, preferential orientation were estimated via XRD. Optical and luminescence properties of the multilayered films were investigated by UV-Vis spectrometry and PL spectroscopy techniques. The obtained results of all thin films are discussed in detail and are compared with other experimental data.

Keywords: Sol-gel technique; Zinc Oxide thin film; Copper Oxide; Structural properties; Optical properties; Luminescence

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A new structure of a-Si:H TFT with Si₃N₄ / HfO₂ double gate layer dielectric

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Abstract:

Electrical characteristics of amorphous silicon thin film transistors with an aluminum gate electrode and an Si₃N₄/HfO₂ double-layer gate insulator are investigated. Performances of this new structure of transistor are modeled using Silvaco software tools. The results show a high electrical performance and low threshold voltage with increasing in the drain current compared with the conventional amorphous silicon based thin film transistors. The importance of the use of Si₃N₄/HfO₂ double-layer gate insulator is then demonstrated.

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Photoconductivity and defects levels in SnO₂ thin films

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Abstract:

In recent years, tin oxide thin films have attracted increasing attention due to their wide domain application. Notable defects in SnO₂ are oxygen vacancies and tin interstitial; these defects may behave like traps for free electrons or holes, such as recombination centre or centre generation. Electron and hole traps (depths) play crucial role in optical and electrical properties, especially in photoconducting properties, moreover persistent photoconductivity (PPC) and existence of low energy below fundamental gap in the spectral dependency of photoconductivity are problematic characteristic that occur as a result of these defects. Several techniques and measurements were used for giving information about deep levels defects in semiconductors such as photo-induced current transient spectroscopy, growth and decay of luminescence emission intensity or photoconductivity.



The impact of the concentration solution on the physical properties of SnO₂ thin films deposited by spin coating

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Abstract:

The aim of this work is to study the solution concentration effect on the SnO₂ thin films properties, which were deposited on glass substrates by spin coating technique and annealed for one hour at 500°C. X ray diffraction spectra show that the films deposited at various solution concentrations (0.5 mol/l, 0.7 mol/l and 1 mol/l) are polycrystalline with a tetragonal rutile type. Grains have two preferred orientations along the directions (110) and (101) corresponding to 2θ equal to 26.74° and 34.11° respectively. We have also noted that the grain size changes between 109 and 178 nm. However, the film coated at 10 deposition cycles and 0.7 mol/l solution concentration has a minimum arithmetic averageroughness of 0.376 nm. The optical transmittance of the films in the visible spectrum was in the range of 77 – 84% and the optical band gap gradually decreases with the decrease of the solution concentration from 4.11eV to 3.56 eV.

Keywords: Thin films; SnO₂; Spin coating; XRD; AFM; Optical properties.



Elaboration of thin layers of Zinc on XC38 steel in the presence of nettle plant extract

ZAABAR Aida

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Abstract: Zinc is currently used in steel coating processes to protect against corrosion. For such reasons, much research has been carried out to improve the corrosion resistance of zinc electrolytic deposits by adding organic additives. Indeed, these additions have an influence on the physical, chemical and mechanical properties of the coating such as grain size, luminosity, chemical composition, etc. The aim of this research is to study the effect of nettle plant extract (notes O1), obtained by the reflux method in water, on the improvement of the quality of zinc deposits obtained by electrodeposition on a steel substrate in a sulphate medium at pH=2. This research is an alternative in order to avoid the addition of polluting chemical additives conventionally used in this type of research. The curves obtained in the cathodic domain show that O1 decreases the kinetics of hydrogen release, a parasitic reaction which is often at the origin of defects observed on metal deposits and which leads to poor performance of the materials obtained. SEM photographs of zinc deposits obtained by chronoamperometry at $E = -1.7 V_{SSE}$ for 30 minutes show that O1 significantly affects the morphology of the zinc deposit and produces a finer-grained deposit (Figure 1).

Keywords: corrosion, coatings, zinc, steel, electrodeposition, nettle, SEM.

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Influence of Fe content on tribologic properties of α - β type Ti-6Al-xFe powders prepared by mechanical milling

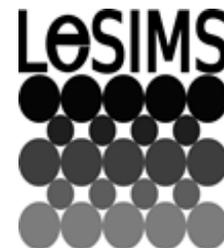
Fouzia fifi hammadi

University abbes laghrour; Algeria

Abstract: In this study, Ti-6Al-4Fe nanomaterials were prepared by high-energy milling using elemental Ti, Al, Fe, powders. The Ti-6Al-4Fe nanomaterials powders were milled for up to 18 h and then hot pressed in vacuum at 300 MPa. The mechanical behavior of the samples was determined as a function of hardness and bending tests and analyzed by scanning electron microscopy, energy dispersive x-ray spectroscopy, optical microscopy and x-ray diffraction (XRD). Our results showed that. The hot pressed density of the Ti-6Al-4Fe nanomaterials decreased with increasing milling time. Milling of titanium powder for 18 h, significant enhance ther hardness and wear resistance due to a grain size refinement. With increasing milling times, the wear rates decreased, which is endorsed to the enhanced powders mechanical properties, due to its particle sizes refinement. At longer milling time, the wear rate and the friction coefficient decreased significantly. At 18 The Ti-6Al-4Fe showd the lowest and the Ti-6Al-4V the highest. According to the presented results, we obtained nanostructured titanium alloys with lower crystallite sizes and higher wear resistance. It seems that the replacement of V by Fe on Ti-6Al-4V alloy would be a good choice in biomaterials for hip prostheses, which means a longer wear life of the components and thus providing the patient a better quality of life.

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Synthesis Of Complex Oxides Composite ZnO/ZnAl₂O₄ By Spray Pyrolysis: Study Of Strain, Structural And Optical Properties

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Abstract: The photo-catalytic activity of the catalysts is highly dependent on the adsorption behavior and the separation efficiency of the pairs e^- and h^+ [1]. The coupling between ZnO, which is an excellent photo-catalyst for the degradation of organic and inorganic pollutants as well as hazardous waste in water and air (due to its photo-sensitivity, no -toxicity and its direct 3.2 eV and indirect 2.45 eV optical gap values), with a second non-sensitive wide band gap semiconductor proved that was an effective method to improve their photo-catalytic activities. In particular the mixing between the ZnO and ZnAl₂O₄ ($E_g = 3.8$ eV) band gap structures ensures the separation efficiency of the e^- and h^+ generated pairs. The ZnO-ZnAl₂O₄ mist has high photo-catalytic activity due the presence of the spinel phase with high surface area and thermal stability [2]. ZnAl₂O₄ is a spinel-type complex oxide. This compound is nontoxic, inexpensive and very stable material. ZnAl₂O₄ is of interest due to its combination of desirable properties such as high mechanical resistance, high thermal stability and low surface acidity [3]. It is used in many catalytic reactions [4]. The aim of this work is the control of the ZnO/ZnAl₂O₄ films synthesis on glass, silicon and ITO substrates (for a better application) as well as the study of their growth and the correlation of the stresses with the structural and optical properties. A simultaneous formation, according to XRD, of ZnO and ZnAl₂O₄ phases on glass substrate from the annealing at 500°C-2h is observed and confirmed by EDX. The (D_{ZnO} and $D_{ZnAl_2O_4}$) crystallites size grown on Si are much higher than those on glass. Tensile stresses between 0,031 and 0,469 GPa for the ZnO layers and compressive one for ZnAl₂O₄ \sim -0,227 and -0,404 GPa in ZnO/ZnAl₂O₄ annealed between 650 and 500 °C. ZnO nanorods are detected by SEM. The ZnO/ZnAl₂O₄ films, as characterized by UV-visible spectroscopy, are highly transparent in the visible and near infrared regions.

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Properties of Short Hollow Recycled PET Fiber Reinforced Crosslinked Polypropylene Composites

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Abstract: The effect of hollow recycled polyethylene terephthalate (PET) fibers reinforced crosslinked polypropylene (XPP) composites on the mechanical and structural properties were investigated. Aiming at improving the adhesion between the PET fibers and the polypropylene (PP), a modification of PP structure was carried out using crosslinking agents. Hollow PET fibers were used in different loading (3,7 and 10 wt%) and the composites were prepared by melt mixing in a Brabender. The obtained results show a significant improvement of the mechanical properties of polypropylene reinforced with PET fibers. The prepared composites are considered for automotive industry.

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Study and characterization of the microstructure, crystallographic texture and mechanical properties of AGS aluminum alloy cold drawn wire

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Abstract : Our study was carried out on an AGS (AA6101) type aluminum alloy wire rod, the most used by the ENICAB company in the manufacture of electrical energy transmission cables. The objective of this work is to study the evolution of deformation texture and the energy stored in the grains during cold drawing of aluminum wire for industrial applications, for an objective to understand the link between the microstructure and the mechanical behavior after wire drawing. We have found that the wire deformation texture of the copper wires is composed mainly of the two fibers $\langle 111 \rangle // DN$ and $\langle 001 \rangle // DN$ ($DN //$ drawing axis) and that the fiber $\langle 111 \rangle // DN$ is a majority and the fiber $\langle 001 \rangle // DN$ is a minority. In addition, we found an increase in hardness, mechanical strength and energy stored in deformed grains of wire drawn with increasing deformation level [1-3]. For this study several experimental techniques of measurement and characterization allowed us to carry out this work. These are Scanning Electron Microscopy (SEM), Back Scattered Electron Diffraction (EBSD), X-ray diffraction, Neutron diffraction, Vickers microhardness and Chemical analysis by EDAX, some of which have allowed to correlate microstructure, mechanical properties to the deformation texture.

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Electrochemical synthesis and characterization of bismuth oxide thin films from alkaline bath: effect of annealing temperature

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Abstract:

In this work, the electrodeposition of bismuth oxide from alkaline bath onto a copper substrate was studied. In order to obtain bismuth oxide with a desired crystallographic structure, the effect of annealing temperature on the morphological and structural properties of Bi_2O_3 was investigated. Cyclic voltammetry and chronoamperometry methods were used to the electrochemical characterization formation of Bi thin layers. The morphological analysis with the scanning electron microscopy (SEM) shows a different surface morphology according to the experimental condition. The X-rays diffraction analysis (XRD) reveals the presence a several Bi_2O_3 phases according to annealing temperature, which also confirmed by Raman spectroscopy.



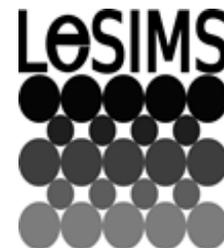
Synthesis and characterization of In-Y codoped ZnO thin films prepared by spin-coating technique

Abdelhamid Bouaine

Laboratoire Physique de la Matière Condensée et Nanomatériaux (LPMCN), Département de Physique, Faculté des Sciences Exactes et Informatique, Université Mohammed Seddik Ben Yahia- Jijel, cité Ouled-Aïssa B.P. 98 Jijel 18000, Algeria

Abstract:

Indium and yttrium codoped zinc oxide thin films were deposited on glass substrates by sol gel spin coating technique. Indium had a constant concentration of 2 at.% whereas yttrium was incorporated with different concentrations of 1, 2, and 3 at.%. X-ray diffraction analysis showed that all the films are polycrystalline with a hexagonal Würtzite structure and a preferred orientation along the (002) plane. UV-visible spectrophotometer showed that all the films have a high transmission of about 94% in the visible zone with band gap energy of about 3.27 eV. The electrical resistivity of the films increases by doping with yttrium.

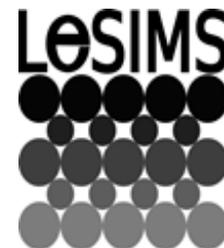


Raman analysis of carbon based thin films

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Centre de Développement des Technologies Avancées; Algeria

Abstract: Raman spectroscopy is now a powerful tool to characterize carbon based thin films materials. The principle is to probe the material with a laser at a given wavelength and energy and record Raman effects as a spectrum which is more sensitive to lengths, strengths and arrangements of bonds within the material. The structure of amorphous hydrogenated carbon (a-C:H) coatings is often described by the bond forms of carbon-carbon and carbon-hydrogen within the carbon matrix mixed with a certain amount of hydrogen content. Therefore, with the presence of hydrogen, carbon forms mainly both sp^3 and sp^2 sites that are at the origin of physical and mechanical properties of the material. The clustering degree of sp^2 sites is also considered as a feature behind optical, electronic and mechanical properties of this kind of material as claimed by Robertson [1]. All these bonds characteristics can be probed by using Raman spectroscopy in the IR, visible and UV energy ranges. To do this, the as deposited DLC films were characterized using Raman laser spectroscopy at 3.81eV of energy ($\lambda=325\text{nm}$) and 1.96eV (632nm). The recorded spectra show the so-called G and D peaks at around 1580 and 1400 cm^{-1} , respectively. The Raman scattering modes that give rise to those peaks are dominated by sp^2 sites and their characteristics according to their size and on whether they are organized in chains or rings. It is known that the G peak originates from the stretching mode of sp^2 sites (E_{2g} mode) formed in chains (olefins) or aromatic or odd-membered rings, while the D peak is due to the breathing mode of (A_{1g} mode) sp^2 sites in rings [2-4]. However, by interpreting Raman spectra on the basis of their parameters such as position, width and intensity leads to more insight and better description of the structure. This can be done through fitting the main feature after baseline correction into two Gaussian peaks in Origin software. From fitting results it has been found that positions of G and D bands and D width are almost with no significant change from one sample to another. However, when comparing these Raman results with those collected in the visible range [5], it is seen that when increasing energy the G peak positions shift towards higher frequencies while the G line width exhibits narrow line and decreases with increasing film thickness. On the other side, the intensity ratio of D and G peaks (I_D/I_G) as a function of residual stress showed a linear relationship and the determined L_a indicate that G width is correlated to the sp^2 clusters organized in rings [6].



Copper oxide synthesis by spray pyrolysis technique: characterizations and application

A. Chetoui^{*1}, A. Zouaoui²

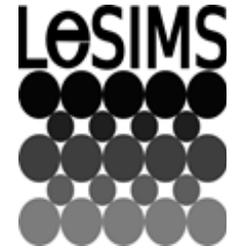
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Abstract: Spray pyrolysis is a very simple and cost-effectiveness chemical deposition method. Its operating principle is based on the atomizing of a starting solution into fine droplets. The generated droplets are subsequently deposited on substrates carried at high temperatures where the pyrolysis process takes place. Among the advantageous presented by this technique is the possibility of deposition of highly adherent and homogeneous films even on large surfaces [1]. Thus, this processing holds strong promise for employment industrially on large scales. However, in order to get films with the previously mentioned properties, an optimization of the different parameters like the air pressure, the temperature, the nozzle-substrate distance, the nature of the precursor, etc. should be studied in detail. The spray pyrolysis technique is used to deposit a variety of materials including the semiconductor metallic oxides such as: SnO₂, TiO₂, ZnO, CuO, Cu₂O, NiO, etc [2]. In this work, we are interested in the study of the spray-pyrolyzed copper oxide properties. Copper oxide is a p-type semiconductor which is used in many technological areas such as photocatalysis, super-capacitors, bio-sensors and gas sensors. This work is intended to study the structural, morphological properties and the use of the obtained copper oxide films in gas sensing. The gas sensor performance is related to three main features: the sensitivity, the selectivity and the stability. We focus here on the enhancement of the sensitivity in terms of the specific surface of detection (SSD). The gas sensitivity is evaluated by measuring the change in one of the electrical properties (current, resistance, capacitance, etc.) of the sensor in the gas atmosphere. It is well known that the sensitivity is as greater as the SSD is large. Hence, we show the different steps which made us able to obtain copper oxide films with a large SSD. As a conclusion, we expose the sensitivity of our sensors towards different CO₂ concentrations.

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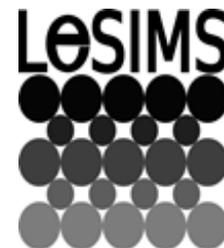
Effect of chemical tempering parameters on the mechanical properties of glass

Oumessad Gridi

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Abstract:

The relationships between the mechanical properties of strengthened glass by ion exchange and the technological parameters of chemical quenching have been investigated. Samples of soda lime silicate float glass were subjected to ion exchange treatment at different temperatures and during different times in a molten salt bath of potassium nitrate in order to create compressive stresses at the surface of these samples. Several techniques were used to evaluate the surface characteristics of these samples; such as Vickers indentation and 4-point bending test. The results obtained show that both the temperature and the time of ion exchange have a significant influence on the characteristics of the surface and consequently on the mechanical properties of the glass.



Sol-Gel Synthesis and Characterization of Monolith and Transparent Sr, Fe and Al-Doped TiO₂.

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Abstract:

Transparent monoliths of Al, Fe and Sr-doped TiO₂ were synthesized through a modified sol-gel way from titanium isopropoxide as precursor. By controlling the hydrolysis of this precursor through the intermediate of the esterification reaction between acetic acid and solvent at room temperature. The monoliths xerogels prepared by this method were transparent in the wavelengths between 500 nm and 800 nm. The Alumina and Iron-doped TiO₂ samples have a crystalline part without calcination. Powder X-ray diffraction confirmed the amorphous-to-anatase and the anatase-rutile/brookite phases transformations. Only anatase TiO₂ could be observed in the samples annealed at T<500°C. BET analysis showed that transparent gels have an important surface area.



Fabrication and characterization of natural dye sensitized solar cell with curcumin and aminothymoquinone

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Abstract: Dye-sensitized solar cells (DSSC) based on natural sensitizers have become a topic of significant research because of their importance in the field of energy conversion. In our study we have used curcumin and aminothymoquinone as natural dye sensitizers. Aminothymoquinone is an important constituent of *Nigella Satvia*. It is very important light sensitizer. The dye molecules are absorbed by TiO₂ nanoparticles at the surface, when submerged in the solution for 24 hrs. When illuminated under 80W/cm² intense light the photovoltaic properties were investigated and the current density-voltage characteristics and current conversion efficiency measurements were carried out. The short-circuit current (I_{sc}), open circuit voltage (V_{oc}), Fill factor (FF) and efficiency (η) for both the dyes were determined. Comparatively the aminothymoquinone dye as light harvesting material was found to be a more promising candidate for future solar cells. Further being natural dyes both these have minimum impact on the environment.

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Copper-Polypyrrole Composite Films for Electrocatalysis of Ascorbic Acid

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Abstract:

In this study, we report the electrochemical synthesis of a composite electrode material based on thin films of polypyrrole (PPy) deposited by electropolymerization method on an indium tin oxide (ITO) substrate which was followed by the insertion of copper (Cu) particles on the PPy film under potentiostatic conditions. For this purpose, two separate solutions were used one is an organic solution containing the monomer pyrrole (Py), and the other is an aqueous solution of the metal salt. The synthesis parameters were carefully examined in order to obtain suitable morphological microstructure of the deposits and thus enhanced electrocatalytic properties of the modified electrode. The electrochemical reactivity of the resulting Cu-PPy/Si electrodes was then examined towards the oxidation of ascorbic acid (AA) in 0.1 M pH 7.0 phosphate buffer solution using cyclic voltammetry and chronoamperometry methods. The results demonstrate that the synergism of the advantages each component in the composite provides an enhancement in catalytic activity of the final material for the determination of ascorbic acid.



Improvement of the characteristics physico-mechanical and durability of the stabilized earth block: a review

Abdelghani Idder, B. Labbaci and A. Hamouine
University Tahri Mohamed Bechar, Algeria

Abstract:

Over a period about 10 000 years, the raw earth is considered as one of the most important building materials, in spite of the development of modern building materials, he is recorded every year increase of the proportion of the construction by the raw earth, where it is estimated that approximately a third of the population today live in traditional houses because of his environmental, social and economic advantages. The raw earth is also a plentiful and unlimited material and at the end to value the local building materials and reduce the price of the construction, this study comes to review on the methods of stabilization of the earth and to study his physico-mechanical properties and their durability after the stabilization. Several studies were led in this domain, where the result was that we can use the raw earth as a building material characterized by the economic, ecological and acceptable performances in the field of the construction.



Structural and optical properties of bismuth sulfide thin films deposited by spray pyrolysis

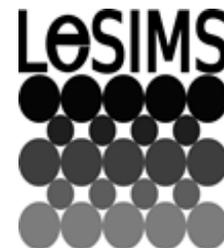
Amara Zeyneb

LECM Laboratory of Djillalil Liabes Sidi Bel Abbes Algeria.

Abstract: Polycrystalline films of Bi_2S_3 compound have been prepared at substrate temperature of 260°C , from Bismuth chloride (BiCl_3) and Thiourea ($\text{CS}(\text{NH}_2)_2$) solutions. The structural characterization has been carried out by the X-ray diffraction analysis (XRD). Study of optical properties shows that Bi_2S_3 compound has a direct transition at 1.64eV energy. The refractive index, extinction coefficient and dielectric constant are calculated by using SPPS (Seed Processing Pattern Search) technique. The absorption coefficient is in the range of 10^5 cm^{-1} .

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Surface Morphology, Electrical Resistivity and Structural Study of Ni/Au/Si(111) Annealed System up to 800°C.

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Abstract: Thermal evaporation was used to deposit Ni/Au bilayers on (111) monocrystalline silicon substrate Si(111). As function of annealing between 200 and 800°C, crystallites size of resulting silicides was calculated. Gold layer thickness of about 64 nm shows that it is not sufficient to prevent interdiffusion of Nickel atoms in silicon lattice. In addition surface morphology, films composition and electrical resistivity of these annealed bilayers was also studied using AFM, SEM, EDS and four probe techniques. After an annealing of 400°C, Nickel textures was missed in X ray spectra which confirm their full consumption to form silicides. Whereas, no interdiffusion of gold was revealed through the different annealing temperatures employed. Consequently, gold precipitations were clearly observed within SEM images on the top of these formed silicided. Ni₂Si is the most easiest formed silicides phase that was formed after only 200 °C. Other silicides such us Ni₂Si, NiSi et NiSi₂ and Ni₃Si were also identified. RMS factors and electrical resistivity were clearly increase when annealing temperature increase.

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The structural and morphological properties of electrodeposited Mo coated onto Cu substrate under current density

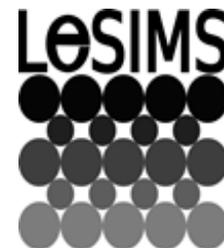
Fatima Nemla

Université Ferhat Abbas Sétif1, Setif, Algeria

Abstract: In this study, we present a successful 1800 seconds electrodeposition experiment of micrometric, bright and rough Mo coating from aqueous electrolyte in an acid bath. XRD analysis and EDS spectrum have been used to confirm the presence of Mo. The crystal structure of deposits was slightly amorphous in nature to body centred cubic structure (bcc) Mo (110), (211) and (220) face. Lattice parameters exhibit some residual tensile stress, and deviate slowly from reference lattice parameter. In addition, calculated lattice parameters agreed well with available works from literature. Surface top was observed at different zoom in order to deep inside the origin of Mo coating properties. Discussions on the grain growth prove that they are constrained by grain boundary energy not the thickness effect. Further discussions were devoted to inspire some relationships and correlations in the view of solar cell application as Molybdenum bottom contact.

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Thermal insulating behaviors of Polypropylene/Spanish Broom flour composites

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Abstract: The present work reviews current research on the field of green composites. The effect of chemical treatment on thermal and thermophysical properties of Polypropylene/Spanish Broom flour composites has been investigated. Polypropylene (PP) is a non-polar matrix; therefore it has a poor adhesion towards polar SB flour. Because an emphasis was put on evaluating the effects of modification, two chemical treatments like sodium hydroxide and silane were performed in order to reduce the hydrophilic behavior of SB flour, and to improve the interfacial adhesion PP-SB. The thermophysical study was performed according to ISO 22007 on transient plane source (TPS 2500S) Hot Disk. The heating powers were 11, 19 and 23 mW for a measurement time of 10 seconds. The thermal conductivity of the flour-reinforced composites increased after every treatment due to improved interfacial interactions. However, for flour ratio low than 20 wt%, we note a decrease of thermal conductivity of composites (i.e., under 19 mW: from 0.2668 W/m.K for neat PP to 0.2699 W/m.K for PP/10 wt% Untreated SB, 0.2562 W/m.K for PP/10 wt% SB-NaOH, and 0.2293 W/m.K for PP/10 wt% SB-VTMS, respectively). For an SB content of 20 wt%, the thermal conductivity values of all PP/SB composites are almost identical to those of neat PP, but beyond 20 wt%, there is a significant increase in thermal conductivity, and this is reflected in a lowering of the total temperature increases.

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Characterization of Ferrite Material's Using Microstrip Ring Resonators in Microwave Frequency Bands

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Abstract:

New microwave electronic technology challenges require integration of many passive components on chips. Among them, isolators and circulators are nonreciprocal passive devices which contain ferrite materials. Hence, it is important to know the magnetic properties as permittivity and permeability. Microstrip ring resonator (MSRR) has proved its efficiency in electromagnetic material characterization in microwave bands. The aim of the work is to characterize ferrite materials using the frequency response of MSRRs. A modelization of the problem allowed to find a relation between the ring resonance frequencies and the electromagnetic properties of ferrite such as effective permittivity and permeability. The measurements made on YIG (101) from 1 to 30 GHz are found to be in good agreement with the theoretical results. And the MSRR technique applied on ferrite materials has been validated.



Ni and Ni/Zn Hydroxide based Nanohybrid Synthesis using Hydrothermal Process

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Abstract: Nano-porous transition metal oxides, hydroxides and carbonate hydroxides based nanomaterial have received increased attention especially due to its electrochemical properties and potential applications and their wide application in many fields. In this work, we focus our investigation on the synthesis of Ni and Ni/Zn based nanocomposites as mono and bi-phase nanoelectroactive materials based of α -Ni(OH)₂ · 2H₂O and α^* -Ni(OH)₂ · 0,75H₂O /Zn₄(CO₃)(OH)₆ · H₂O, respectively, using a simple and low cost free template urea based hydrothermal process at 120 °C growth temperature during 18 hours. The morphological, textural and the structural selectivity of the as-prepared materials were characterized with different techniques such as: XRD, FTIR, FESEM, BET and Raman analysis in order to investigate their physico-chemical properties. These obtained mono (Ni) and bi-phase (Ni/Zn) nanohybrids have shown the formation of heterostructures based of quasi-microsphere-like structure consisting of overlapping filaments and regular or irregular nanoflakes shape with two kind of pores with an important specific surface area around 97 m²/g and 34.64 m²/g, pore volume around 0.38 cm³/g and 0.10 cm³/g and pore size around 12 nm and 14.86 nm, respectively.

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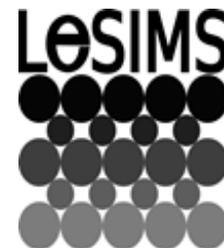
Investigation of corrosion inhibition effect of vitamin B1 on copper in 1M HNO₃ solution: electrochemical study and surface analysis

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Abstract: Corrosion prevention systems favor the usage of chemicals with low or no environmental impacts. In this content, the usage of some of the inhibitors has been restricted due to the toxicity, and their insufficient inhibitory efficiencies at low dosages. Therefore, the studies have begun to focus on finding novel, cheap, non-toxic, healthy and extracted from natural foods. VitB1 molecule contains many π electrons as well as one oxygen, one sulphur, and four nitrogen atoms which are assumed to be adsorption centers. The presence of such adsorption centers in the molecular structure is expected to cause an easier electron transfer from the functional groups to the metal surface which provides greater adsorption ability and corrosion inhibitory efficiency. Due to its unique advantages, which are describes above, the VitB6 was investigated as potential corrosion inhibitor for copper which are widely used in industrial applications as and could exposed to corrosion medium. For this aim, potentiodynamic polarization, electrochemical impedance spectroscopy (EIS) and linear polarization resistance techniques were used. Surface of the metal exposed to corrosive medium was investigated by Scanning Electron Microscopy (SEM) and atomic force microscopy (AFM). It was found that the VitB1 provided satisfactory inhibition on the corrosion of copper and the inhibitory efficiency of this compound depends on its concentration. The high inhibition efficiency was explained by adsorption of the VitB1 molecules on the copper surface and a protective film formation. The results obtained by SEM and AFM confirm the results obtained previously.

key words: Corrosion , copper, Vitamin B1, SEM



Synthesis, nonlinear optics properties of new thin films of schiff bases ligands containing O-tolidine.

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Abstract:

This paper explores the synthesis, structure characterization and nonlinear optics properties of new schiff bases. These compounds were obtained by condensation of o-tolidine with salicylaldehyde and cinnamaldehyde. The obtained ligands were characterized by UV, ^1H and NMR. Their third order NLO properties were measured using the third harmonic generation technique on thin films at 1064 nm [1]. The electric dipole moment (μ), the polarizability (α) and the first hyperpolarizability (β) were calculated using the density functional B3LYP method with the lan12dz basis set. For the results, the title compound shows nonzero β value revealing second order NLO behaviour.

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Deposition of zeolite films on metal surfaces and studies of their corrosion inhibiting effects in NaCl medium

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Abstract:

Corrosion in industrial environments is one of the main factors limiting the life of materials. ZSM-5 has been synthesized and characterized by DRX and FTIR and its behavior as a studied corrosion inhibitor. In this study metal plates were covered with different zeolite films using the dip coating method. They were then introduced into NaCl solutions of different concentrations. The treated samples were studied by gravimetric and electrochemical methods to determine the corrosion inhibiting effect of their zeolite layers. The results show that the zeolite layers have exhibited high corrosion resistance and have great potential to become ecological alternatives to conventional coatings.

Keywords: *ZSM5, zeolitic films; inhibitor; corrosion, gravimetric; electrochemical*



Electrodeposition behavior of nickel–zinc alloys from citrate bath.

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Abstract:

In this work, electrodeposited Ni-Zn alloy was studied using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) methods from aqueous solutions with different molar ratios of Ni/ Zn and different cathodic applied potentials. The morphological and structural characterizations of the electrodeposited films were performed by scanning electron microscopy, EDX and DRX analysis. The results showed an anomaly during the as-deposition process [1], three phases obtained of as-deposited Ni-Zn alloy η , γ and α [2]. The Ni percentage in the obtained alloys increase with molar ratio of Ni/ Zn (until 18.80 % of alloy at molar ratio equal 10) and when the cathodic potentials shifted to more negatives values. The surface of the all coatings is spherical nodular, and compact without cracks.



Study of the effect of temperature and time on the anticorrosive power of a Schiff base molecule named {4, 4' Bis (2-Furane Carboxaldehyde) Diimino Diphenyl Sulfide} on mild steel in acidic medium.

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Abstract: Inhibitory effect of a Schiff base molecule {4, 4' Bis (2-Furane carboxaldehyde) diimino diphenyl sulfide} on corrosion of mild steel in 1M HCl solution has been studied using weight loss measurements and polarization curves methods. The results of the investigation show that the studied compound with mean efficiency of 92% at 5.10^{-3} M additive concentration have fairly good inhibiting properties for mild steel corrosion in hydrochloric acid, and it is as mixed inhibitor. All measurements show that inhibition efficiency increase with increase in inhibitor concentration. This reveals that inhibitive action of inhibitor were mainly due to adsorption on mild steel surface. Analysis of the temperature dependence of inhibition efficiency as well as comparison of corrosion activation energies in the absence and presence of inhibitor gives some insights into the possible mechanism of inhibitor adsorption [1]. In order to evaluate the adsorption of inhibitor and to calculate thermodynamic and activation parameters of the corrosion processes of steel in acidic media, the effect of temperature on the polarization curves and corrosion parameters (E_{corr} (vs. SCE), I_{corr} , b_a , b_c , IE% and q) in the absence and presence of various concentrations of inhibitors were studied. Activation parameters of the corrosion process such as activation energies, E_a , activation enthalpies, ΔH°_a , and activation entropies, ΔS°_a , were calculated by the obtained corrosion currents at different temperatures (25-35-45 and 55°C). The results obtained from the polarization curves show an increase in the current density with increasing temperature followed by an increase in the inhibitory efficiency at 35 °C. Beyond this temperature the inhibitory efficiency begins to decrease with the increasing temperature with analogous increase in corrosion activation energy in the presence of inhibitor compared to its absence. The time effect on inhibitory efficiency was studied using gravimetric measurements for different times (8h, 16h, 24h, 48h and 72h). The results also indicated that the inhibitory efficiency increased with immersion time to 94% at 72 hours and that the studied Schiff base compound retarded the corrosion of mild steel in the 1 M HCl medium. **Keywords: Corrosion, mild steel, HCl, Schiff base, inhibitory efficiency.**

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Radical scavenging activity of ascorbic acid analogs: kinetics and mechanisms

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Abstract :

In the present work, the antioxidant activity of four ascorbic acid analogs have been studied at the M05-2X/6-31G+(d) computational level using the conventional transition state theory in different solvents, with different polarity and taking into account all possible mechanisms (see Scheme 1) . Scheme 1. Structure and site numbering of analogs Ascorbic (1, 2, 3, 4) and Ascorbic Acid (AA). The obtained results indicate that the antioxidant activity of the ascorbic acid analogs increases with the polarity of the environment. Additionally, their antioxidant activity is higher than ascorbic acid. This result is in line with experimental finding [1] which supports the hypothesis that the analogs that had an endocyclic nitrogen atom instead of a ring oxygen may have a higher antioxidant activity than ascorbic acid. On other hand, the results also indicate that compound 4 (designed by us) [2] is predicted to be more antioxidant than ascorbic acid and the other analogs 1-3, in both lipid and aqueous solution. Finally, for the first time, pKa values, branching ratios and the rate constants for the reactions of ascorbic acid analogs with methylperoxyl radical $\text{CH}_3\text{OO}\bullet$ are reported.

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Effect of the nature of the solution on optical and mechanical properties of ZnO thin films deposited by the spray pyrolysis technique on a local glass production.

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Abstract: Zinc oxide thin films were deposited by spray pyrolysis technique on a local production glass substrate. Two solutions have been used for this purpose. Zinc chlorides and acetate with a molarity of 0.1M For both solutions. The focus was on the effect of the nature of the solution on the structural, optical and mechanical properties of the films. The results show that the thickness of the deposited films is of the order of 152 nm for the films obtained by the solution of zinc chloride, and 125 nm for those deposited with the zinc acetates. The spectrophotometer UV-Visible confirms that samples keep a good transparency. A considerable improvement of the mechanical strength of the samples with the films deposited by zinc chloride solution compared to the raw glass. Its value is 150MPa for the first case and does not exceed 110MPa for the second one.

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Kinetic and Equilibrium Studies of adsorption of methylene blue from aqueous medium by porous heterostructures adsorbents

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Abstract: Industrial wastewater contains many contaminating organic and inorganic materials, such as aromatic compounds and dyes. Many compounds have been classified as hazardous pollutants because of their potential toxicity both to human health and environment. There are many methods for the removal of organic pollutants from aqueous solutions, such as adsorption, chemical precipitation, ion exchange, membrane processes, biological degradation, chemical oxidation and solvent extraction. Adsorption is the most popular method in which activated carbon or ion exchange resins are usually applied. Activated carbons have the advantage of high adsorption capacity for organic compounds. However, because of its relatively high cost, there have been attempts to utilize low cost, naturally occurring adsorbents, to remove contaminants from wastewater. Recently, the usage of natural mineral sorbents for wastewater treatment is increasing because of their abundance and low price. The adsorption was carried out according to the following parameters: pH, initial concentration, contact time, temperature and mass. Several kinetic and equilibrium models were used to determine the parameters of the adsorption of benzoic acid and salicylic acid by the two organobentonites. Also, the thermodynamic parameters and the nature of the mechanism governing the adsorption of the two acidic pollutants were estimated. Understanding the composition and structure of porous clay heterostructures (PCHs) is of great importance in clarifying the topological design and performance of PCHs in applications. PCHs are new materials, having many favorable characteristics, such as large surface area ($400\text{--}900\text{m}^2/\text{g}$), unique combined micro-and mesopores, high adsorption capacities and high mass transfer rates. In this study, methyl blue (MB) as a typical dye was used to evaluate the effect of different preparation of PCHs on the adsorption of this dye.



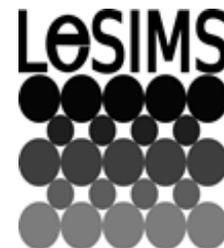
Elaboration and characterisation of porous silicon thin films for solar cells application

Oussidhoum Samira

Abstract: Porous silicon is one of the spongy materials, capable of absorbing gaseous or liquid substances without deteriorating. Thanks to this property, the matrix of the material reacts with the environment; the optical, electrical, mechanical and thermal properties can change. Thin films of porous silicon are used in the field of chemical sensors [1] (liquid, gas and biological material), and also in the field of solar cells as antireflection layers on the surface of silicon [2] or as heterojunction PS / c- Si [3] that offer an additional absorption zone to the solar cell. In our work thin films of porous silicon are developed using two inexpensive methods: chemical etching and electrochemical etching using solutions based on hydrofluoric acid [4]. In order to study the morphological, optical and electrical properties of these thin films of porous silicon, we have used several characterization techniques such as: SEM and AFM that show the formation of dense and homogenous porous layer of thickness 1.2 μm with nano-pores of size of 12 nm. The Raman spectra of porous layer show a peak at 530 cm^{-1} with different intensities depending on crystallite size. The XRD results confirm that porous silicon has the same crystallographic orientation as silicon substrates. The electrical resistivity of the porous layers was measured with four-point probe method. The UV-Visible spectroscopy showed the considerable improvement in the porous silicon absorption in the visible. The reflectivity of PS/c-Si heterojunction was reduced from 35% to 6%. The optical band gap of porous silicon was found to be 1,85 eV. These results show the great potential of porous silicon as intersecting material for improving the performances of high efficiency solar cells.

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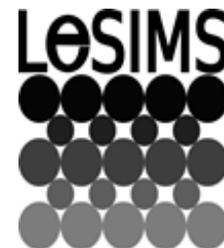


Characterization of Thin Films of CZTS using Transmission Electron Microscopy

Charif Tamin

Abstract:

The Kesterite ($\text{Cu}_2\text{ZnSnS}_4$), named CZTS, is a potential semiconductor for use as an absorber layer in thin-film solar cells because of its optical and electrical properties. The basic materials for the synthesis of this semiconductor are not expensive and less toxic, compared to other candidates such as (CdTe and CIGS). However, the optimization of this material requires works to obtain the pure Kesterite structure, which is not stable after thermal annealing. This work concerns the development and characterization of CZTS thin films. The colloidal solution of CZTS was synthesized from metal chloride salts and thiourea, dissolved in methoxyethanol with ethylenediamine (EDA) as a stabilizer. The CZTS thin films were deposited on glass substrates by the sol-gel spin coating method. Then the samples were heated at 500°C , using a graphite box under vacuum with a small amount of sulfur for the sulfurization process. The microstructure of CZTS thin film were characterize by transmission electron microscopy (TEM) and selected area electron diffraction (SAED). The Scanning transmission electron microscopy (STEM) images shows a homogeneous morphology. Identification of the different crystallographic structure was realized by using electron diffraction patterns and Fast Fourier Transformation of High Resolution image (HRTEM). Meanly pure $\text{Cu}_2\text{ZnSnS}_4$ crystallites were found with some secondary phase such as SnO_2 . With this work, it is shown that films deposited by spin coating and sulfurized at 500°C under vacuum with solid sulfure, are Kesterite structure of $\text{Cu}_2\text{ZnSnS}_4$ with some residual phases of SnO_2 Cassiterite.



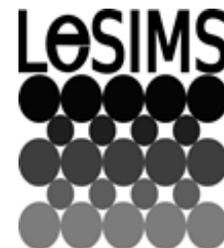
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Polythiophene (PTh) nanoparticles was synthesized by cationic surfactant assisted dilute polymerization method using FeCl_3 as oxidant. The physical characterizations of the synthesized PTh nanoparticles were studied by FT-IR and XRD, DSC, SEM. Polythiophene (PTh)/clay nanocomposites were successfully synthesized with montmorillonite modified with Cetyl-Trimethyl - Ammonium Bromide (CTAB) and Didocyl Diméth hyl-Ammonium Bromide (DDAB), 1-bromohexadecane (MSAB). The thermal degradation behavior of polythiophene (PTh) in PTh/ Na^+ -montmorillonite (Na^+ -MMT) nanocomposites prepared by in-situ intercalative polymerization of thiophene into Na^+ -MMT has been investigated by thermogravimetric analysis (TGA), X-ray diffraction (XRD) and SEM. It was found that the PTh obtained by cationic surfactant assisted dilute polymerization method had better capacitor performances than the same obtained by the conventional chemical and electrochemical polymerization methods. The nanocomposites suggest that the PTh chains for PTh/ Na^+ -MMT nanocomposites are more thermally stable than those for a pure PTh. This improvement in the thermal stability for the nanocomposites is attributed to the presence of Na^+ -MMT nanolayers with a high aspect ratio acting as barriers, thus shielding the degradation of PTh in the nanogalleries and also hindering the diffusion of degraded PTh from the nanocomposites. The shielding effect of the nanolayers is found to be significant as the Na^+ -MMT content in the PTh/ Na^+ -MMT nanocomposites is increased. The XRD patterns of the nanocomposites after TGA measurements indicate that the basal spacing (d_{001}) of the PTh/ Na^+ -MMT nanocomposites is almost intact, implying that the thermal decomposition of the PTh chains is believed to occur mainly outside the silicate layers.

Keywords: Nanocomposite, Polythiophene, Thermal stability.



Electrochemical and Mechanical characterization of composite Ni / SiC coatings produced by electrodeposition on XC45 steel.

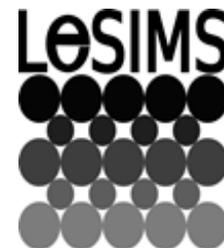
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Abstract: The need to improve coatings for better properties lead to the development of composite electrolytic deposition, by the incorporation of solid particles in the nickel structure. The aim of this work is to produce a composite coating with silicon carbide (SiC) which a high hardness and a good chemical stability. The coating is performed in a Watts bath of electroplating chloride, consisting of an electrolytic nickel matrix (binder) with different concentrations of silicon carbide micro particles (mean diameter 0.8mm). The coating analysis is performed by RX diffraction and atomic force microscopy (AFM). The characterizations of the deposited layers are carried out in 3.5% NaCl solution. The weight loss, the polarization and the micro hardness results highlighted a silicon carbide concentration which can be included in the overall expression of a good composite coating. This concentration improves the corrosion resistance and the micro hardness.

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Elaboration and characterization of a refractory based on algerian kaolin: evolution with heat treatments up to 1450 °C

Ladjama Sabrina Ladjama

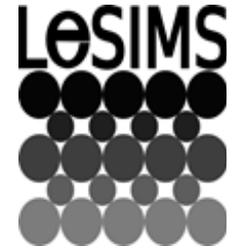
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Abstract:

In order to meet the needs of the local market in terms of renovation of ovens for different uses, we propose the valorization of natural resources through the development of local products that meet industrial requirements and international standards and therefore the reduction of the import bill. Refractory ceramics based on silica-alumina are the subject of our study. The chemical characteristics of a kaolin known as DD1, from eastern Algeria were examined. The results showed that kaolin DD1 has an alumina content of 40%, and 37.23% of silica. Thermogravimetric and thermogravimetric analysis (ATD and ATG) confirm the mineralogical results obtained by X-ray diffraction (XRD) of the sintered samples at different temperatures namely 1200, 1300, 1350, 1400 and 1450 ° C; ATD peaks characteristic of a kaolinite are present. X-ray diffraction analysis showed that the refractory samples are composed of mullite and cristobalite. The different treatments lead to the formation of mullite, from 1200 ° C the beginning of the crystallization of the mullite and the densification of the sample due to the sintering phenomenon are marked. At sintering temperature greater than or equal to 1200 ° C, mullite constitutes the dominant phase of the material. The intensity of the peak at 21.6 °, corresponding to the cristobalite that remains and its intensity increases as the cooking temperature increases, according to the literature at a temperature > 1400 ° C cristobalite melts in the amorphous phase which leads to the formation of the vitreous phase which causes the degradation of the refractoriness, which encourages us to work more on this phenomenon because the refractory ceramics containing more cristobalite, and working in continuous thermal cycles, are deteriorated by cracking and fragmentation.

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Analysis, characterization and application of the acoustic microwave signal in piezoelectric materials on lithium niobate (LiNbO_3) substrate

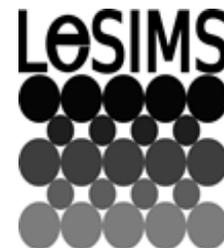
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Abstract: In this work we propose a technique for analyzing microwave acoustic we use as analysis tool analysis the famous wavelet transform, it can analyze the signal locally and know its characteristics in a more precisely way. The signal to be processed represents the propagation of the microwaves acoustic in a piezoelectric structure excited by an interdigital transducer when the electroelastic wave propagation by surface deformation of this structure. As an application, these structures are used for the modeling of various electronic components in microwave such as filters and Acoustic wave amplifiers.

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Deposition and characterization of Mg-doped ZnO nanostructured thin films

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Abstract: Magnesium-doped zinc oxide thin films were prepared by the sol–gel method. Magnesium chloride hexahydrate ($\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$), Zinc acetate dihydrate ($\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$), isopropanol and monoethanolamine (MEA) were used as a precursors, solvent and stabilizer, respectively. Results from X-ray diffraction indicated that the films exhibited a hexagonal wurtzite structure and were highly oriented along the c-axis. The intensity of the (002) diffraction peak increased with increasing the Mg doping concentration. Morphological studies by AFM indicated the uniform thin film growth and the decreasing of grain size and surface roughness with Mg doping. Optical analysis showed that the average transmittance of all films was above 90% in the visible range and Mg-doping has significantly enhanced the bandgap energy of ZnO. UV emission peak and three defect emission peaks in the visible region were observed by photoluminescence measurements at room temperature. The intensity ratio of UV emission to the visible emission increased with the Mg concentration.

Keywords: Sol–gel processes; Mg-doped ZnO thin film; Structural properties; Optical properties; Luminescence; defects

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Effect of aluminium ions as dopant on physical, optical properties of electrodeposited ZnO nanorod arrays.

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Abstract:

Transparent and semi transparent conductive Al-doped ZnO (AZO) thin films were electrodeposited on indium doped tin oxide (ITO) coated glass substrates from aqueous mixed bath of zinc nitrate and potassium chloride with 2%, 4%, 6%, 8% of $\text{Al}(\text{NO}_3)_3$ as doping at 70°C using chronoamperometry technique. Thin and adherent films were obtained after same deposited time of 60 min and under different applied potentials (-1V/ Ag/AgCl) chosen. The structural properties have been performed using X ray diffraction which showed that all obtained AZO thin films present wurtzite phase with highly c-axis preferred orientation. AZO films with 4%, 6% and 8% exhibit other weak peaks with other orientations (101) and (100) suggesting that those later AZO films are polycrystalline. Generally crystallites sizes calculated using Deby Sherrer formulae decreased with the enhancement of doping concentration. The presence of compression stress plays critical role in determining the crystalline structure of AZO films, which tends to stretch the lattice constant c and enlarge the (002) diffraction angle. Sample obtained with large amount of doping 8% of Al^{3+} exhibit a compressive stress ($\epsilon < 0$) parallel to the growth plane (002). The morphological characterization of the pure and doped deposits was carried out by MEB whereas the optical characterization was realized by UV-visible spectroscopy. Indeed, it was noted that the increase in the concentration of the doping agent supports promotes growth in transmittance of deposits and a variation of the gap. In parallel one observed by MEB a specific growth of structure in the form of nanorods which differs from the morphology of pure ZnO. It is also alternative with the concentration of the doping agent.

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The influence of the oxygen percentage on the properties of ZrO₂ thin films deposited by radio-frequency magnetron sputtering

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Abstract:

Zirconium dioxide is one of the most suitable materials for biomedical application. The influence of the oxygen percentage in the gas mixture on the properties of ZrO₂ thin films deposited by radio-frequency magnetron sputtering (RFMS) was studied in this work. The ZrO₂ films were deposited steel substrate using 316L stainless as a substrate by RFMS from a pure zirconium target in Ar-O₂ gas mixture. The oxygen percentage was varied from 10 to 30% which produced a variations of structure, electrochemical and mechanical properties of the films. The deposited films were characterized by X-Rays Diffraction, scanning electron microscopy, nano-indentation and potentiodynamic polarization. Experimental results showed the increase of the thickness of the deposited films with the increase of the percentage of the oxygen. All structures of the films are crystalline as shown by the XRD results. The monoclinic phase is predominant in obtained films. For the study of the electrochemical properties, HANK's solution was used as the electrolyte in order to simulate natural biological conditions. Comparison between the corrosion resistance of the uncoated and coated samples showed a reduction in corrosion current density for coated samples compared to the uncoated one in addition to its improvement of the corrosion resistance and the mechanical properties with the increases of the oxygen percentage.

Keywords: ZrO₂, magnetron sputtering, DRX, nano-indentation, Corrosion.



Synthesis of Cu_2SnO_3 , Structural and Morphological Studies

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Abstract:

Nanocrystalline of CuSnO_3 was prepared from sol gel solutions and spray technique deposition. The composition, structural and morphological properties of the nanaopowder was characterized by X-ray fluorescence (XRF), X-ray diffraction (XRD), *atomic force microscopy* (AFM), and Infrared Spectroscopy (IFR) respectively. XRD results showed the predominant peaks associated to Cu_2SnO_3 with monoclinic structure and the crystallite size value was calculated to be 109.46 nm. We note here that all the films crystallized at 500°C.

Keywords: compound semiconductor, Composition Structural and morphological properties, thin film solar cells

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The Influence of glycine on the formation of calcium carbonate polymorphs

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Abstract: Calcium carbonate is one of the most abundant minerals in nature. It is found at the level of limestone rocks, molluscs shells, oceans, and bones of several animal species. Natural or precipitated CaCO_3 have been used as filler and pigment in the paper, food, cosmetics and pharmaceutical industry [3]. It can be found in three different allotropic forms: calcite, aragonite and vaterite. The most stable thermodynamical polymorph is the calcite, followed by aragonite and then vaterite [1,2]. In this work, we have studied the effect of glycine as an additive on the growth of calcium carbonate polymorphs. CaCO_3 was elaborated by mixing two salt solutions CaCl_2 and NaCO_3 , in the presence and absence of glycine. The samples prepared are examined by X-ray diffraction and infrared spectroscopy for the identification of the crystalline phases. In the absence of glycine at 30°C , the Rietveld quantitative phase analysis shows that the volume fraction of calcite is 100%. In contrast, in the presence of glycine at 30°C , remarkable changes in phase proportions are observed. In fact, the Rietveld quantitative phase analysis shows that the volume fraction of calcite decreases to 2% and that of vaterite represents 98%.

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Synthesis and characterization of new composite films (ITO/PBTh-MnO₂) and their luminescence properties

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Abstract: Polythiophenes constitute a particularly important class of conjugated polymers, which has been extensively studied for the relation between the geometrical structure and the optic and electronic properties. They are, furthermore, chemically and thermally stable materials, and are very attractive for exploitation of their physical properties [1]. The observation of photocurrents from polythiophene-modified metal electrodes has been reported by several groups of investigators [2, 3]. In this work, a composite thin film containing polybithiophene (PBTh) and manganese dioxide (MnO₂) on indium tin oxide (ITO) glass substrates was prepared by electro-polymerization of bithiophene in the presence of MnO₂ nanoparticles. The films ITO/PBTh-MnO₂ are characterized by AFM and SEM, the analyses show an increase in roughness and the incorporated MnO₂ particles are of size in the range of 50 nm. As a result, the optical gap is shifted by the incorporation of MnO₂ nanoparticles from 2.23 eV for ITO/PBTh to 2.03 eV for ITO/PBTh-MnO₂. The photocurrent measurements indicate that the ITO/PBTh-MnO₂ films show a value that is three times higher than that of polybithiophene substrate, so that such a composite can be used as a new active material in solar cells.

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Effects of saccharin additive on properties of electrodeposited nanocrystalline Ni–Co alloy coatings

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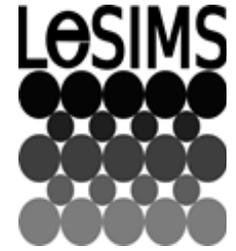
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Abstract: Owing to their exceptional magnetic properties, the Co-Ni alloy thin films are used as magnetic recording media and as hard magnetic materials for microelectromechanical systems (MEMS) applications [1]. Generally, these materials are elaborated by physical vapor deposition techniques such as sputtering or molecular beam epitaxy (MBE). Electrochemical deposition is an attractive method for the elaboration of thin films alloys. This latter method has a great advantage in preparing Cu₂O thin films over conductive substrates due to the low cost and simple equipment used [2-4]. In our research, we will study the effect of saccharin additive in the chloride bath on the mechanism of electrodeposition, microstructure and magnetic properties of Co-Ni alloy coatings. In order to investigate this effect, different analytical techniques had been used through atomic force microscopy (AFM), X-ray diffraction (XRD) and alternating gradient force magnetometer techniques. The conditions of electrodeposition of Co–Ni alloys were determined using the cyclic voltametry (clearly show the presences of cathodic peaks that correspond to deposition are observed around 1.20 V). From AFM analysis when saccharin concentration increased from 0 to 0.005 M, the RMS roughness (root mean square) decreases from 88 down to 14 nm. XRD measurements indicate a small crystallite size with the presence of a mixture of hcp and fcc Co–Ni structures. Also, from XRD measurements, the average size of crystallites decreases with increasing saccharin additive concentration in the chloride baths. It can be suggested that adsorption of saccharin molecules can block the active growth centers during electrodeposition and acts as a grain refiner. Effectively, the presence of the saccharin in the bath also causes notable changes in. Indeed, because of the presence of saccharin the deposits exhibit lower values of coercivity and magnetization saturation compared to those without saccharin. The coercivity values decrease to 1.4 Oe and magnetization saturation decreases in comparison to the film without saccharin, although the decrease in Ms is considerably lower at the highest saccharin content of 0.00 M. The magnetic properties of the deposits can be related to the grain refinement and the internal stress.

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Fabrication of A2024-T3/Al₂O₃ and A2024-T3/Ti₃SiC₂ surface composites by friction stir processing

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Abstract:

Herein we present the fabrication of metal matrix composites (MMC) through Friction Stir Processing (FSP). The latter is one of new methods of fabricating surface composites through stirring process of a soft materials as Aluminium alloys, magnesium and copper. MAX phases are new Nano laminated ternary ceramics, which combines some of best metals and ceramics properties, this later make them good enhancement phases for MMC. In this work, new A2024-T3 composites reinforced with Al₂O₃ and Ti₃SiC₂ hard phases are used to investigate their effect on microstructure, hardness and tribological properties. A ball-on-disc tribometer under dry sliding conditions, at room temperature, were used to study the wear and friction properties of these new composites. Scanning Electron Microscopy were used to analyse and determine the wear mechanisms occurring in the worn surfaces under different applied normal loads.



Inhibition effects of a synthesized novel 3,5-diphenyl pyrazole derivatives on the corrosion of mild steel in hydrochloric acid solution together with quantum chemical studies

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Abstract: Heterocyclic compounds are widely used in acid solutions to prevent the metal corrosion in the process of acid pickling, industrial cleaning, acid descaling and oil-well acidizing [1]. These compounds rich in heteroatoms, such as sulphur, nitrogen and oxygen, can be regarded as environmental friendly inhibitors because of their characteristics of strong chemical activity and low toxicity [2, 3]. So research on new types of thiadiazole derivative inhibitors has been a hot topic in recent years. However, the inhibitive efficiency usually has a close relationship with its concentration and the environmental temperature. Therefore, studying the behavior of inhibition of thiadiazole derivatives has great value for the selection and application of inhibitors [4, 5]. In this work, we focused on the synthesis and study of the inhibition efficiency of new 3,5-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide derivatives on corrosion inhibition of mild steel in HCl solutions. The study of the electrochemical behavior (polarization curve, polarization resistance and electrochemical impedance spectroscopy) and gravimetric measurements of the inhibitors under investigation has shown that the variation of the inhibition efficiency increases as a function of the concentration of inhibitors to achieve 99% at a temperature equal to 30 °C. The results of the gravimetric method and electrochemical methods are in good agreement and the adsorption isotherm was evaluated to explain the mechanism of inhibition and interactions metal-inhibitor. Activation energy and Gibbs free energy for adsorption of inhibitors are calculated. Molecular modeling has been conducted to correlate the corrosion inhibition properties with the calculated quantum chemical parameters.

Keywords: corrosion, mild steel, pyrazole

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Electrochemical synthesis and characterization of bismuth oxide thin films from alkaline bath: effect of annealing temperature

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Abstract:

In this work, the electrodeposition of bismuth oxide from alkaline bath onto a copper substrate was studied. In order to obtain bismuth oxide with a desired crystallographic structure, the effect of annealing temperature on the morphological and structural properties of Bi_2O_3 was investigated. Cyclic voltammetry and chronoamperometry methods were used to the electrochemical characterization formation of Bi thin layers. The morphological analysis with the scanning electron microscopy (SEM) shows a different surface morphology according to the experimental condition. The X-rays diffraction analysis (XRD) reveals the presence a several Bi_2O_3 phases according to annealing temperature, which also confirmed by Raman spectroscopy.

Key words: Bismuth oxide, Electrodeposition, SEM, XRD, Raman spectroscopy.



Synthesis and characterization of new pyrazole heterocyclic derivatives using as a protective organic film for mild steel corrosion in acidic media

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Abstract: Heterocyclic compounds are widely used in acid solutions to prevent the metal corrosion in the process of acid pickling, industrial cleaning acid descaling and oil-well acidizing [1]. These compounds rich in heteroatoms, such as Sulphur, nitrogen and oxygen, can be regarded as environmental friendly inhibitors because of their characteristics of strong chemical activity and low toxicity [2, 3]. So research on new types of thiadiazole derivative inhibitors has been a hot topic in recent years. However, the inhibitive efficiency usually has a close relationship with its concentration and the environmental temperature. Therefore, studying the behavior of inhibition of thiadiazole derivatives has great value for the selection and application of inhibitors [4]. In this work, we focused on the synthesis and study of the inhibition efficiency of new 3,5-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide derivatives on corrosion inhibition of mild steel in HCl solutions. The study of gravimetric measurements of the inhibitors under investigation has shown that the variation of the inhibition efficiency increases as a function of the concentration of inhibitors to achieve 98% at a temperature equal to 30 °C. The results of the gravimetric method and electrochemical methods are in good agreement and the adsorption isotherm was evaluated to explain the mechanism of inhibition and interactions metal-inhibitor. Activation energy and Gibbs free energy for adsorption of inhibitors are calculated. Molecular modeling has been conducted to correlate the corrosion inhibition properties with the calculated quantum chemical parameters.

References

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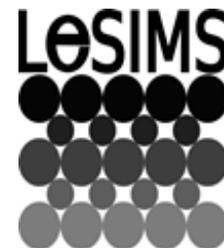


Experimental and quantum chemical analysis of 4, 4'-bis(2,4-dihydroxybenzaldehyde) diphenylethanedimine as new corrosion inhibitor for mild steel in 1M hydrochloric acid solution

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Abstract: Iron and its alloys play crucial roles in our daily lives due to their excellent properties. These materials are used in many industrial processes such as acid cleaning, acid pickling, acid descaling, and oil well acidizing [1,2]. To prevent from acidic solutions aggression, the use of inhibitors is one of the most practical methods to control the corrosion of steel [3]. A new corrosion inhibitor namely, 4,4'-bis(2,4-dihydroxybenzaldehyde) diphenylethanedimine (L1) has been synthesized and chemical structure was confirmed using elemental analysis, FT- IR, ¹H-NMR and mass spectral studies. Inhibition action on corrosion of mild steel in 1M HCl has been investigated using Weight loss, Electrochemical impedance spectroscopy (EIS), Potentiodynamic polarization, Scanning electron microscopy (SEM) and Energy-dispersive X-ray spectroscopy (EDX) methods. Compared to the parent amine, 4,4'-diaminodiphenylethane (M1), the Schiff base L1 exhibited a high inhibition efficiency. The results obtained from above methods reveal that L1 is an excellent inhibitor. It gives a maximum inhibition efficiency of 95.33 % at 5×10^{-4} M. Polarization study suggested that L1 acts as mixed type inhibitor with some cathodic predominance. The adsorption of inhibitor on the surfaces of the corroding metal obeys Langmuir isotherm. SEM analyses showed improved morphology of the mild steel surface in presence L1. The calculated quantum chemical parameters are performed using DFT method such as energy gaps support the good inhibiting performance of the Schiff base molecule. Local reactive sites of the present molecule have been analyzed through Fukui indices [4,5].



The role of chloride and carbonate ions on carbon steel passivity studied in simulating concrete pore solutions

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Abstract: Corrosion of steel in reinforcement concrete is complex. When chloride ions and oxygen reach reinforcing steel, corrosion is initiated. The deterioration process starts with expansions of the bare steel substrate then after cracks in the concrete are developed. The aim of this work is to determine firstly, through the electrochemical technic, the critical concentration of chloride ions which are responsible for the initiation of the dissolution step. Then, the effect of the external parameters on the rate of penetration of the chloride ions into the concrete is also evaluated. For this propose, the electrochemical behavior of the steel of construction “E24” is studied in carbonate medium without and with different concentrations of chloride ions. The effect of various parameters such as temperature, ions concentration, and solution pH was also evaluated through the evolution of the open circuit potential, d.c polarisation measurement and electrochemical impedance spectroscopy. The d.c polarisation and EIS results show that the addition of 0.5M CaCl_2 (as critical concentration) to the saturated $\text{Ca}(\text{OH})_2$ solution, brings to a rapid and a continuous dissolution of the substrate where after 3 hours of immersion time the whole surface of the substrate was covered the corrosion products. This is may be due to specific adsorption of Cl^- . According to Raman, SEM and EDS analyses of the surface after immersion in the corrosive media, the composition of rust layer is mainly composed of g- FeOOH , b- FeOOH , and a- Fe_2O_3 .



Effect of the Al thickness layer on the structural, optical and electrical properties of ZnO/Al/ZnO multilayer structures grown by DC sputtering at room temperature

Saad Amara¹, Mohamed Bouafia²

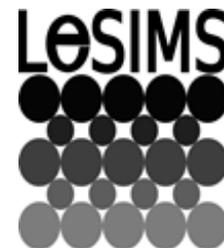
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Abstract : The development of multiple layers structures combining thin metal oxide and metal films (oxide/metal/oxide) is the most interesting alternative to improve the opto-electrical performances [1]. These structures have globally better characteristics than the attainable ones with a single type of material [2]. Previous research on ZnO/Metal/ZnO multilayer structures [3-10] have shown that the metal layer thicknesses of 5nm [11, 6, 12-14] and 10nm [15] exhibit the best opto-electrical performances. In this work, ZnO/Al/ZnO multilayer films have successfully deposited on glass substrates by DC magnetron sputtering, at different ZnO thickness layers and Al thickness (5nm and 10nm). The XRD patterns have shown that the films were polycrystalline and hexagonal like Wurtzite structures, with preferential growth in the (002) plane. The results of the AFM roughness revealed that the Al layer addition makes the surface smoother that it meets the required conditions as the bottom electrode of organic light emitting diodes. The effects of Al film thickness on resistivity and optical transmittance are characterized and discussed. The maximum figure of merit value achieved is $(3.92 \cdot 10^{-4} \text{ W}^{-1})$ corresponding at the thicknesses (50nm/10nm/50nm) of ZnO/Al/ZnO structure respectively.

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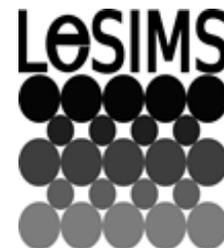
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Improvement in corrosion protection of electrodeposits zinc by ceria based coatings: elaboration, analytical and electrochemical characterization

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Abstract: To avoid corrosion problems, different methods have been used such as protective lacquers, corrosion inhibitors and coatings. Surface passivation based on the use of chromates has been success fully applied on a large number of metals and alloys. The success of these pre-treatments is mainly due to their high protection efficiency/cost ratio. Toxicity and carcinogenic properties of Cr(VI) compounds ought to develop effective and safer alternatives. In this regards, cerium based conversion coatings were found to be a possible solution. The first studies were conducted by Hinton et al. [1]. The authors used cerium chloride for corrosion inhibition on zinc and aluminum and proposed a cathodic mechanism to explain the formation of the rare earth metals (RE) oxide film. In previous works [2-3] devoted to the preparation of ceria coatings on platinum, stainless steel and aluminum it was reported that the formation of the cerium films depends on the reduction kinetics of oxygen. In aerated solution, cerium is initially deposited as Ce(III) with further evolution to Ce(IV). In this work, as first step, we studied the effect of the applied current densities on the morphology and on the texture of electrodeposits zinc. From X-ray diffraction results, it has shown that the preferential orientation of the film is found to be sensitive to the applied current density. Next, as second step, a cerium oxide thin layer was deposited onto electrogalvanized steel by cathodic electrodeposition, from 0.1M cerium nitrate solution. In our previous works, we have shown that electrodeposition of ceria based coating on steel substrate from concentrated cerium slats leads to the dissolution of the substrate where the quality of the deposits is altered [4,5]. This partial dissolution occurring mainly during the electrodeposition process is due to the acidic pH of the solution (pH = 3.8) [4]. In this work, the influence of polyethylene glycol (PEG) addition on the composition and morphology of the deposits is examined. The corrosion protective capabilities of the superficially modified steels were evaluated through cyclic voltammetry, linear polarization resistance (R_p), and electrochemical impedance spectroscopy (EIS). The composition and structure of the surface products were analyzed through Raman spectroscopy and Scanning electron microscopy (SEM) coupled to chemical EDS analysis. The results showed that the addition of PEG to the cerium nitrate solutions lead to a decrease of the cracks in the deposits by decreasing the hydrogen reduction reaction and by decreasing the film thickness which provided enhanced corrosion protection. Moreover, the substrate dissolution reaction is inhibited.



Corrosion inhibition of carbon steel in 1M HCl solution by *Lamium flexuosum* ten extract

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Abstract:

Methylene dichloride extract of *Lamium flexuosum* was investigated as corrosion inhibitors for carbon steel (CS) in 1.0 M HCl using weight loss and potentiodynamic polarization measurements, electrochemical impedance spectroscopy techniques. The effect of temperature on the corrosion behavior of CS was studied in the range of 293–323 K. The experimental results show that the extract is a good corrosion inhibitor and the protection efficiency increased with increasing concentration of the extract, but decreased with rise in temperature. The extract behaved as mixed-type corrosion inhibitor with highest inhibition at 900 ppm. The adsorption of the extract on the CS surface was found to follow the Freundlich isotherm, and the adsorption mode was found to be physisorption.



Evaluation of the corrosion inhibiting efficacy of two thiazolines derivatives against XC38 steel corrosion in acidic medium

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Abstract: In the oil and gas industry, steel is largely utilized for diverse applications such as fluid transportation line, storage tank, drilling pipe, etc. In many cases, industrial practices like mill scale removal, acid cleaning and oil well acidizing, bring metals in contact with corrosive solutions. It is therefore a common practice to add corrosion inhibitors into corrosive solutions before metal pre-treatment [1]. The compounds containing hetero atoms and particularly those containing both the nitrogen and the sulfur are of remarkable significance as they often provide excellent inhibition [2-4]. The corrosion inhibiting property of these compounds is specified in their molecular structure. The planarity and lone pair of electrons present on heteroatoms are the significant characteristics that ascertain the adsorption of these molecules on the metal surface [5-9]. In this work, we are interested in studying the inhibition efficiency of two thiazolines: 2-amino-5-mercapto-1,3,4-thiadiazole (AMT) and 2,5-dimercapto-1,3,4-thiadiazole (DMT) of XC38 steel in 0.5M sulfuric acid at 303 K was studied practicing weight loss. The obtained results showed that these two compounds were an effective inhibitor. The inhibition efficiency, $\eta(\%)$, increased with the increase in concentration inhibitor. Isotherm adsorption was evaluated to explain the mechanism of inhibition and inhibitor metal reactions. The effect of temperature for both compounds studied and discussed.

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Comparison of linear and non-linear method for modeling CO₂ adsorption over impregnated zeolite (mgo)-nay

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Abstract: The greenhouse gas emissions in the environment are recently the major problem all over the world. Carbon dioxide (CO₂) is the most important greenhouse gas (GHG) emitted in the atmosphere [1]. Various CO₂ capture technologies have been proposed to retain this gas, in particular by adsorption. The zeolitic adsorbents prove to be more interesting for the selectivity, which they offer towards the CO₂. In this work, we studied the adsorption of CO₂ at 30°C (P = 0 to 1 bar) on impregnated NaY zeolite at different mass levels of MgO (2, 5, 10 and 15%). The experimental data was analyzed using the Sips isotherm equations by linear and non-linear method. The coefficient of determination (r²) and the sum of the squares of the errors were used to predict the best method. The determination coefficients obtained from non-linear method were higher than those obtained from linear one. Error values indicated that non-linear method is a better way to obtain the isotherm parameters describing the CO₂ adsorption onto NaY impregnated zeolite.



Deposition of zeolite films on metal surfaces and studies of their corrosion inhibiting effects in NaCl medium

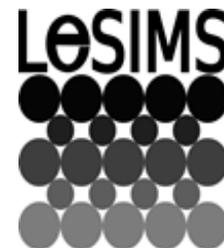
Hamblisamiha, Benbouzid Mohammed, Nacer Houria

Laboratory of Materials and Environment Analytical Sciences (SAME). Faculty of the exact sciences. University Larbi Ben M'Hidi. Oum El Bouaghi. Algeria.

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Abstract: Corrosion in industrial environments is one of the main factors limiting the life of materials. ZSM-5 has been synthesized and characterized by DRX and FTIR and its behavior as a studied corrosion inhibitor. In this study metal plates were covered with different zeolite films using the dip coating method. They were then introduced into NaCl solutions of different concentrations. The treated samples were studied by gravimetric and electrochemical methods to determine the corrosion inhibiting effect of their zeolite layers. The results show that the zeolite layers have exhibited high corrosion resistance and have great potential to become ecological alternatives to conventional coatings.

Keywords: ZSM5, zeolitic films; inhibitor; corrosion, gravimetric; electrochemical



ZnO: M (M = Mg, Ag and Mn)/ZnAl₂O₄ Heterostructures Formation on Silicon Substrate for Gas Detection

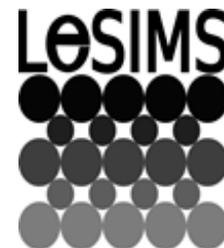
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Abstract: Considering the issues being caused by various gases which are emitted in the environment and can cause lethal damage to humans and environment, proper sensors are to be deployed for detection. So, gas sensors with excellent efficient sensitivity and stability are required. Before few years mixed oxides are used in pollution control via adsorption and/or catalysis, they are also frequently superior to simple oxides with regards to the catalytic performance, long lifetime and resistance to sintering [1]. Among different metal oxides, zinc oxide (ZnO) is the most preferable candidate because its wide band gap (3.37 eV), enhanced electron mobility of 200 cm²/V s [2, 3], good chemical and thermal stability [2], photoelectric response and tunable transport properties [4]. In addition, it is robust, has a fast response with a possibility of miniaturization [5]. However, it presents some disadvantages, such as the high working temperature, between 400 and 500 °C, poor gas selectivity and comparatively low gas sensitivity [5, 6]. In general, to improve sensor performances the control of material morphology, doping by additives which act as a catalyst for the solid-gas reaction [7] are an issue and the use of multiple oxide heterostructures may also be another effective mean that may have been used [6]. Undoped and 0.002, 0.006 and 0.008 molar concentrations of Mg, Ag and Mn, respectively, doped and co-doped ZnO/ZnAl₂O₄ thin films are successively deposited on Si substrate by chemical spray method. X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) confirmed that ZnO: Mg Ag/ZnAl₂O₄ coating has the best crystallinity and the lower estimated electrical resistance. Response and the gaz sensing characteristics of the mists are discussed.

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Effect of potential deposition on the Cu-Zn alloys thin films properties

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Abstract:

Cu-Zn alloy thin films were electrodeposited on a steel substrate from a sulfate solution at different applied potentials. Voltammetric studies showed that the composition and consequently the potential dissolution of Zn depend greatly on the applied potentials. The morphological study by atomic force microscopy (AFM) shows that the roughness of the deposits depends on the applied potential. X-ray diffraction analysis showed that the films is consistent a secondary phase β and γ phase, greatly related to applied potential. The increase of the applied potential induces a decrease in the grain size and the lattice constant.

Keywords: Cuivre-zinc; Electrodeposition; AFM; X-ray diffraction.



New unsymmetrical organic materials: ultrasound assisted synthesis, spectral characterization, X-ray structures, electrochemical and catalytic oxidation.

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Abstract

The present work describe the ultrasound assisted synthesis of new unsymmetrical monomeric Oxovanadium materials VOL^Z , where L^Z is a tetradentate ligand, prepared by refluxing 2-hydroxy-1-naphthaldehyde with different diamines [1-2].

The characterization of the structures were carried out by elemental analysis, ^1H NMR, SM, FT-IR, UV-Vis spectroscopy and conductance measurement. The crystal structures of the synthesized materials were solved by X-ray diffraction, which revealed a square pyramidal N_2O_3 geometry around the metallic centers.

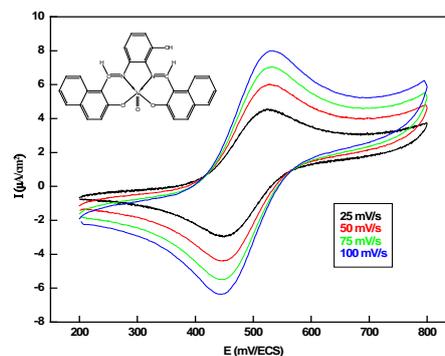
Cyclic voltammetry studies of complexes, investigated in DMF on a glassy carbon (GC) electrode under nitrogen atmosphere, revealed that all of the complexes showed a single electron quasi-reversible redox waves through diffusion controlled processes [3]. The diffusion coefficients are determined using GC rotating disk electrode.

The catalytic activity of the oxovanadium materials in the epoxidation of cyclohexene, in the presence of a greener oxidant hydrogen peroxide H_2O_2 , was also investigated. The results are promising for the use of the complexes as catalysts in optimized conditions [4-5].

Keywords: Ultrasound synthesis, Oxovanadium materials, X-ray Diffraction, Electrochemical, Green epoxidation.

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Ni and Ni/Zn Hydroxide based Nanohybrid Synthesis using Hydrothermal Process

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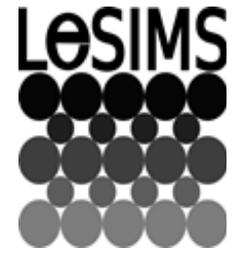
Nano-porous transition metal oxides, hydroxides and carbonate hydroxides based nanomaterial have received increased attention especially due to its electrochemical properties and potential applications and their wide application in many fields. In this work, we focus our investigation on the synthesis of Ni and Ni/Zn based nanocomposites as mono and bi-phase nanoelectroactive materials based of α -Ni(OH)₂·2H₂O and α^* -Ni(OH)₂·0,75H₂O / Zn₄(CO₃)(OH)₆·H₂O, respectively, using a simple and low cost free template urea based hydrothermal process at 120 °C growth temperature during 18 hours. The morphological, textural and the structural selectivity of the as-prepared materials were characterized with different techniques such as: XRD, FTIR, FESEM, BET and Raman analysis in order to investigate their physico-chemical properties. These obtained mono (Ni) and bi-phase (Ni/Zn) nanohybrids have shown the formation of heterostructures based of quasi-microsphere-like structure consisting of overlapping filaments and regular or irregular nanoflakes shape with two kind of pores with an important specific surface area around 97 m²/g and 34.64 m²/g, pore volume around 0.38 cm³/g and 0.10 cm³/g and pore size around 12 nm and 14.86 nm, respectively.

Keywords: Nanohybrid, Nanocomposite, Hydroxide, Hydrothermal synthesis, Energy storage.

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SOFT CONDENSED MATTER



Structural phases of a flexible polymer chain in the presence of internal adhesive contacts

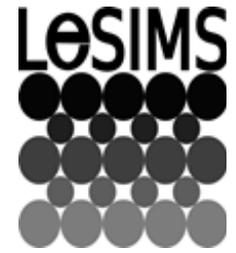
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Abstract

The influence of hydrogen bonding on the formation of ordered secondary structures like alpha helices and beta sheets in proteins has attracted much attention recently. In this work, we present a new potential model that includes the build of internal adhesive contacts between non bonded monomers and mimics hydrogen bonding in proteins. We investigate the structural phases of a flexible polymer chain in the presence of internal adhesive contacts due to the change in temperature and adhesive contacts strength. Stable alpha helices and beta sheets phases are successfully characterized by the new potential model.



Effect of polymer topology on the dynamics behavior of polymer melts

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Abstract

We perform a comparative study of the scaling of polymer size and diffusion dynamics with changing molecular weight N for melts comprised of ring- and linear polymers in a broad interval of chain lengths, $10 \leq N \leq 2048$ and observe a qualitative difference caused by distinct topology. Using large-scale molecular dynamics simulations of a bead-spring coarse grained model, we find that the Flory exponent for linear chains in a dense solution, $\nu_L = 1/2$, varies in the case of rings from $\nu_R = 1/2$ for short rings, over $\nu_R = 2/5$ for rings with intermediate length, down to $\nu_R = 1/3$ for long rings $800 \leq N \leq 2048$, confirming thus recent findings of the behavior of such long rings in a melt effectively as compact globules. In our studies of ring dynamics we allow for the hydrodynamic interactions in the system by using Dissipative Particle Dynamics (DPD) and find that cyclic polymers (rings) diffuse faster than linear chains with the same molecular weight owing to the absence of chain ends that would otherwise lead to reptation dynamics as for linear chains. In presence of hydrodynamics interactions when the Zimm model of polymer dynamics is valid, we find that the relaxation time τ_R scales as $\tau_R \propto N^{-7/3}$ for big rings in agreement with recent theoretical prediction.



Breakdown of the electron-spin motion upon reflection at metal-organic or metal-carbon interfaces

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Abstract

For a better understanding of the spin-dependent electron transport across an organic/ferromagnetic interface, we study the spin motion of the electrons when they are reflected from an organic film deposited on a ferromagnetic surface. Our experiment is distinguished from other experiments using spin-polarized electrons by the fact that the spin polarization \mathbf{P}_0 of the incident electrons is perpendicularly oriented with respect to the magnetization \mathbf{M} of the ferromagnetic material. It is only with this non-collinear initial configuration that the motion of the polarization \mathbf{P} can be observed. The spin motion consists of two sub-motions, namely a precession of \mathbf{P} around \mathbf{M} by an angle ε , and a rotation of \mathbf{P} by an angle φ either into the direction of \mathbf{M} or antiparallel to it.

In this attempt, spin-polarized electron scattering experiments on different metal-organic and metal-carbon interfaces have been performed. We observe a completely unexpected behavior of the spin-polarized reflection properties of these interfaces. Submonolayer amounts of organic molecules or pure carbon makes the reflection of electrons independent of the spin; i.e., both the reflectivity and the reflection phase become spin independent. Such a behavior is expected for non-magnetic organic films of several monolayers (ML) thickness, but not for such low coverage as studied in this work. Our findings show that this behavior is a very general phenomenon which is independent of the electron energy and the choice of the metal as well as of the organic molecules and thus does not depend on the choice of the specific interface. This breakdown phenomenon (BP) appears in experiments with ferromagnetic systems, as well as in experiments with heavy nonmagnetic materials in which only spin-orbit interaction can lead to a spin dependence of the reflected intensity. Despite this extensive study, we have no physical explanation for this intriguing behavior at the moment.

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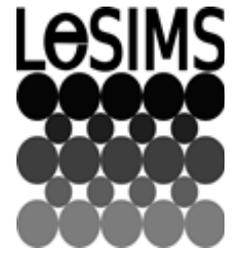
Influence of thickness on the photocatalytic activity, structural and optical properties of TiO₂ thin films

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Algeria

Abstract

In this work, TiO₂ thin films were prepared using sol-gel spin-coating method deposited on glass substrate and annealed at various temperatures (450, 500 and 550 °C) for 2 h. According to XRD and Raman analysis, TiO₂ films show only anatase phases. The crystallites sizes were increased with annealing temperature whereas the optical transmittance was higher than 80 % in the visible region. The reflective index, thickness and the gap energy values were deduced from transmittance data. The gap energy was decrease with the increase of annealing temperature. The photocatalytic activity of TiO₂ was tested and shows the degradation of methylene blue (MB) under UV light irradiation.



Modeling and optimization of piezoelectric energy harvesting system

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²Automatic Laboratory of Setif, Electrical Engineering Department, University of Setif1, Algeria.

Abstract

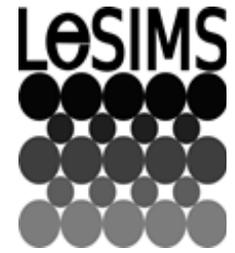
Vibration-based energy harvesting has been investigated by several researchers over the last decade. The goal in this research field is to power small electronic components by converting the waste vibration energy available in their environment into electrical energy. Piezoelectric energy harvesting is a promising technique for powering small-scale standalone electronic devices.

We further proposed an effective and efficient optimization method based on bond graph for optimizing physical aspects of the piezoelectric energy harvesting systems without intensive human effort.

Since the time constant of the mechanical cantilever system and internal piezoelectric inertia are far apart, a simple model of the piezoelectric element is sufficient for this analysis. More detailed models of piezoelectric transducers are available and could be of interest in future works.

This enables the piezoelectric layer to be model as a simple current source, an internal capacitance and an internal resistance. The electrode and substructure of the harvester create a capacitor C_p with the piezoelectric material as a dielectric. The internal resistance of the dielectric is expressed by R_p . The internal capacitance and resistance for each layer can be obtained.

This paper proposes a bond graph approach that is capable of modeling piezoelectric energy harvesters. The model is parameterized enabling simple introduction of relevant physical parameters. The bond graph model is verified by comparison to examples for which analytical and graphical solutions has been published. The bond graph model is valid close to the analysed mode centre frequency and delivers results compared to analytical data.



Yttrium Iron Garnet Ferrites (YIG) Magnetic Photonic Crystal Fiber Infiltrated with Fe₃O₄ Magnetic fluid

Saker khadidja, Bouchemat Touraya, Lahoubi Mahieddine, Bouchemat Mohamed

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Abstract

Magneto photonic crystals (MPCs) give the possibilities for optical signal modulation via external magnetic fields through magneto-optical effects. They provide significant enhancement of the magneto-optical effects, such as Faraday and Kerr effects, with relatively small optical losses. These noticeable optical properties of the MPCs are used for high-sensitive biosensors and magnetic field detectors [1]. Ferrite materials with garnet structures have impact on the electronic industry because of their application in diverse technological fields and devices, such as in isolators, phase shifters, oscillators, IC fabrications, sensors, antennas, etc.. The efficiency and performance of these devices have been improved using the yttrium iron garnet ferrites (Y₃Fe₅O₁₂, YIG) [2], which have been widely applied for circulators, isolators, phase shifters, nonlinear devices... [3]. Given that YIG has large Faraday rotation and high saturation magnetization, this ferromagnetic garnet can be potentially applied in electronic devices with a high melting point, large resistivity, high electromagnetic properties, high thermal stability, low thermal expansion, high chemical stability, and high thermal conductivity [2]. Magnetic fluid (MF) is a kind of stable colloidal mixture of magnetic nanoparticles dispersing in a suitable fluid carrier. MF possesses both the features of the magnetism of a solid ferromagnetic matter and the fluid behavior of a liquid matter with various attractive magneto-optical properties including tunable refractive index (RI), magnetically controllable birefringence [4]. In this work, we proposed a magnetic photonic crystal fiber (MPCF) with a triangular lattice of air holes, filled with MF (Fe₃O₄) at several external magnetic fields strength and at Temperature T=60°C [5] in YIG fiber at $\lambda = 1.55 \mu\text{m}$. An analysis of the magneto photonic properties of the structure such mode conversion, Faraday rotation, and modal birefringence is reported using the Beam Propagation Method (BPM). The mode conversion efficiency introduced by the gyrotropy and the coupling length are also investigated for TE and TM polarizations. This study shows a large Faraday rotation and small modal birefringence which improves the performance of optical isolators. From the results, a novel isolator based on YIG MPCF is developed.



Elastic Properties of Ikaite and their Pressure Dependence: a DFT Corrected Van Der Waals Study

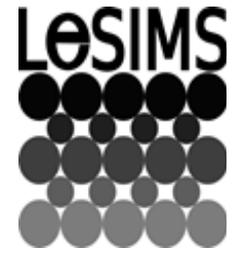
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Abstract

Calcium carbonate (CaCO_3) is one of the most abundant minerals in the earth crust. This mineral has attracted too much interest in several different fields, such as biology, geology, climatology and environmental science. CaCO_3 has both anhydrous (calcite, aragonite, vaterite) and hydrated polymorphs (Ikaite and monohydrate calcite). Among all the anhydrous allotropic forms exhibited by CaCO_3 , calcite is the most stable one at ambient conditions of pressure and temperature. Ikaite is a hexahydrated phase of calcium carbonate ($\text{CaCO}_3 \cdot 6\text{H}_2\text{O}$) which crystallizes in the monoclinic system. Its name is derived from that of the “Ikka” fjord, in Greenland, where it was discovered for the first time in 1963, as submarine columns. It has also discovered in marine sediments in Arctic, Antarctic, Congo and Japan. At variance with the anhydrous polymorphs of CaCO_3 , for which the physical properties are well documented, few reports are available in literature concerning hydrated polymorphs, namely Ikaite.

We have performed atomistic computer simulations based on Density Functional Theory (DFT) to investigate structural and elastic properties of Ikaite as well as their pressure dependence up to 5 GPa. Our calculations were carried out by using the ABINIT code, which uses plane waves to expand valence orbitals and pseudopotentials to account for the interaction between core and valence electrons. The PBE exchange and correlations functional with an empirical correction of the dispersion interactions introduced by Grimme [5] (D2) were adopted. We first investigated the evolution of cell parameters over pressure. The obtained values are in good agreement with the experimental data. The elastic constants were evaluated in the framework of Density Functional Perturbations Theory (DFPT). These were used to evaluate the different elastic moduli (the the bulk modulus (B), the shear modulus (G), the Young modulus (E) and the Poisson ratio (ν)) by mean of the averages of Reuss, Voigt and Hill. The elastic constants and elastic moduli exhibit a quadratic evolution over to pressure. Finally, Graphical representations were used to analyze the directional dependence and the degree of anisotropy of the elastic properties of Ikaite



Synthesis and Characterization of Special Optronic Glasses

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Abstract

Sb_2O_3 antimony oxide glasses have low phonon energy and non nonlinear optical properties χ^3 . They have potential optronic applications. This work deals with the synthesis and characterization of a glassy system based on antimony trioxide Sb_2O_3 - $ZnBr_2$ - $LiCl$. In this context differential scanning calorimetric analysis (DSC); thermo-mechanical analysis (TMA); the optical transmission and the elastic modulus have been made. The variation of physical properties has been discussed, in relation to the variation of the chemical composition. The good stability of some glasses qualified them to have a technological application.



Simulation of Ruthenium Metal Production by Technetium Transmutation in High Flux Reactors

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Abstract

Ruthenium is a one rare transition metal present in platinum group. Ruthenium is inert to most chemical reactions. This element is generally found in ores of other platinum group metals in the Ural Mountains of South and North America. Naturally occurring ruthenium consists of seven stable isotopes. It reacts with molten alkali and halogens and oxidizes explosively. The metal remains unaffected by air, acids and water. Ruthenium has several applications in industries, chemistry, informatics and also jewelry.

In this paper we simulated numerically the production of Ruthenium-100 in nuclear reactor by neutron irradiation of long lived radioactive Technetium-99 in different nuclear reactors. The results were compared with the experimental data obtained previously. The concentration and the evolution of Ruthenium production under irradiation are also presented.



Structural, Electrical and Optical Properties of Transparent Conducting ZnO films: Doping Effect

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Abstract

Zinc oxide (ZnO) is a TCO material with interesting physical properties, which places it among the most promising materials for the use in various fields such as piezoelectricity, photovoltaic effect, optoelectronics...

In this work of experimental nature, the aim is to study the effect of doping on the structural, electrical and optical properties of thin films. To accomplish this, we have deposited Al-doped ZnO thin films by spray pyrolysis technique from an aqueous solution of zinc chloride doped from hydrated aluminum chloride. Transparent conductive thin films of zinc oxide were deposited on ordinary glass substrate preheated at the temperature of 350°C. The effect of doping percentage (1%, 3% and 5%) has been investigated. X-ray diffraction showed that all films are polycrystalline with a hexagonal wurtzite structure, and revealed the effect of doping on grain size. Spectrophotometric measurements showed that the ZnO: Al is transparent (60%-70%) in the visible zone. Hall effect measurements showed p-type electrical conductivity.

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Non-aqueous Sol-Gel Routes to Magnetic Nanoparticles

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Abstract

General interest in magnetic nanoparticles (MNPs) has grown due to the need generated by novel biomedical, diagnostic, and therapeutic applications. Nanosized magnetic materials play a major role in the development of functional nanoscaled devices. It is essential to understand the relationship between NPs synthesis and the resultant magnetic properties. Moreover, the tendency is to achieve the goal of a single domain within one NPs, which will allow the tailoring of resulting magnetic properties. Therefore, making ultrasized NPs (below the single magnetic domain size limit), with a narrow size distribution (monodisperse), is crucial to increase the maximum information density in magnetic recording, to optimize the magnetic coupling, and to increase the volume of soft magnetic phase in permanent magnet nanocomposites. Non-aqueous sol-gel routes are remarkably successful for the synthesis of bimetallic and multi-metal oxide nanoparticles. Solvent assisted synthesis and especially the “benzyl alcohol route” have several advantages such as a low reaction temperature and a high crystallinity and purity of the as synthesized oxides.^[1-3] Here, we present the synthesis, characterization and magnetic properties of bimetallic CoPt_3 and multi metal oxide CoFe_2O_4 nanoparticles achieved by the “benzyl alcohol route”. This non-aqueous sol-gel method is suitable in this case as it allow the synthesis of high quality nanocrystals where no others solvent were involved on the reactions. The highly monodisperse powder CoPt_3 and CoFe_2O_4 nanoparticles were investigated with innovative advanced X-ray methods (XRD), whole powder pattern modeling (WPPM), high-resolution scanning transmission electron microscopy (HR-STEM), energy dispersive X-ray spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS), Raman, Mössbauer spectroscopy and superconducting quantum interference device (SQUID) magnetometry. In these systems, the magnetic properties seem to be strongly dependent on the metal oxide precursor and thus, on the synthetic conditions. The magnetic properties were studied and were correlated to the oxidation state of the NPs.

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MAGNETIC MATERIALS



Modeling of the Magnetic Properties of Materials

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Abstract

This article studies the different magnetic behaviors that can appear in a material. It represents a theoretical modeling of the purely magnetic properties that are due to the macroscopic magnetic field existing outside the materials, and also to the internal and intrinsic properties of these materials that are related to the presence of spin and of magnetic moments in their volume.

In the first place, the description of macroscopic magnetism, or macromagnetism, is essential in order to understand the functioning of the device and the work equipment. This step is treated by modeling the macroscopic magnetic field created by the electromagnet at any point in space. Through this step we get to know better the magnetization and magnetic susceptibility that are generated by the external magnetic field.

In a second step, the modeling is dedicated to the micromagnetism which describes the magnetic behavior within the materials, by the knowledge of the distribution of the spins and the magnetic moments in all the space of the interior of the materials to be studied.



Thickness Effect on the Physical Properties of $\text{Co}_{0.9}\text{Pd}_{0.1}$ Thin Films

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Abstract

The structural and magnetic properties of $\text{Co}_{0.9}\text{Pd}_{0.1}$ thin films grown under vacuum by physical vapor deposition (PVD) on Si (100) are reported. Before evaporation the pressure in the chamber was 10^{-7} mbar. During evaporation, the base pressure was better than 10^{-6} mbar. The thicknesses of the samples were measured with a DEKTAK 150 profilometer and ranges from 50 to 220 nm, The atomic concentration was determined by EDX measurements, microscopic characterizations of the films were done with X-Ray diffraction (XRD) and infer that all the samples were polycrystalline with an hcp structure. The hysteresis loops were performed by means of vibrating sample magnetometer (VSM) and infer that all the samples present a planar ferromagnetic anisotropy. The thickness dependence of in plane squareness showed a similar trend with corresponding coercivity. All these results will be presented and discussed.



Permeability Tensor of M-Type Hexagonal Ferrite Films

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Abstract

Presently, there is a critical need for millimeter wave devices, which operate in the frequency range from about 30GHz to 100GHz. This need for broadband telecommunication capabilities will mandate the use of mm-wave frequencies in next-generation satellite. One important strategy for the above described frequency extension is the use of $\text{BaFe}_{12}\text{O}_{19}$ films (BaM). The goal of our work is the characterization of BaM films over frequency range of 0.4 to 65GHz. The theoretical method adopted to determine the different elements of permeability tensor use the scattering parameters S and Maxwell equations. Polder's model, consider ferrite in its saturated state. The BaM films shows the presence of a gyroresonance phenomenon and the resonance frequency reaches a very high value of about 45GHz. The non-reciprocal effect is greater than 10dB and the line width is very wide. BaM ferrite has a high value of uniaxial anisotropy, its saturation magnetization is about 500mT and the remnant magnetization reached 270mT. The coercive field value ranges between 200KA/m and 330KA/m. It may be useful when the magnetic device is to function at high frequency.



Magnetic and Structural Properties of $\text{Co}_x\text{Fe}_{100-x}$ Thin Films Thermally Evaporated onto Glass substrate

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Abstract

The structural and magnetic properties of $\text{Co}_x\text{Fe}_{100-x}$ thin films evaporated onto glass substrate have been investigated. The atomic composition has been evaluated from X-Ray Fluorescence analysis. The structural properties have been performed by X-Ray diffractometry technique. The static magnetic properties have been carried out using Vibrating Sample Magnetometer (VSM) tools. x ranges from 38 to 65 at.%. The X-Ray patterns present (110), (200) and (211) textures with a grain size varying with the composition. Saturation magnetization evolution versus cobalt content has been studied. M_s decreases with cobalt content increasing; this dependence has been interpreted as a transition from strong to weak ferromagnetism.

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Study of the Corrosion of Neodymium-Iron-Boron Magnets at Different Solution

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Abstract

Sintered Nd–Fe–B permanent magnets exhibit excellent magnetic properties and are widely used in industry as essential components of energy applications [1]. However, these types of magnets could not be used for some commercial applications due to their very low resistance against corrosion in various ambient environments.

This work lies on a comparative study of the effect of the magnetized fields on the corrosion behavior of NdFeB permanent magnets at different solutions, which are NaCl and Na₂SO₄. Corrosion resistance was investigated by electrochemical techniques in the aim to monitor the open-circuit potential, the impedance spectroscopy (EIS) and the polarization curves. We observe that during corrosion the electrochemical process is influenced by the existence of the magnetic field.



New Diluted Magnetic Semiconductor for Application in the Field of Spintronics

Ouafa Hamidane

Abstract

We have used first principle methods of density functional theory within the full potential linearized augmented plane wave scheme to investigate the electronic and magnetic properties of cubic rock-salt SrO doped with vanadium (V) impurity as $\text{Sr}_{1-x}\text{V}_x\text{O}$ at various concentration, $x = 0.25$, 0.50 and 0.75 . We have found that the ferromagnetic state arrangement of $\text{Sr}_{1-x}\text{V}_x\text{O}$ is more stable compared to the anti-ferromagnetic state configuration. The electronic structures have a half metallic (HM) ferromagnetic behavior for $\text{Sr}_{0.75}\text{V}_{0.25}\text{O}$ and $\text{Sr}_{0.5}\text{V}_{0.5}\text{O}$. The value of half metallic gap of ferromagnetic phase decreases with the increasing concentration of vanadium atoms due to the broadening of 3d (V) level in the gap, and hence the $\text{Sr}_{0.25}\text{V}_{0.75}\text{O}$ becomes metallic ferromagnetic. The $\text{Sr}_{0.75}\text{V}_{0.25}\text{O}$ compound revealed a large gap with spin polarization of 100% at Fermi level. The $\text{Sr}_{1-x}\text{V}_x\text{O}$ compounds, at low concentrations, seems a better candidate to explore the half-metallicity for practical spintronic application.



Stability and Magnetic Properties of Cr-Substituted ScN from First Principles

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Abstract

Recently, many efforts have been focused to obtaining III-V dilute magnetic semiconductors (DMS) by doping semiconductors. Among these latter, nitride based diluted magnetic semiconductors are attracting increasing attention, such scandium nitride (ScN) doped with transition metal elements.

We have studied the structural, electronic and magnetic properties of Rocksalt scandium nitride (ScN) and chromium doping $Sc_{1-x}Cr_xN$ (with $x=0.25$). We used density functional theory (DFT) [1] framework as implemented in the projector augmented wave method (CP-PAW)[2]. The generalized gradient approximation (GGA)[3], as well as hybrid functional have been employed for the electronic exchange and correlation effects.

The equilibrium structural parameters, density of states (DOS) and magnetic moment are analyzed and discussed.

Keywords: DFT, spintronic, magnetic semiconductors

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The Elaboration of Nanoparticle Composite Magnetite Multi-Walled Carbon Nanotubes as Catalyst

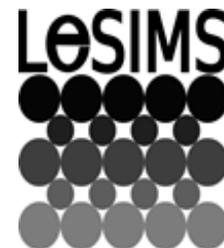
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Abstract

Environmental pollution is the most serious issues facing this world today, especially when we talk about several contaminants which invaded waste water and caused health hazards. Therefore, we have focused on the elaboration of nanocomposite as catalyst to eliminate dyes from aqueous solutions by using adsorption process. We have succeeded in synthesizing magnetite multi-walled carbon nanotubes by co-precipitation method, the characterization of this material by the X-Ray diffraction (XRD) showed a presence of the magnetite on the surface of the carbon nanotubes. Kinetic study indicated a rapid increase in the adsorption capacity of Bromocresol purple (BCP) dye, the equilibrium time took about 25 minutes. Besides, thermodynamic study indicated that adsorption of the organic pollutant on magnetic-MWCNT was a spontaneous and exothermic process. Furthermore, the adsorption isotherm represented perfectly by the Langmuir model and the value calculated by Freundlich model indicated that the adsorption was favorable. In conclusion, our study showed that the catalyst could be manipulated magnetically and exhibited good and fast adsorption capacity because of the magnetite properties and the huge specific area of carbon nanotubes.

Keywords: Magnetite carbon nanotubes, catalyst, adsorption.



Structural and Magnetic Properties of Fe/Si (100) Thin Films

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Abstract

In this work we have studied the structural and magnetic properties of Fe thin films evaporated onto Si (100) substrates. The film thickness ranges from 10 to 70 nm. The characterizations of the obtained thin film were performed by X-ray diffraction (XRD), atomic force microscopy (AFM), and vibrating sample magnetometer (VSM) techniques. XRD measurements show that the films are polycrystalline with centered cubic structures and grow with $\langle 110 \rangle$ texture. The grain size values range from 29.3 to 37.5 nm. Atomic force microscopy (AFM) observations reveal smooth surfaces for the most of the films, whereas some films present small roughness, the root mean square (rms) roughness ranging from 0.4 and 4 nm.

Carried out by means of VSM, the hysteresis curves show that the easy magnetization axis lies in the film plane for all the samples, with no in-plane magnetic anisotropy within the plane. The coercive field values seem to decrease with increasing thickness, till a critical value where an increase of H_c appears for $t > t_c$. H_c value ranges from 15 to 96 Oe, influenced by a number of parameters such as magnetic layer thickness, stress, as well as grain size. The saturation field ranges from 35 to 270 Oe. The value of squareness for most of samples are greater than 0.7. All these results will be presented and discussed.

Keywords: Thin films; XRD; Fe; Magnetization; Coercive field.

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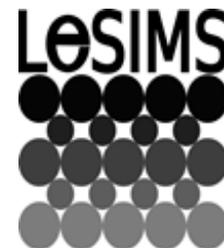
Comparative Study on Adsorption of Methylene Blue By KDD3-Fe₃O₄ Magnetic Composite and KDD3 Purified Clay

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Abstract

The aim of this work was to compare two sorbent, before and after modification by magnetite particles for removal of cationic dye methylene blue from aqueous solution. The magnetic composite was characterized by XRD and ATG. The influence of contact time, initial concentration of dye, and the effect of temperature were studied. The amounts of MB adsorbed at equilibrium for the different concentrations were respectively 10.33, 11.93mg/g by KDD3-Fe₃O₄, was less than by KDD3 purified clay with 26.73 36.46 mg/g, according to deposition of magnetite particles on surface of KDD3 purified clay. Kinetics, thermodynamic studies and adsorption isotherm models were affected to evaluate experimental data. The results exhibit that the adsorption of MB is well described by the second order model. Furthermore, the thermodynamic study revealed that the adsorption is spontaneous and exothermic.



Structural, Electric and Magnetic Properties of Evaporated Ni/Co Thin Films on Si (111) substrate

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Abstract

In this work, we studied the formation and the thermal stability of a ternary silicide ($\text{Ni}_x\text{Co}_{1-x}$) Si_2 , obtained by thermal annealing. Ni and Co thin films were deposited on Si (111) substrate. The performed annealing of 500Å- Ni/100Å-Co/Si (111) samples is carried out by means of a conventional furnace during 20 minutes and a temperature range 300, 600 and 800°C. The obtained specimens were investigated using grazing incidence X-Ray diffraction (GIXRD), X-ray fluorescence spectrometer, electric resistance square measurement and vibrating sample magnetometer. XRD spectrum showed that the formation temperature of the ternary ($\text{Ni}_x\text{Co}_{1-x}$) Si_2 phase was relatively lower compared with those of the NiSi_2 and CoSi_2 disilicides and it maintained its sheet resistance below 2.2Ω/sq, X-ray fluorescence spectrometer analysis shows a composition about 85 atm% for Ni and 15atm% of Co. Furthermore, hysteresis loop displays a ferromagnetic behavior of ours deposited films.



Effect of the Boron Content on the Amorphization Process and Magnetic Properties of the Mechanically Alloyed $\text{Fe}_{92-x}\text{Nb}_8\text{B}_x$ Powders

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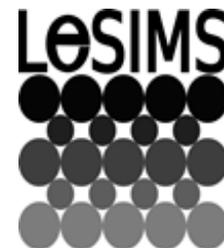
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Abstract

The effect of the B content on the microstructural, structural and magnetic properties of partially amorphous $\text{Fe}_{92-x}\text{Nb}_8\text{B}_x$ ($x = 5, 10, 15$ and 20) alloys has been investigated by means of scanning electron microscopy, X-ray diffraction, high and low temperature extraction-type magnetometers. The XRD results reveal the formation of a nanocomposite structure where nanocrystalline bcc α -Fe and Fe_2B phases are embedded into an amorphous matrix. The FeB boride is observed for higher boron content ($x = 15$ and 20), and the crystallite sizes are in range of 7-24nm. As the B content increases, the amorphous phases-relative proportion and coercivity increase, whereas the saturation magnetization decreases. An important magnetic hardening occurs by lowering the temperature from 400 to 5 K for $x = 20\%$ B. the variation of the Curie temperature can be attributed to the heterogeneity of the amorphous matrix.

Keywords: Nanocrystalline materials; Mechanical alloying; Fe-Nb-B alloys; X-ray diffraction; Magnetic properties.



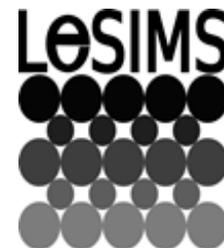
Modeling of Electromagnetic Shielding Effectiveness of Novel Multilayer arrangement of conductive Composites layers in the far Field

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University Amar Telidji Laghouat

Abstract

Frequency dependence of the electromagnetic interference shielding effectiveness (EMI SE) of Nickel fibre (NiF)-Polyimide (PI) composite have been investigated on the basis of attenuation due to absorption and reflection mechanism in the range 1 to 10 GHz. This paper aims to a good understanding the relations between the parameters of shield: magnetic permeability, electrical conductivity, thickness, and the shielding effectiveness SE of the shielding materials composite against the electromagnetic interference (EMI). We suppose that our multilayer built contains a three-layered conductive composite of Nickel fibre (NiF/PI) separated by a two-dielectric layer of Polyimide (PI), to see how the our multilayered work against the electromagnetic interference (EMI). The simulation results prove that the proposed multilayer structure shows more effectiveness of electromagnetic shielding, and a good performance in the frequency rang 1 to 10GHz, which is achieved due to the impedance mismatch of proposed composite. So many-layered composites can be used for many industrial and commercial shielding applications.



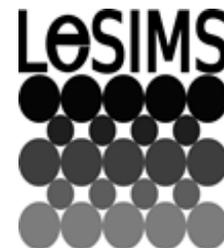
Structural and Magnetic Properties of Co/SiO₂ Nanocomposites

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Abstract

In the present work, SiO₂ nanocomposites were synthesised by wet impregnation, calcined at various temperatures (T = 200, 350, 500, 700 °C) and reduced under thermal H₂- treatment (T = 350°C). X-ray diffraction (XRD), transmission electronic microscopy (TEM) and vibrating sample magnetometer (VSM) were used to characterize the samples.



Structural, Electronic and Magnetics Properties of EuMnPF

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Abstract

In this work, structural, electronic and magnetics properties of EuMnPF were investigated using density functional theory within the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA)¹ of the exchange-correlation energy implemented, in the Vienna ab-initio simulation package (VASP)².

The optimized lattice parameters and bulk modulus of the parent compound are determined by fitting a set of data points to the Birsh-Murnaghan equation of state and compared with experimental data³ using GGA ,vdW-DF,rev-vdW-DF2 and vdW-SCAN+rVV10 methods.

The vdW-SCAN+rVV10 density can predict perfectly the lattice parameters which are in excellent agreement with experimental value.

The magnetic behavior of the compound is clearly shown from partial density figures.



Structural and Magnetic Properties of evaporated $\text{Fe}_x\text{Pd}_{1-x}$ Thin Films on Si(111) substrates

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Abstract

Various structural and magnetic characterization techniques have been used to investigate FePd thin films onto different substrates. Series of $\text{Fe}_x\text{Pd}_{1-x}$ ($x = 18, 24, 26, 27$ and 34 at. %) thin film were deposited onto Si(111) by thermal evaporation technique. X-ray diffraction (XRD), atomic force microscopy (AFM) experiments were performed to study the structure and the surface morphology of these films. The evaporated layers crystallized in the face centered cubic structures for different composition of palladium. The images issued from AFM present flat surface for most of the films. The atomic compositions of these films obtained by Energy dispersive analysis showed that the films are rich in Fe. The magnetic properties were obtained by VSM, the magnetization curves display hysteresis loops allowing to infer that the magnetization axis lies in the plane of the film with a total absence of in-plane anisotropy. The samples of FePd films with a Pd content with in 18–34at. % are ferromagnetic at room temperature. The magnetization of the films depends on the Pd content and decreases linearly with increasing Pd concentration; however, the coercivity does not exhibit any monotonic dependence. The different physical parameters were investigated as a function of composition of palladium.

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SEMICONDUCTOR MATERIALS



Effect of the Sol-Gel Dip-Coating Method on the Optical Properties of ZnO Thin Films

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Abstract

Today, the technological development that has been concentrated on the front 99% on the use of silicon as a base material for the photovoltaic industry [1], went even further by exploiting other materials such as layered oxides thin and more particularly the oxides of semiconductors. These materials are very have found various applications, for example we mention SAW-based thin films of ZnO [2, 3], for electroacoustic sensor technology. Zinc oxide (ZnO) is a direct gap material [4], the gap at room temperature of ZnO can be placed in the range 3.2 to 3.3 eV [5].

The main advantage of ZnO is the fact that its components are non-toxic and very abundant on Earth [6]. ZnO is part of the family of transparent semiconductor oxides and has a high absorption and diffusion of ultraviolet radiation. Zinc oxide is a transparent material whose refractive index is equal to 2. In the form of a thin layer, the refractive index and the absorption coefficient vary according to the production conditions. The refractive index of Thin ZnO varies between 1.90 and 2.20 [7]. The optical properties of thin films are strongly dependent on the elaboration method, the quality of the layers, the heat treatment applied, the type and concentration of the dopant [8].

The deposition procedure (sol-gel) (dip-coating) makes it possible to obtain coats of ZnO that are rough and thus effectively scatter the light that passes through them. Thin layers of ZnO allow to lengthen the path that the light so the optical parameters studied are measuring: the optical gap, the disorder the index of refraction.

We studied the influence of the elaboration method on the optical properties of the ZnO layers; we realized 2 series of samples that we characterized on the optical level,



The Study of Annealing Temperature Effect on Cu₂O Nanostructures Prepared by Electrochemical Deposition

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Abstract

Copper oxides are known as p-type semiconductors, and their applications in optoelectronic devices have attracted much attention because of their low cost, low thermal emittance, high solar absorbance, and simple process of manufacture [1]. Both oxides CuO and Cu₂O were p-type semiconductors having an optical band gap of 1.9 to 2.1 eV and 2.1 to 2.6 eV, respectively [2], depending on the preparation methods. Hence, careful regulation of temperature and oxygen pressure is required to obtain pure CuO and Cu₂O. In this study, we investigate the growth of Cu₂O nanostructures on FTO glass substrate by electrochemical deposition. The applied potential, bath temperature and pH were fixed at -0.5 V/SCE, 60 °C and 11, respectively. We examined the effect of annealing temperatures on the morphological, structural, optical and photoelectrochemical properties of Cu₂O nanostructures. Cu₂O nanostructures were annealed in air at different temperature of 200 to 500 °C and as-deposited sample was used as reference. The XRD patterns showed that the films as-deposited and annealed at 300 °C were cuprite structure with Cu₂O composition. Cu₂O thin films annealed at 400 and 500 °C are completely converts tenorite structure with composition of CuO. The surface properties were characterized using atomic force microscopy. AFM images present a remarkable change in the form of grains of Cu₂O, beans in the nodular form at high temperature. Mott-Schottky measurements showed that the Cu₂O nanostructures before and after annealing have a p-type conductivity. Increasing the annealing temperature resulted in a shifting of the carrier density from 2.11×10^{20} to $2.7 \times 10^{19} \text{ cm}^{-3}$. UV-Vis transmittance spectra confirmed the results from the XRD by a decrease in the optical band gap from 2.5 to 1.9 eV. Photo-electrochemical measurements of both oxides confirmed that these films behave as a semiconductor of p-type. Significantly, the CuO nanostructures obtained at 500 °C exhibit a high enhancement of photocurrent in comparison with as-deposited sample.

Keywords: Annealing temperature, Cu₂O, CuO, Electrodeposition, Nanostructures.

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Photoactivity of Nitrogen- Doped Mesoporous TiO₂ in the Degradation of Orange Methyl

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Abstract

Significant pollution of aquatic environments is caused by highly polluted industrial discharges. The dyes used in the textile industry are among the pollutants encountered in these discharges and are known for their toxicity and low biodegradability [1] ($t_{1/2} > 2000$ h). Current treatment technologies for these releases (Adsorption, coagulation) do not solve this problem satisfactorily, which leads to the progressive degradation of freshwater resources, the lack of which is already being felt in a large number of countries. Recently, heterogeneous photocatalysis using semiconductor oxides has been of great interest because of its potential to mineralize at ambient temperature and pressure a wide range of recalcitrant organic pollutants [2]. Among the many semiconductors studied, TiO₂ is considered to be the best photocatalyst because of its photochemical stability, its chemical and biological inertness, its non-toxicity and its relatively cheap price. The use of mesoporous TiO₂ allows the conjugation of the specific properties of TiO₂ and the advantages of a mesostructure, in particular a large specific surface which could lead to a better dispersion of active sites compared to P25. The photoactivity of TiO₂ is limited to UV radiation, which represents an average of 5% of the solar spectrum. It has been reported that the doping of the semiconductor with metals or non-metals leads to a narrowing of the forbidden band and thus to the absorption in the visible [3]. As the sun is a source of renewable energy, solar photocatalysis for the depollution of water, particularly in countries with high levels of sunshine, such as Algeria, is part of a sustainable development perspective.

This work concerns on the one hand the development of photopatterns based on nitrogen-doped mesoporous TiO₂ at different molar ratios N/TiO₂ and at two calcination temperatures 500 °C and 700 °C and secondly their implementation in the photodegradation of a model molecule methyl orange under UV and solar irradiation.



The Effect of Deposition Time on the Optoelectronic Proprieties of Fluorine Doped SnO₂ Thin Films Deposited by Spray Pyrolysis for Solar Cells

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Abstract

In present work, Fluorine doped tin oxide (FTO) were prepared. This films exhibits good visible transparency owing to its wide band-gap ($E_g > 3$ eV) while retaining a low electrical resistivity due to the high carrier concentration (N_d) caused by the oxygen vacancies and the substitutional fluorine dopant [1]. FTO films are mechanically, chemically and electrochemically stable [2].

Spray pyrolysis technique has been employed to deposit the films because it is a low cost and requires simple equipments [3]. The samples were prepared from ($\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$) precursor on glass substrate at 450°C . The dependence of optical and electrical properties of films on the deposition time is investigated. Films structural properties were determined by XRD using Philips X'Pert system with $\text{Cu K}\alpha$ radiation ($\lambda_{\text{Cu}} = 0.154056$ nm). The x-ray diffraction spectra show that all films are polycrystalline with (110) as a preferred growth orientation. The presence of other peaks such as (101), (200), (220) and (211) confirm the cassiterite tetragonal SnO_2 crystal structure (JCPDS N^o. 41-1445) [4]. The optical transmission in the UV-visible range measurements was performed using Shimadzu UV-3101 PC spectrophotometer. The U-Visible spectra showed high transparency of the films in the visible region and the optical gap is ranged from 3.35 to 3.8 eV this is in the order than the reported values in the literature [3-5].

Films electrical character-ization was performed using Hall Effect measurement system, at room temperature (27 °C), to determine carriers concentration, mobility and electrical conductivity.

Study reveals that the sprayed films doped at 12 wt.% has the minimum resistivity of $4.3 \cdot 10^{-4} \Omega \text{ cm}$ whereas the carrier concentration and mobility were about $6 \cdot 10^{20} \text{ cm}^{-3}$ and $3 \text{ cm}^2 \text{ v}^{-1} \text{ s}^{-1}$ respectively.



Electron Distribution of ZnO and ZnSe by mBJ-GGA Approximation associated to like electron-matter and photon-matter interactions in Experimental Analysis (Auger electron spectroscopy and X-Ray photoelectron Spectroscopy)

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Abstract

The zinc oxide (ZnO) and zinc selenide (ZnSe) are important II-VI semiconductors appropriate for optoelectronic devices applications. Their electronic properties are related to the electron distribution in the core levels and in the valence band. In this respect, we used the ab-initio simulation to predict the density of states (DOS) of both materials. Our calculations are based on the mBJ-GGA approximation implemented in the Wien2K program. In order to validate the theoretical simulation, we associate to this study the experimental results related to the characterization by Auger electron spectroscopy (AES) and X-rays Photoelectron Spectroscopy (XPS). The XPS technique is useful for proving the clean state of ZnO and ZnSe compounds. The electron distribution revealed by XPS approve the theoretical results DOS obtained by calculations.

In other hand, Biosensors have shown great potential for health care and environmental monitoring. The performance of biosensors depends on their components, among which the matrix material, i.e., the layer between the recognition layer of biomolecule and transducer, plays a crucial role in defining the stability, sensitivity and shelf-life of a biosensor. Recently, zinc oxide and zinc selenide (ZnO, ZnSe) nanostructures and thin films have attracted much interest as materials for biosensors due to their biocompatibility, chemical stability, high isoelectric point, electrochemical activity, high electron mobility and so on.



Microstructure and Electrical Properties of ZnO-Based Varistors Prepared by Spark Plasma Sintering

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Abstract

The study deals with for the elaboration of varistors by spark plasma sintering (SPS) are investigated, using 70 nm zinc oxide nanoparticles. A system constituted of zinc oxide, bismuth oxide and other metal oxide nanoparticles are used for this purpose. Sintering of this materials is performed by SPS at various temperatures and dwell times. Different, characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) equipped with energy dispersive X-ray (EDX) have been used. Microstructural analysis revealed the presence of ZnO, spinel and bismuth rich phases. Varistor samples prepared from the nano-ZnO sintered within climb speed $900^{\circ}\text{C}-100^{\circ}\text{C}/\text{min}$ at have a smaller grain size than the samples sintered within climb speed $1200^{\circ}\text{C}-100^{\circ}\text{C}/\text{min}$; The nonlinear electrical characteristics are evidenced by current-voltage measurements. The breakdown voltage of these varistors strongly depends on grain sizes. The results show that the best varistors are obtained by SPS at sintering temperature ranging 1200°C .



Theoretical Prediction of Structural and Electronic Properties of $\text{BeSe}_{1-x}\text{Te}_x$ ternary alloys

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Abstract

Structural and electronic properties of $\text{BeSe}_{1-x}\text{Te}_x$ compounds in cubic phase are investigated using the First-Principles Full Potential Linearized Augmented Plane Wave method (FP-LAPW) within the framework of the density functional theory (DFT) using the Wien 2k code package. The exchange-correlation potential is treated with the Generalized Gradient Approximation (GGA-PBE).

The calculated structural properties of previous compounds are in reasonable agreement with available Vegard's law values. We have also carried out the calculation of the electronic band structure for $\text{BeSe}_{1-x}\text{Te}_x$ alloys. Therefore, they have a direct band gap. A reasonable agreement is found in comparing our results with Vegard's law values.

It should be noted that's our compounds are predicted to be a promising tools for novel materials: Nano and optoelectronic devices, especially for quantum well lasers.



Electrical Properties of Au/n-InP Schottky Diode with InN Interfacial Layer

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Abstract

Group-III nitrides, as InN are very important materials for optoelectronics and electronics. It is essential for the realization of such devices to grow high quality nitride. In this paper, we study electrically thin InN films realized by the nitridation of InP (100) substrates using a glow discharge source (GDS) in ultra-high vacuum. The current-voltage characteristic of Au/InN/n-InP Schottky diode is analyzed by using different methods at room temperature. The barrier height and ideality factor of the diode are determined by using the conventional current-voltage method as 0.69 eV and 3.80, respectively. The series resistance (R_s) is evaluated to 4.58 Ω from Cheung functions.



The use of a piezoelectric material in the treatment of liquid discharges

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ABSTRACT

The main purpose of this research is the study of the influence of the ultrasounds generated by a piezoelectric material on the treatment of seepage waters, specifically the leachates stemming from the Technical burying center of Souk-Ahras city, by coagulation-flocculation process, thus to know the performance of the three coagulants, namely, ferric chloride, aluminum sulphates, and ordinary alum, of the polluting load contained in these waters.

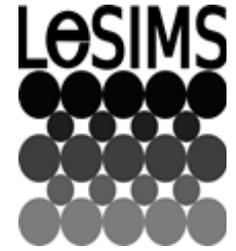
To do this, leachate samples were collected and analyzed during a limited duration, also physicochemical and biochemical analyses such as conductivity, turbidity, pH, refractive index, oxygen below, Biochemical oxygen demand (DBO₅) and organic matter, were applied to this polluted water before and after treatment.

The optimal conditions found are: a time exposure to the ultrasounds equal to 5 minutes for both aluminum sulphates and ordinary alum; a time exposure equal to 15 minutes for ferric chloride, a ratio of (volume coagulant / volume leachate) equal to 1 for a coagulant dose of 15 %. The best clarity was obtained by a treatment based on Fe Cl₃, resulting a turbidity of the order of 1.07 NTU.

The effect of the temperature of the ultrasounds bath was also approached, a temperature of 20°C was found better for the clarification of waters of infiltration by coagulation-flocculation process.

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Doping Effect on the Parameter In II-VI Based Quantum Well Laser

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Abstract

Optical properties of a semiconductor structure are the key to the understanding of semiconductor optical devices. Of great importance is the linear optical susceptibility because it represents intrinsic material or structure properties without being masked by the interaction with light. When the densities of charge carriers vary only slightly around some given values, important parameters such as the gain coefficient and the so-called Linewidth enhancement factor can be introduced to characterize the optical susceptibility [1].

The aim of this article is the study of the doping effect on the variation of the Linewidth enhancement factor of CdZnSe/ZnSSe quantum well laser. a is defined as [2]:

Where λ , Δn , Δg are the lasing wavelength, the differential gain, and the differential refractive index, respectively.

We assume that all radiative transitions take place between the first conduction sub-band and the first valence band. We found that the a shows the typical behaviour of the Linewidth enhancement factor, and decreases with carrier density mainly because of the decreasing differential gain.

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Effect of Anti-Reflective Films on the Characteristics of CdS/SnS Solar Cells

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Abstract

Thin film solar cell is a second generation solar cell that is made by depositing one or more thin layers. Debutant analysis of the parameters impeding the efficiency of the CdS/SnS based photovoltaic device is the chief novelty of the present report. In this work, we investigated the effect of anti-reflective films (ARC) on the characteristics of CdS/SnS solar cell (Current density J_{sc} short circuit, open circuit voltage V_{CO} , $P(V)$, $QE(\%)$, and $C(V)$). All these options are implemented in the one-dimensional numerical simulation program SCAPS-1D [1-3].

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Numerical Simulation Study of Current–Voltage Characteristics of a Molybdenum/4H-SiC Schottky Diode Containing Barrier Inhomogeneities Using SILVACO-TCAD Software

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Abstract

Silicon carbide SiC poses excellent electrical, mechanical, and chemical properties. Thus, devices based on silicon carbide can be used in harsh environments at high temperature and pressure. In this paper, SILVACO-TCAD software is used to calculate the current–voltage (I–V) characteristic of the Schottky diode (Mo/4H-SiC) in the temperature range of 303–498 K. This is to examine the influence of temperature on the current–voltage (I–V) curves. Simulation results showed a good agreement with measurements. The current–voltage (I–V) characteristics are parsed according to the standard thermionic emission (TE) theory and the inhomogeneous barrier heights (BHs) supposing a Gaussian distribution. It is found that the ideality factor increases while the barrier height decreases with decreasing temperature, on the basis of thermionic emission theory. Furthermore, the homogeneous BHs value of about 1.29 eV for the device has been obtained from the linear relation between the temperatures dependent effective (BHs) and ideality factors. The modified Richardson plot considering Gaussian distribution of the BHs, has quite a good linearity over the temperature range. The evaluated Richardson constant A^* was $141.86 \text{ A cm}^{-2} \cdot \text{K}^{-2}$, which is close agreement with the theoretical value of $146 \text{ A cm}^{-2} \cdot \text{K}^{-2}$ for electrons in n-type 4H-SiC. The temperature dependence of the I–V characteristics of the Mo/4H-SiC Schottky diode have been successfully explicated on the basis of thermionic emission (TE) mechanism with Gaussian distribution of the Schottky barrier heights (SBHs).



Vibrational and Thermodynamic Properties of Copper Halides CuCl, CuBr and their Ternary Alloys $\text{CuCl}_x\text{-1Br}_x$ in B3 (ZnS) and B1 (NaCl) Structures

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Abstract

The structural, lattice dynamical and thermodynamic properties of copper halides CuCl and CuBr and their ternary alloys ${}^1\text{CuCl}_{x-1}\text{Br}_x$ have been studied using first principles calculations. The density functional perturbation theory (DFPT) and the virtual crystal approximation² (VCA) are employed. The variation of the structural parameters, the optical and acoustic phonon frequencies at the high symmetry points, the electronic and static dielectric constants, the Born effective charge are studied as a function of the concentration (x). Using the quasi harmonic approximation the thermodynamic functions : free energy, thermal expansion and specific heat are evaluated.



Spin-Orbit Effect On The Electronic Structure Of Mose₂/Wse₂ Heterobilayer

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Abstract

Investigating the electronic structures of the single-layer and heterobilayer of dichalcogenides MoSe₂ and WSe₂ we observe an unusual nature of their excitations. To do so, we used first-principles methods based on density-functional theory (DFT) [1,2] and many-body perturbation theory (MBPT - the *GW* approximation and the Bethe-Salpeter equation) [3,4]. The specific properties of the subunits, which play the role of building blocks in this van der Waals heterostructures are basically preserved. For example, the semiconducting character of the monolayers is maintained in the heterostructure and only the nature of the band gap was changed. Indeed, our calculations show clearly that the building blocks are direct semiconductor at K point of the Brillouin zone in the visible range while the heterostructure shows type -II band alignment with an indirect gap. Our results open up perspectives to create new low-dimensional materials with customized characteristics.



Preparation and Characterization of Thin Layers of Chalcogenide (CdS, CuxS) Prepared by Chemical Bath Technique

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Abstract

Metal chalcogenides are semiconductors increasingly studied and used because of their remarkable physical properties in optoelectronic applications as well as in the manufacture of solar cells as thin buffer layers such as cadmium sulphide (CdS) or absorbents such as: copper sulphide (CuxS), cadmium telluride (CdTe) and indium selenium copper (CuInSe₂). In our work, we have been interested in the elaboration and characterization of thin layers of CdS and CuxS deposited by chemical bath. The transmittance of the films is determined by the UV-Visible spectrophotometer of the type (Jasco V-630 Spectrophotometer). The structural properties of the films are determined by X-ray diffraction (XRD), using a BRUKER D8 ADVANCE diffractometer (D8 X-ray diffractometer). The morphology of the films is analyzed by atomic force microscopy (A100 - AFM, APE Research Italy) and the scanning electron microscope (SEM - LEOL). The results obtained show the deposited films have good physical properties.



The Temperature Effect on Electrical Parameters of CIGS Thin Films Grown by CSVT

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Abstract

CuIn_{0.7}Ga_{0.3}Se₂ (CIGS) thin films are deposited on glass (SLG) substrate, by close-spaced vapor transport technique (CSVT) [1]. Pure copper (Cu) contacts are deposited on the front side of SLG/CIGS thin films by physical vapor deposition (PVD). Hall Effect measurements [2], on these samples, named CIGS1 and CIGS2 and grown at substrate temperature (T_s) of 470 °C and 510 °C, respectively, are performed in the temperature range (300 K – 438 K), in order to investigate the temperature effect on the electrical parameters such as carrier concentration (p), conductivity (σ) and mobility (μ). The bandgap energy (E_g) of about 1.38eV and 1.24 eV are extracted from Arrhenius diagram of (p) and (σ), respectively. Activation energies (E_a) at 563.9 meV and 239.4 meV for CIGS1 thin film and 584.2 meV and 72.7 meV for CIGS2 thin film are also determined. Moreover, average mobilities of 1.83 cm²/Vs and 1.77 cm²/Vs are deduced for CIGS1 and CIGS2 thin films, respectively.



Structural Stability and Electronic Properties of Silver Halides (Ag-VII) Ternaries and Superlattices

BELACEL Rabia

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Abstract

We have investigated the structural and electronic properties of AgCl and AgBr binary compounds, their ternaries $\text{AgCl}_x\text{Br}_{1-x}$ and superlattices $(\text{AgCl})_n/(\text{AgBr})_n$ for specific cases of $x=0.25, 0.5$ and 0.75 and $n=1, 2,$ and 3 by using first principles with full potential linear muffin-tin orbital (FP-LMTO) method, in the framework of the density functional theory (DFT) within the local density approximation (LDA). The ground-state properties are determined in the cubic phase Rocksalt and zinc-blend for comparison.

Calculation of the electronic properties in the Rocksalt (B_1) phase shows that ternaries have a semiconductor behavior with an indirect band gap while the superlattices have a metallic behavior.

In the Zinc-blend (B_3) phase, results show that our superlattices exhibit a semiconductor behavior with a direct gap for the three configurations mentioned above.



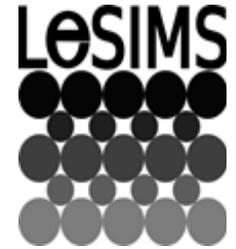
Photoelectrochemical Study of PbO Doped With Sn

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Abstract

It well known that during the anodic polarization of lead and lead tin alloys are dipped in a H_2SO_4 solution in the lead oxide potential region (-0.40 to + 0.95 V vs a Hg/Hg₂SO₄ reference electrode), the electrode system Pb/PbO layer/Pb₂SO₄ membrane/H₂SO₄ solution is formed. It was determined by X-ray diffraction that mainly the tetragonal PbO is formed, as well as small amounts of orthorhombic PbO and basic lead sulphates. It was established that the Pb/PbO/Pb₂SO₄/H₂SO₄ electrode is photoactive in the visible band (up to 650 nm) of the spectrum. In this work, the corrosion layer formed in dark on pure Pb and Pb-Sn alloys was photo electrochemically studied using: AC voltammetry, Cyclic voltammetry CV, Electrochemical Impedance Spectroscopy (EIS), Mott-Schottky plots and Photocurrent measurements. The composition was determined by XRD analysis. It was found that tin reduces the thickness and enhances the conductivity of the corrosion layer by formation of conductive and no photoactive tin oxides. A mechanism of action of tin was proposed.



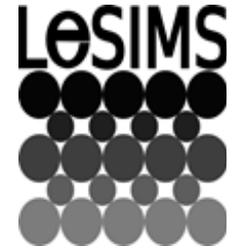
Variation of Effective Permittivity as a Function of Frequency for Concentration in Air Makes and for a Report E/C Makes

Amina Reziouk
Constantine University
Algeria

Abstract

Two types of material characterization tests are known: Destructive tests and non-destructive tests. In this work, we will try to approach this characterization by a nondestructive test. It consists in the use of a dielectric characteristic of the material to follow the variation of its resistance through its porosity. . The electrical characteristic used is the dielectric permittivity. The material concerned by this study is the cement mortar.

Key Words: Non Destructive Testing, Resistance, Dielectric Permittivity, Porosity, Cement Mortar.



Modeling of Surrounding Gate MOSFETs with Interface trapped charges

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Abstract

The impact of Interface trapped charges on the performance of Junction Less Triangular Material Cylindrical Surrounding-gate (JLTMCSTG) metal-oxide-semiconductor field-effect transistors (MOSFETs) has been studied by using an analytical model. This model is based on solving the two-dimensional Poisson's equation in two continuous cylindrical regions with any simplifying assumption. Using the superposition technique, the Poisson equation is divided into two different equations; a two dimensions (2D) homogeneous Laplace equation with its boundary conditions and a Poisson equation in one dimension (1D), where the general solution is obtained by using the series of Fourier-Bessel.

The device performance is investigated in terms of surface potential, electrical field and subthreshold current. This study is carried out over a wide range.



Effect of the Laser Wavelength on the Light Current in The Optically-Gated CNTFET

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Abstract

In this work, we have presented a compact model of the I-V and optoelectronic characteristics of optical gated CNTFET, Our study is based on a physical modeling and a numerical simulation of the electrical and optical properties of the carbon nanotubes in OG-CNTFET component. We firstly presented a mathematical modeling of current voltage characteristics as well as the optical characteristics of an OG-CNTEFT transistors, in this optic , I-V results were presented , the effect of the laser wavelength on the drain current of the component were investigated. The results obtained showed that our component had a high response when the laser wavelength took the value of 445nm .This study open several perspectives either on the scientific or technological side and it will encourage us to continue to work in this important and recent scientific field.



Structural and Optical Properties of SnS Thin Films Deposited by Spray Pyrolysis

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Abstract

Thin layers of tin sulphide (SnS) have been grown, by spray pyrolysis technique, on glass substrates at different substrate temperatures ranged from 250 to 400°C. The used solution is a mixture of $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ and thiourea precursors dissolved in distilled water. The structural, electrical, and optical properties of film are determined using Raman spectroscopy, scanning electron microscopy (SEM), Hall Effect measurement and UV visible transmittance. X-ray diffraction (XRD) analysis indicates that films are mainly composed with orthorhombic SnS phase. The SEM observation reveals that films are dense and continuous structure. The Hall Effect measurements indicate that SnS thin film exhibits p-type conduction with a conductivity varied from 5.91×10^{-4} to $34 (\Omega \cdot \text{cm})^{-1}$. We concluded that the deposited SnS films have suitable properties to be used as absorbent layer in thin films solar cells.



Study of the CISE Absorbent Layer Deposited by Spray Pyrolysis on Glass and Stainless Steel 316 Substrates

Bachir Eddine MESSAID^{1,2}, Razika Zair Talaighil^{1,3}, Claire Le Paven², Faycal Bensouici¹, Ratiba Benzerga², Laurent Le Gendre², Florent Marlec².

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Abstract

Currently, chalcopyrite CuInSe_2 (CISE) solar cells based on thin films have been imposed in the photovoltaic market, especially those deposited on Glass substrate [1], but the use of these solar cells is limited to regular support, In order to widen the range of its application, a stainless steel 316 is used as substrate with a glass substrates, a comparative study was carried out. In this work, the spray pyrolysis presents the technique of elaboration, the CISE layers deposited on Glass have been optimized, the deposited layers are heated at 550 for 10 min, One can remark the presence of four peaks in all diffractograms, indexed as (112), (220), (400), and (424) according to the JCPDS 23-0209 file of CISE chalcopyrite [2,3], This confirms that films are polycrystalline, however this crystallization is totally lost by using the stainless steel 316 substrate, that the peaks of Iron and stainless steel 316 were found, these results are confirmed by the EDS analysis which shows a non-stoichiometric CISE layer at 550 ° C, the ratio $\text{Se} / \text{Cu} = 1$, However, a different surface observed on the images SEM, The films surface deposited on stainless steel 316 looks like a spider canvas, the CISE grains are bigger on stainless steel 316 (900 nm to 1200 nm) than those observed on glass (200 nm to 400 nm).

OPTOELECTRONIC MATERIALS



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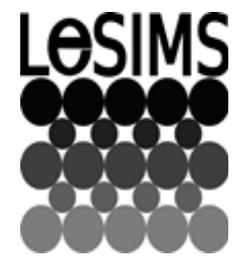


Simulation of LED using SILVACO TCAD

Ahmid Djelloul

Abstract:

White light generation using InGaN based light-emitting diodes (LEDs) with two different Quantum well active region layers that emit in two wavelength with fixed proportionality and double anodes common cathode have been numerically investigated using the SILVACO TCAD simulation software. It is found that the proposed structure shows higher light output power, lower current leakage, and smaller efficiency droop. Based on numerical simulation and analysis, these improvements of the electrical and optical characteristics are mainly attributed to the homogenous carrier distribution in the active regions of the two quantum wells (QWs), in the other hand because each QW active region has its own p-AlInN electron blocking layer EBL the electron overflow in the p-type region is greatly reduced in both active regions



ZnO thin films for solar cells application

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Abstract: Zinc oxide (ZnO) has a wide band gap of 3.37 eV at room temperature. It is a piezoelectric material with high electrical mobility and high luminescence at room temperature. According to that, ZnO thin films have attracted attention in several modern devices like solar cells, gas detectors, optical and gas sensors, laser diodes, light emitting diodes and optoelectronic devices operating in the UV-visible (violet and blue) spectral range. In this work, we are interested in developing ZnO thin films that elaborated by magnetron reactive sputtering. This technique process has high deposition rate, low-cost, good adhesion with the substrate, low deposition temperatures required, and a good parameters control. We try to optimize the conditions of elaboration and to study the influence of flow of oxygen on the different properties ZnO thin films. As well as their optimal flow rate, which gives it better physical properties necessary for applications in the field of optics and photovoltaics. We have deposited the ZnO films using a D.C reactive magnetron sputtering a different O₂ flow rates. The correlation between optical and structural proprieties was investigated.

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Prediction study of structural, optoelectronic and magnetic properties of the cubic Samarium oxide perovskite from first principal calculation

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Abstract:

The structural, optoelectronic, and magnetic properties of the cubic Samarium oxide perovskite SmCrO_3 have been investigated by the full potential linearized augmented plane wave (FP-LAPW) method with the generalized gradient approximation (GGA) based on the Density Functional Theory (DFT). The calculated ground state properties of the investigated compound agree quite well with the available experimental data. The calculated densities of states presented in this study identify the half-metallic character with an integer magnetic moment of $8 \mu_B$ per formula unit at its equilibrium volume. Calculations of the optical spectra, viz., the dielectric function, optical reflectivity, absorption coefficient, and real part of optical conductivity, refractive index and extinction coefficient are performed for the energy range 0–30 eV. The results obtained, make the cubic SmCrO_3 a promising candidate for application in spintronic.



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Milling effect on the photo-activated properties of TiO₂ Nanoparticles : electronic and structural investigations

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²Emerging materials research unit, Ferhat Abbas Setif1 University, Algeria

Abstract: Commercial PC105 titanium dioxide nanoparticles were studied under mechanical milling process. The effect of milling time and speed on the structural and electronic properties of TiO₂ powder was then investigated using X-ray powder diffraction (XRD), dynamic light scattering (DLS), transmission electronic microscopy (TEM), electron paramagnetic resonance (EPR) and UV-visible spectroscopy. The related photo-catalytic properties of the milled nanoparticles were probed following the degradation rate of methylene orange (MO) under UV-light irradiation and through EPR spin-scavenging approach[1]. Comparison with pristine powder shows that milled nanoparticles are significantly less reactive upon illumination, despite decreased radius and hence, higher specific area. Such low yield of reactive species is attributed to the apparition of the amorphous TiO₂ and brookite phase upon milling, as well as increased charge carrier recombination as pointed out by the presence of sacrificial electron donor[2].

Keywords : TiO₂ powder, PC105, Photocatalysis, EPR spectroscopy.

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Improvement of the opto-electrical properties of ZnO/Al/ZnO structures by the low Al doping of the ZnO layers

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Abstract: At present, the main objective of developing new materials for TCO films is to achieve lower resistivity and higher transmittance in the visible range spectrum. Recently, a combination of dielectrics, semiconductors and metals were used to fabricate transparent conducting oxides offering highly opto-electric performances, combined with excellent environmental stability, reproducibility, and good surface morphology [1, 2]. These structures were influenced by many factors that can effectively improve the opto-electrical performance, such as the nature and the percentage of dopant used [3, 4]. Some research mentioned that doping ZnO with Al at 0.5% produce layers possess good opto-electric performances [5, 6]. The present paper study the influence of the low Al doping (0.5%) on opto-electric performances in two ZnO/Al/ZnO structures with thickness (25nm/5nm/25nm) and (50nm/10nm/50nm), respectively. Thin AZO (ZnO doped with Al at 0.5%) and Al films were deposited on non-ferrous glass (10cm ´10cm) as (AZO/Al/AZO) multilayer structure using magnetron sputtering in DC mode. The layers were deposited successively on glass substrate at room temperature by rotating the substrate holder without breaking the vacuum. The XRD patterns show that the peaks of the spectra correspond to ZnO wurtzite structure. Both films are polycrystalline and have a preferred crystallographic orientation in the (002) plane along the c-axis perpendicular to the substrate surface. In order to show the effects of Al doping in the multilayer structure, the resistivity and optical transmittance are characterized and discussed. It is found that the low Al doping (0.5%) of the ZnO layers in AZO/Al/AZO tri-layer film present higher opto-electric performances compared at ZnO/Al/ZnO multilayer films. The maximum figure of merit value achieved of AZO/Al/AZO structure is $11.87 \times 10^{-4} W^{-1}$ corresponding at the thicknesses (50/10/50 nm), much higher than that obtained with the same thickness of the ZnO/Al/ZnO ($3.92 \times 10^{-4} W^{-1}$).

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Investigation of the optical interband transitions of the copper halide CuCl and CuBr compounds in B3 (ZnS) and B1 (NaCl) structures

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Laboratory of physics at Guelma; Algeria

Abstract:

First principles calculations by means of the potential linearized augmented plane wave method within generalized gradient approximation (GGA) were carried out for the electronic and optical properties of the copper halide CuCl and CuBr compounds. The CuX have zinc blende structure (ZnS) and show direct band gap, the density of states and band gap pressure coefficients are given. On the other hand, an accurate calculation of linear optical functions like refraction index and both parts of dielectric function is performed. The assignment of the peaks and structures to the different interband transitions is analyzed in detail. The results are compared with previous calculations and experimental measurements, we show that our calculated values compare acceptably well with values reported in the literature.



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An optimized photonic crystals sensor based on a selective geometric and optimal fill factor parameters

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Abstract :

The components based on photonic crystals attract a great interest in the scientific community, the kind of these components are like guides [1], fibres [2], cavities [3] and sensors. The development of photonic crystal sensors has become a major challenge to meet the needs of today in various fields such as medicine, industry and security, with an ever-higher level of requirements. Among these sensors, we find gas sensors [4] biochemical sensors [5] and pressure sensors [6]. In this work, we studied by simulation the index variation detection sensor, based on a photonic crystal ring resonator. We used the Plane Wave Expansion (PWE) method to find the phonic band gap and the Finite-Difference Time-Domain (FDTD) method to determine the output spectrum of this sensor, we have optimized in this paper the sensor sensitivity for a selective geometric parameters and an optimal fill factor.



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Electrodeposition of semiconductors for optoelectronic devices: Results on Cu₂O thin films

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Abstract:

Cuprous oxide (Cu₂O) is an attractive material for applications in solar energy converting devices, it can be used as a p-type semiconductor material due to the Cu vacancies created in the crystal lattice during the growth with a direct band gap (E_g) of 1.9 to 2.2 eV [1]. Although the theoretical efficiency of Cu₂O solar cells is about 18 %, and the best-reported efficiency is only 2.05% [2]. This material has been synthesized by different methods including chemical vapor deposition (CVD) [3], Sol-Gel [4], and electrochemical deposition [5,6]. Among these methods, electrodeposition is a simple and low-cost technique for preparing nanostructures of oxide semiconductors on conductive substrates. It provides advantages such as, low synthesis temperature, and large area deposition [7,8]. Many researchers using the electrodeposition method for the elaboration of Cu₂O nanostructures only consider the effect of the precursor concentration or make a comparative study between precursors, forgetting that temperature has a considerable influence on the optical and structure of Cu₂O. In this work, we have electrodeposited a series of Cu₂O thin films on FTO coated glass substrates in pH = 9.5 by using copper sulphate electrolyte through potentiostatic electrodeposition with different temperatures (40, 50, 60 and 70°C). It was found that the optimum deposition temperature was 70°C. The electrochemical, structural, morphological and optical properties were characterized using Mott-Schottky plots (MS), photocurrent measurements (PC), X-ray diffraction (XRD), scanning electron, microscopy (MEB) and Ultraviolet and visible transmission Spectroscopy (UV-Vis), respectively.



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Characterization of transparent polycrystalline MgAl₂O₄ Spinel fabricated by Spark plasma sintering

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Abstract:

Transparency is a highly sought-after property in the materials for optical applications (lenses, windows, laser power...). It is therefore particularly interesting to develop transparent ceramics that combine the specific properties of ceramics with the advantages of a transparent medium [1-2]. Among these transparent polycrystalline ceramics, we find that the spinel MgAl₂O₄ has an excellent optical and mechanical properties such as: high hardness, high resistance to erosion, low thermal expansion, high resistance to chemical attack and good transparency in the ranges of visible wavelengths and IR. The development of transparent polycrystalline ceramics is a very important technological challenge, so the interest is obvious. Spark Plasma Sintering is an alternative technique to fabricate a transparent spinel [3]. The aim of this work is to elucidate the effect of sintering temperatures on the optical properties of sintered transparent ceramics. For this reason, Spinel pellets were prepared by SPS at different temperatures (1300 °C, 1350 °C, 1400 °C) based on two types of magnesium aluminate nano-powders (S25 CRX 14 and S25 CRX 12). The heat treatment was carried out at different temperatures under a pressure of 73 MPa. Then, these samples were polished and subjected to optical characterizations. We followed the evolution of the optical transmission, the optical diffusion, the optical gap and the change of the refractive index. The results obtained show that S25 CRX 12 Spinel samples have a good optical property (optical transmission is about 84% at 550 nm, the optical gap is 5.6 eV and the refractive index expect 1.6553) with respect to this S25 CRX 14 Spinel samples (RIT = 73% at 550 nm, E_g = 4.9 eV). In addition, it is shown that the 1350 °C temperature which allow good optical properties for both types of Spinel. Moreover, the sintered samples at 1400 °C, have a large diffusion coefficient due to carbon contamination are remarkable in this sample.



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Study of light transmission by PDMS microlens fabricated using chemical etching

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Abstract:

Optical fiber micro-collimators are Optical fibers equipped with microlenses, become essential end components in the field of optoelectronics. They ensure the transfer of light energy in a connection. Several studies have been proposed in order to optimize this optical coupling and have led to the proposal of various solutions. However, it remains difficult to increase the coupling efficiency due to the difference between the mode field diameters (MFD) of the laser diode and the optical fiber. The microlenses at the end of the fibers are using to increase the coupling efficiency. The microlenses can have different surface morphology to modulate the incident waist of the laser diode (LD) and transmit it into the SMF. This provides better-collimated beams for coupling applications. In this work, we will represent the Manufacturing Methodology of the micro-collimator involves etching a conical microcavity at the end of an optical fiber. The selective etching [1] process produces a concave cone centered on the axis of the core of the fiber [2]. We will highlight the peculiarities of the process. In the microcavity is inserted a quantity of PDMS (Polymer of good optical properties). The micro-collimators obtained are equipped with microlenses [3]. Depending on the amount of PDMS, different radii of curvature (focal) are obtained. The second part of this work is dedicated to the coupling of a laser diode to a spherical microlens in PDMS on the end of a single mode fiber (SMF) (9 / 125 μ m, telecom). The light transmission through a micro-collimator was digitally analyzed in 2D using the COMSOL Multiphysics finite element software. The simulation results shows the optical focusing characteristics (Waist, Working distance) and shows optical coupling performance.



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Elaboration, Structural and optical properties of KCl:Y2O3 single crystal

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Abstract:

Recently, many research teams have been interested in the application of nanomaterials in different disciplines of technology, especially in the optical field. In this context, we suggest this investigation where the nanocrystallites of Y2O3 were dispersed inside of a transparent crystalline matrix (KCl), the composite material KCl:Y2O3 (2 weight%) was elaborated using the Czochralski technic. In order to measure confidently, the obtained crystal was cleaved parallel to the (100) plane. The XRD structural results prove that the Y2O3 are incorporated inside of KCl with two phases monoclinic and cubic. In addition, the Raman spectrum demonstrates that the two phases of Y2O3 (monoclinic and cubic) are present. Moreover, the optical properties prove that the KCl:Y2O3 single crystal exhibits a significant optical activity in the UV region, this feature makes this sample as a good candidate to integrate them in the optical devices which work in the UV range.



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Photonic Crystal Based Bio-Sensor for Detection Cancer Cell

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Abstract:

Les biocapteurs qui fonctionnent dans la région térahertz du spectre électromagnétique attirent de nos jours de plus en plus d'intérêts de recherche en raison des applications possibles dans le diagnostic médical et les soins de santé [1]. Les cristaux photoniques sont des matériaux nanostructurés dont les dimensions caractéristiques submicroniques permettent un contrôle sans précédent du confinement de la lumière et rendent possible la miniaturisation de plusieurs fonctions optiques [2]. Du fait que les molécules et nanoparticules sont beaucoup plus petites que la longueur d'onde, leur absorption est très faible aux fréquences de Terahertz, ce qui rend leur détection difficile à moins qu'elles ne soient présentes en grandes quantités. Cependant, il a récemment été démontré que leur absorption peut être améliorée en plaçant les macros à l'intérieur des résonateurs à nano-intervalles. Cela donne un coefficient d'absorption considérablement accru, permettant de détecter de plus petites quantités [3]. Nous présentons dans cet article un ensemble de résultats sur la conception et le développement de nouveaux composants à base de cristaux photoniques pour le guidage de la lumière et la détection haute sensibilité des analytes en utilisant la méthode de résolution des équations de Maxwell méthode de domaine en deux dimensions (FDTD-2D). Dans cet article, nous proposons une plate-forme de Bio-détection basée sur un cristal photonique infiltré mis en place par des trous en forme d'anneau pour détecter de nombreux types de cancer dans le corps humain comme l'estomac, colorectal, foie, sein, cervical, prostate etc. les caractéristiques de la lumière dans le biocapteur sous différents indices de réfraction correspondant à différents types d'indice de réfraction de l'échantillon de cellules cancéreuses entraînent un décalage de la longueur d'onde résonante au niveau de la borne de sortie.



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Fabrication of a micro sensor in optical fiber using chemical etching

Amina Nezzar

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Abstract:

Since a long time, sensors are widely used in many fields, but the increasing need of a compact, small size, high sensitivity, and low-cost, gave a rise to a new technological solution, especially with the optical fibers. In this work, we propose to fabricate a micro sensor based on a chemical etching and metalized optical fibers. Firstly, a small part of the single mode fiber SMF (Core diameter $9\mu\text{m}$, Cladding diameter $125\mu\text{m}$) was cleaved and dipped in an etchant solution of 65% ionized water, 35% HF acid, and organic solvent, then the same fiber was dipped in another etchant solution but in this time with a 5% of HF acid. After etching process, the obtained diameter of the reduced part around $8\mu\text{m}$, two samples with the same fiber have been prepared. Secondly, one of the reduced parts covered with a thin layer of gold with thickness of 30 nm, deposited using the vacuum evaporation technique, and the other sample is covered with a thin layer of silver, by a chemical process. As results we found that, the layer of silver obtained by this process is very thick, and of high roughness, but for the gold layer is uniform with a more adapted thickness.



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Design and simulation of optical filter based on photonic crystal ring resonator

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Abstract:

In this paper, we proposed the design of optical filter with ring resonator based on two-dimensional photonic crystals. The filter is designed in two-dimensional photonic crystals (2D PCs) with square lattice of silicon rods in air. The lattice constant and the rod radius are designed to achieve maximum operating range of frequencies. The Plane Wave Expansion (PWE) method is used to obtain the band structure of the proposed model. The numerical simulation results through finite difference time domain method show that the electrical field distribution, high transmission efficiency are achievable at the resonant wavelength, which is an important for optical communication systems. Also, the effect of different parameters such as refractive index, lattice constant, the radius of the rods and the resonant wavelength on the filtering behavior of the structure is investigated. The obtained high transmission efficiency and the electrical field distribution of the filter are presented in this work. The proposed filter is characterized by its design simplicity and high transmission efficiency.

Keywords: Photonic crystal, optical filter, photonic crystal ring resonator, FDTD, PWE, transmission efficiency.



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Photonic crystals for Malaria Detection

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Farhat Abbas University; Algeria

Abstract: Cell refractive index is a key biophysical parameter, which has been extensively studied. Healthy red blood cells have a homogeneous distribution in refractive index, while infected red blood cells in malaria disease show non-homogeneous refractive index throughout the cytoplasm of the cell. In this paper we design and simulate a 2D photonic crystal ring resonator based refractive index biosensor for malaria detection. The simulation results have analyzed by using the finite difference time domain (FDTD) method, the band gap calculation is performed using the plane wave expansion method. The grating design, incorporated in the photonic crystal waveguide increases the efficiency and sensitivity of the designed sensor.

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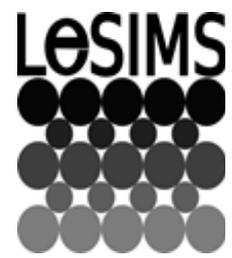
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Polarized second harmonic response from gold nanocylinders

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Abstract:

In this work, the non linear optical properties of gold nanocylinders arrays of various sizes arranged according to square geometrical configuration on a substrate are studied. For this purpose, the technique of polarization resolved second harmonic generation in on-axis transmission configuration is used. The results demonstrate that the second harmonic response of the nanocylinders is shown to be mainly incoherent, of pure electric dipole nature resulting from the breaking of the centrosymmetric shape of the body of the nanocylinders, in a plane parallel to the substrate surface, by surface defects.



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The role of seed layer thickness on ZnO nanowires deposited by electrochemical method

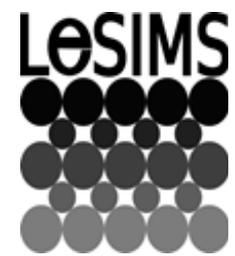
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Abstract: Zinc oxide (ZnO) is a very important semiconductor with a direct wide band gap of (~ 3.37 eV) and large exciton binding energy (60 meV) at room temperature [1], ZnO has a wide range of structural morphologies of such as nanobelts, nanorods [2,3] and nanowires [4]. Due to its important characteristics, ZnO is an ideal material for various applications in future electronic and photonic devices, such as solar cells, light emitting diodes and photoconductive sensors [5]. In this study, we reported the growth of ZnO nanowires directly on (ITO) coated glass substrates by electrodeposition route from aqueous solution under different thicknesses of ZnO seed layer ranging from 0 nm to 150 nm. The variation of the electrochemical, structural and optical properties of the ZnO nanowires grown at different thicknesses of ZnO seed layer were investigated. The Mott-Schottky analysis demonstrates an n-type semiconductor character for all the samples with a carrier density varied between $4,27 \times 10^{-20}$ and $9,27 \times 10^{-20} \text{ cm}^{-3}$ when the thickness of ZnO seed layer increases. From the electrochemical impedance spectroscopy (EIS), a low charge transfer resistance (R_{ct}) of 100,44 Ω was obtained. The XRD patterns indicated that ZnO nanowires crystallize in a hexagonal Würtzite structure along (002) crystallographic plane with a preferential orientation along c-axis and an average crystallite size ranging from 95.816 to 97.23 nm when the ZnO seed layer thickness increases. UV-Vis spectra showed a significant optical transmission (up to 70%), which increased with ZnO seed layer thickness. The energy band gap values (E_g) have been estimated to be between 3.3 and 3.13 eV.

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Characterization of nanostructured Ti₈₀Ni₂₀ elaborated by mechanical alloying

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Abstract: Nanostructured Ti₈₀Ni₂₀ material was prepared by mechanical alloying from pure Ti and Ni powders in a planetary ball-mill P7 under argon atmosphere. Morphological change, microstructural and structural variation, formability and mechanical properties were studied by scanning electron microscopy, X-ray diffraction, cold compaction followed by sintering and nanoindentation technique. The Morphological observations shows the predominance of the welding phenomenon during the milling process. The Rietveld refinement of the X-ray diffraction pattern reveals after 4 h of milling, the formation of disordered hcp-Ti(Ni) solid solution, intermetallic fcc-Ti₂Ni in addition of unreacted Ti and Ni. The interdiffusion of Ti and Ni leads to a heterogeneous solid solution with Ti-rich and Ni-rich environments after 9 h of milling. The end product is a mixture of a highly disordered structure, hcp-Ti(Ni), fcc-Ni(Ti) and hcp-Ti(Ni) phases having different microstructural and structural parameters. The porosity of the compacted powder (milled for 9 h) which is about 15 % after cold compacting reaches 5 % after sintering at 1000 °C for 1 hour. The maximum values of nanohardness and elastic modulus are of about 5,98 and 164,53 GPa respectively.



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Application of multiwall carbon nanotubes in waste water treatment

Nait Merzoug Assia

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Abstract: Important challenges in the global water situation, mainly resulting from worldwide population growth and climate change, require novel innovative water technologies in order to ensure a supply of drinking water and reduce global water pollution. The development of cost-effective and stable materials and methods for providing the fresh water in adequate amounts is the need of the water industry. Traditional water/wastewater treatment technologies remain ineffective for providing adequate safe water due to increasing demand of water coupled with stringent health guidelines and emerging contaminants. Nanotechnology-based multifunctional and highly efficient processes are providing affordable solutions to water/wastewater treatments that do not rely on large infrastructures or centralized systems. The aim of the present work is to study the possible applications of nanostructured adsorbent based on carbon which is functionalized multi wall carbon nanotubes synthesized in Algeria at LEREC laboratory in Annaba University, for the removal of organic pollutants from wastewater. Before the study of adsorption processes, our adsorbent was characterized by different methods such us DRX, MEB, IR and BET. The effect of different operational parameters like contact time, initial dye concentration , adsorbent dose, pH and temperature on the sorption of behavior was studied in batch mode. Experiments showed that the O-MWCNTs was efficient for the removal of the organic pollutant and the equilibrium can be reached in 60 minutes. The removal efficiency was found to be dependent on the initial micropollutant concentration and there is no significant effect of temperature on the adsorption process. Also, acidic pH was found the favor disperse dyes removal, while the adsorption capacity decreases proportionately with the functionalized multi wall carbon nanotubes dosage.



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Effect of Hygrothermal aging on Morphology and Thermo-Mechanical Properties of PHBV/ Cloisite 30B Bionanocomposites

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Abstract: Hygrothermal degradation is one of environmental aging process which combines the effects of both moisture and temperature; leading to irreversible changes in the molecular structure, chemical and mechanical properties of polymers [1]. So it is crucial to study the degradation mechanism and to predict the service life of materials. Among the biodegradable polymers, Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) which is a bacterial polyester belonging to the polyhydroxyalkanoates (PHA) family was developed primarily as a renewable and biodegradable replacement material for petroleum-derived plastic [2]. It is widely exploited in consumer markets, especially in food packaging and biomedical applications [3]. The use of organomodified montmorillonite such as Cloisite 30B to reinforce the functional properties of PHBV can affect the inherent hydrophilicity of the polymers and subsequently the mechanisms of degradation. Therefore, the objective of this work was to investigate the effects of Cloisite 30B (3 wt%) on the morphology and thermal and mechanical properties of bionanocomposite based PHBV under hygrothermal ageing. The property changes of the aged samples were evaluated by several techniques, involving size exclusion chromatography (SEC), differential scanning calorimetry (DSC), scanning electron microscopy (SEM) and tensile tests.

Keywords: Poly (3-hydroxybutyrate-co-3-hydroxyvalerate), bionanocomposites, Hygrothermal aging.



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Green synthesis of nanocomposite Polyethylene glycol dimethacrylate/ Algerian clay (Maghnite-CTAB)

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Abstract:

A reactive cationic surfactant cetyltrim-ethyl-ammonium bromide (CTAB) was synthesized for intercalation of montmorillonite Mmt, a Maghnite type of clay. The pristine montmorillonite (Mmt) was obtained from Algerian plant with a cation exchange, Organophilic Mmt, was prepared by ion exchange between Na^+ ions in the clay. CTAB-intercalated Mmt particles were easily dispersed and swollen in Polyethylene glycol dimethacrylate. This method is based on the swelling of the silicate layers with the liquid polymer. The polymer composites were characterized using different techniques such as X-ray diffraction (XRD), FT-IR, thermal gravimetric analysis (TGA) and scanning electron microscopy (SEM). Five types of composites of different compositions (2, 3, 5, 7 and 10 wt% MMT-CTAB) were prepared by melt compounding at room temperature. Each tube contained a mixture of 1 g of Polyethylene glycol dimethacrylate and an amount of montmorillonite-CTAB. The desired amount of cation exchanged MMT was dispersed in the polymer. The mixtures were held at under ambient temperature and stirred with a magnetic stirrer. The effect of organoclay (Maghnite-CTAB), prepared and used with different ratios, on the properties of Polyethylene glycol dimethacrylate/Algerian clay nanocomposites was studied. The results of thermogravimetry indicated that the nanocomposites showed a higher thermal stability. This is attributed to interactions between the set of polymer chains and the organic compounds of the modified clays.



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Bottom-up process for elaboration of ZnO nanoparticles and photocatalytic applications

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Abstract :

The nanoparticles compared to massive, present new physical properties which open promising perspectives for new applications. In the present work, bottom-up process are used for ZnO elaboration passing by lamellar hydroxide as stable structures stage, the X-ray diffraction is used to follow the developing of the crystalline structure and the infrared spectrometry reveals the existing chemical bonds in samples and proving the CO₂ fixation on nanoparticles surfaces offering to the materials a possibility to be air purifier. The photocatalytic properties are proved according to the semiconductive properties of ZnO nanoparticles, this interesting property open a new access to the water purification, the last applications can be interesting in the environment domain.

Nanohybrid materials based on the graphene oxide functionalized covalently and decorated by the silver nanoparticles

Keywords : ZnO nanopartiles, hydrothermal method, CO₂ fixation, photocatalysis



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Nanohybrid materials based on the graphene oxide functionalized covalently and decorated by the silver nanoparticles

Lhadi Otmani, Rachida Doufnoune

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Abstract:

Nanohybrid materials were developed by the decoration of the support material, currently called graphene oxide (GO). These materials were further functionalized and decorated with sulfonic and silver, respectively. The functionalization process involves a covalent and non-covalent linking in which the chemical sulfonation and solvothermal reactions are implicated, respectively. The structure of the graphene oxide (GO) was used as the starting material to develop sulfonated graphene oxide (SGO), sulfonated non-reduced and reduced graphene oxide in which the silver nanoparticles (SGOAg, SrGOAg) were incorporated. These materials were identified using different characterization techniques. The TEM images and X-ray spectra confirmed the high degree of oxidation despite the decrease of the crystallite size. The TEM images also showed a uniform distribution of the silver nanoparticles on the surface of GO sheets.



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Mechanical and physical study on the aging of a polymer resin in an organic solvent

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Abstract: The durability of PE structures is also an important concept to consider in estimating their service life. Indeed, they are often exposed to severe environmental constraints (exposure to UV, chemicals, etc ...), which generally induce a modification of their microstructure, physical state, and even their chemical composition. The challenge then rests on a rationalist evaluation of the lifespan of these structures, considering the "aging" aspect of the material. The difficulties associated with this type of prediction are difficult because of the limited time available to the experimenter to analyse the phenomena involved. We will study the effect of an organic solvent on the degradation of mechanical and physical properties. This work is based on a macroscopic approach realized with uniaxial tensile tests, and a thermal analysis. The results provided by these two approaches are discussed to better understand the behavior of this type of polymer. Mechanical tests and thermal analysis show that the toluene-methanol mixture is much more absorbed compared to water. In addition, the study shows the evolution of changes as a function of the thickness of the tube in order to have an idea on the structural heterogeneity. An amplification in crystallinity was detected which is established by the literature for other organic solvents.

Keywords: HDPE, Aging, organic solvent, uniaxial stress, thermal analysis.



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Synthesis and characterization of Zn/Al layer double hydroxide materials and their application in organic pollutant removal

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Abstract:

The nanostructural materials Zn/Al layer double hydroxide (Zn-Al /LDH) were prepared via a one-pot co-precipitation method, with different (Zn^{2+}/Al^{3+}) molar ratios (2, 3 and 4). The synthesized samples were characterized by X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Nitrogen Physisorption (BET) and Scanning Electron Microscopy coupled with Energy Dispersive X-ray Spectroscopy (SEM/EDX). The XRD spectra obtained for the synthesized samples exhibits a series of characteristic reflections of well-crystallized hydrotalcite-like structure and the Brunauer-Emmer-Teller analysis (BET) confirm that the samples exhibit a strong characteristic of mesoporous materials. The synthesized materials were assayed in the adsorption of organic pollutant in aqueous solution. Experimental results indicated that the adsorption of pollutant onto Zn(2)Al-LDH followed the Freundlich isotherm model. The Zn^{2+}/Al^{3+} molar ratio was found to affect the adsorption process. The facile, low-cost preparation and efficient removal of pollutants makes the LDH materials advantageous.



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Ab initio DFT study of the properties of the Gen+1 and GaGen nanomaterials

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Abstract: This work is an ab initio theoretical investigation of the physicochemical properties of pure germanium nanomaterials (clusters) (Gen+1) and germanium doped with gallium (GaGen) in the range of 1 to 19 atoms through the density functional theory (DFT) with the generalized gradient (GGA) approximation, implemented in the SIESTA program. We show the relationship between the electronic and chemical behavior of these small systems with their structural properties. For each size, several initial structures have been relaxed to determine the most stable one. The structural relaxation and the search of the ground states energies of the Gen+1 and GaGen clusters are performed using the conjugate gradient method with the polarized spin option. Our results show the considerable influence of the sizes of the systems on the structure and the electronic properties of the GaGen clusters. We have also shown the influence of doping with a gallium atom on the stability and other physicochemical properties of pure germanium clusters and the relationship between binding energies and the size of new clusters. The values of the HOMO-LUMO gaps decrease with the increasing of their sizes. For each GaGen clusters, the HOMO-LUMO spin-up gaps are higher than the HOMO-LUMO spin-down gaps. This characteristic provides these clusters with properties that can have many potential applications, especially in the field of spin electronics applications in the coming years. The small clusters with high HOMO-LUMO gaps are higher stability and low reactivity than those with large sizes having very small gaps. The very small values of HOMO-LUMO gaps indicates that the gallium atom enhance the metallic character and the chemical activity during the crystal growth. In order to give more information on the electronic and chemical behavior of these systems, the ionization potentials, electron affinities, chemical hardness, total and partial densities of states are calculated and analyzed. The vertical electron affinity (VEA) and vertical ionization potential (VIP) of GaGen clusters are used to determine the energies needed to add or remove an electron from a cluster without any structural relaxation. The results obtained show that the values of the AEVs show an increasing tendency with the increase of the cluster sizes. This indicates that the clusters GaGen of great size will capture electrons more readily compared to those of small sizes. However, the values of the VIP increase with increasing of size. This implies that the clusters of great sizes require more energy to lose an electron compared to the clusters of small sizes indicating their high stabilities.

Keywords: nanomaterials, ab initio, DFT, SIESTA, germanium-gallium, physicochemical properties.



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Elaboration and study mechanics of a Gibbsite $\text{Li}(\text{OH})_3$ Hybrid Material

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Abstract : A hybrid material may be defined broadly as the association between two partners of different chemical nature, related to the nano-scale (hybrid nanocomposites) or microscopic (hybrid composite) [1]. The combination of a mineral matrix and organic matter, presents multiple and varied interests. From a chemical point of view, it allows the obtaining of bifunctional materials, combining the chemical properties of the two partners. Developing new materials with specific properties and nanostructured HDLs (lamellar double hydroxides) has widely been investigated in the last few years and still remains of great importance. In this frame work, study and valorization of hybrid materials HDL was one of the major areas of our activity [2]. This study focused on the development of a hybrid material consisting of a matrix of alumina trihydrate $\text{Al}(\text{OH})_3$ (gibbsite) [3]. Previous studies to synthesize suspension lamellar double hydroxides (HDLs) by lithium salts intercalation in a gibbsite matrix was examined, the obtained samples were characterized by different physicochemical characterization methods, and study mechanical properties of these different composites.



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Effect of TiO₂ nanoparticles on the mechanical Properties of Low- Density Polyethylene (LDPE)

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Abstract:

In the recent years, composites using nanoparticles (nanocomposites) have gained much attention and been intensively investigated owing to their remarkable enhanced properties including mechanical, optical, thermal properties and their wide spread, potential applications [1]. Different inorganic nanoparticles have been used to improve polymer properties, such as titanium dioxide (TiO₂), silicon dioxide (SiO₂) and aluminum trioxide (Al₂O₃). Polymer-based TiO₂ composites have been extensively studied in the literature in order to develop mechanical and thermal properties of the polymer [2]. In this work, effect of TiO₂ nanoparticles on the mechanical properties of low density polyethylene (LDPE) was investigated.

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Synthesis, Characterization and Crystal Structure of a New Schiff Base Ligand and Hydrolytic Cleavage of the Imine Bond Induced by a Copper(II) Cation

Kamel Mokhnache

University Farhat Abbas of Sétif-1; Algeria

Abstract:

A Schiff base ligand 2-[(1E)-N-{2-[(2-[(Z)-[1-(2-hydroxyphenyl) ethylidene] amino)ethyl]amino]ethyl}ethanimidoyl]phenol L was hydrolyzed by copper cation which lead to formation of 8,8-dichloro-2H,3H,5H,6H-1,3-diaza-2-cupracyclopenta[1,3-a]1,3-diaza-2-cupracyclopentane hydrate (Complex), characterized by UV, IR, Powder XRD and by elemental analysis. The study of quantum chemical calculations shown, stability and reducing character of L. In vitro antioxidant, anticoagulant, and hemolytic activities of L were evaluated. Antioxidant potential of L was assessed by DPPH scavenging, β -carotene bleaching test, hydroxyl radical scavenging method, ABTS radical scavenging test, and by reducing power test. In vitro anticoagulant effect of L at the 84 $\mu\text{g/mL}$, showed the maximum prolongation of plasma recalcification time. Schiff base L showed no toxic effect (hemolytic activity) in vitro. For anti-denaturation effect, L exhibited significant activity against denaturation of egg proteins with I% decreasing with increase of temperature. In conclusion, results of the present investigation indicate that the ligand L can be a potential anticoagulant and anti-denaturant agent.



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Structural and optical properties studies of pure and Al-doped ZnO aerogel elaborated in supercritical drying conditions of isopropanol

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Université de Bejaia; Algeria

Abstract :

Pure and Al-doped ZnO were synthesized in supercritical isopropanol using zinc acetate dihydrate, aluminum nitrates and methanol as precursor, dopant source and solvent, respectively. The atomic ratio [Al]/[Zn] was fixed to be 0.03 (3%). The aerogels were characterized without any chemical or heat treatments. X-ray diffraction (XRD), infrared spectroscopy (FTIR), UV-visible spectrophotometry, photoluminescence spectroscopy and scanning electronic microscopy (SEM) were used to characterize the aerogels. XRD results showed a single phase with hexagonal wurtzite structure of ZnO. The introduction of 3% at. Al-doped ZnO ameliorates the crystalline quality of the doped ZnO aerogel by the occupation of Zn²⁺ sites by Al³⁺. The crystallites size increases from 31 nm in undoped to 50 nm in doped aerogel. FT-IR results show the bands intensity decreases after Al-doping. UV-visible measurements show the increase of the absorption band intensity and a slight shift towards long wavelength side after the introduction of Al atoms. Room temperature photoluminescence spectra show that Al-doping increases the emissions bands intensity. SEM images reveal the spherical grains morphology of pure ZnO aerogel and random forms of the grains of the doped aerogel. The grains have the same size in pure ZnO and different sizes for Al-doped ZnO grains were observed.



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Simultaneous complete phononic and photonic band gaps in periodic structures

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Abstract:

The photonic crystal (PC) is a periodic dielectric structure that can exhibit a forbidden band of frequencies, or a band gap, in its electromagnetic dispersion relation. The first realization of a band gap in a three-dimensional photonic crystal occurred in 1989 [1]. The photonic crystal capability to control the flow of the light makes this kind of structures very attractive for several applications in the field of integrated optics and telecommunications. A wide range of application of these materials include, wave guide, filter, microcavities, photonic crystal fiber and high efficiency LEDs [2]. Two-dimensional PC slabs can be fabricated by electron beam lithography [3,4] or holographic lithography [5]. In this paper we present a theoretical study of two-dimensional crystal constituted by a square array of holes drilled in a matrix of Si using COMSOL Multiphysics software based Finite Element Method (FEM) with MATLAB programme integration. The results show that it is possible to obtain a complete photonic and phononic band gaps in a two-dimensional crystal of Si. Moreover, the phononic band gap width depended with the height of silicon pillars deposited on a homogeneous thin silica plate.



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Structural study of amorphous silicon nitride matrix containing silicon nanocrystals

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Abstract: The reflectance combined with photoluminescence (PL) and Raman spectroscopy are a very sensitive tool for probing silicon nanocrystals (Si-ncs) characterization. Indeed, the structure of a thin film SiN_x ($x=0.12$) containing Si-ncs in terms of composition, Si-ncs size distribution and defects is studied. The elastic and inelastic light scattering by the silicon nanocrystals (Si-nc) embedded in amorphous silicon nitride matrix are also investigated in this work. Results shows that the PL spectrum can be deconvoluted into several peaks attributed to the quantum confinement effect, the surface effect and the photocarriers recombination between band tail states in the amorphous matrix. The PL peak broadening is attributed to the Rayleigh scattering and the PL peaks positions are affected by the Raman scattering. Here we offer also a new approach to describe the coordination of the silicon surface atoms. From a parameter called the ratio of surface bonding contribution in Raman red shifts, we demonstrated that the silicon surface atoms are hyper coordinated under a sp^3d^2 hybridization.



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Crystallization kinetics of α -cordierite ceramic from MgO–Al₂O₃–SiO₂–TiO₂ glasses using DTA analysis

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Abstract: The results of studies of crystallization kinetics of α -cordierite ceramics from MgO–Al₂O₃–SiO₂–TiO₂ glasses that are obtained via melt cooling using Differential thermal analysis (DTA), Thermogravimetric analysis (TG), X-ray diffraction (XRD) and scanning electron microscopy (SEM) are presented. DTA experiments were carried out on samples between room temperature and 1400 °C under argon gasflowing at a rate of 40 cm³/min. Heating rates of 10, 20, 30, 40, and 50 °C/min were used in this investigation. X-ray diffraction was used to characterize the phase transformations of the sintered powders. The average activation energy values for α -cordierite formation, using DTA results was measured under both isothermal (Johnson–Mehl–Avrami (JMA) theory using Ligeró method) and non-isothermal (using Kissinger, Boswell, and Ozawa methods) treatments were found to be equal to 845 and 720 kJ mol⁻¹, respectively. The growth morphology parameters n (Avrami parameter) were found to be almost equal to 1.5, using non-isothermal treatments, and equal to 1.5 using isothermal (Ligeró method) and m (the numerical factor) was 1.5 obtained by Matusita et al. equation. The growth morphology parameters n and m are both approximated as 1.5, which is an indication of a three dimensional growth from a constant number of nuclei and resulting in a polyhedron -like morphology controlled by diffusion.

Keywords: Cordierite, Differential thermal analysis, Avrami parameter, numerical factor, Activation energy.



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Sodium effect on the hydroxyapatite synthesis by the sol-gel route

Imane Sassaoui, Fatima Zohra Mezahi

Abstract:

Hydroxyapatite (HA) $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ is a very important inorganic material; first mineral constituent of bones, tooth enamel and dentin. It is very flexible in terms of composition and morphology. HA is known as a non-resorbable and surface-active bioceramic and is mainly used for many medical applications thanks to its biocompatibility and bioactivity. The aim of this work is devoted to study of the effect of the sodium addition (Na) with different molar ratio (0, 1, 5, 10, 15 and 20%) on the synthesis of hydroxyapatite by the sol-gel route. From the obtained results, it was possible to obtain well crystallized hydroxyapatite at 700°C ; synthesized from the precursors: the calcium nitrate and tri-ethyl phosphate. Sodium nitrates were used as a source of Na. The synthesis was carried out for 3 days; one day for aging the prepared solutions; one day to obtain a gel, one day to dry the gel. The obtained results showed that the addition of sodium stabilize the hydroxyapatite synthesized by the sol-gel route. As ratio of Na increases, the intensity of the XR peaks of HA increases and that of CaO decreases. Thus, DRX has shown the apparition of a new phase (b- CaNaPO_4) at 1000°C and 1300°C for the large concentrations of Na (15 % and 20 %).



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Effect of Ag doping on the physical properties of TiO₂ nanopowders prepared by sol-gel

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Abstract:

Pure TiO₂ nanopowders and doped with silver for 1% and 5% concentrations were synthesized by sol-gel method, using titanium tetra n-butoxide and silver nitrate as precursors. The obtained powders were annealed at 500 °C. The effects of silver incorporation on structural and optical properties were investigated by X-ray diffraction (XRD), UV-Vis spectroscopy and Fourier transform infrared spectroscopy (FT-IR). XRD characterization showed that grain size decreases with Ag concentration. The absorption edge obtained by UV-visible is shifted to the lower energies for doped TiO₂. FTIR spectra indicated that all peaks are almost the same.

Keywords: Nanopowders; Sol-gel; TiO₂; Silver.



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Preparation and synthesis of a hybrid based on graphene oxide

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Abstract:

The production of graphene oxide by Hummers' method from the natural graphite powder has been confirmed by IRTE, AFM and ATG. Following an experimental protocol for the synthesis and preparation of the GO - Zn hybrid was carried out. The pyrrole was used as an intermediate agent which provides the link between graphene oxide and zinc oxide. The material obtained has been characterized through conventional investigative means such as Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM). The study made it possible to highlight that the important properties obtained by the oxidation of graphite give us the motivation to use it as a basic element for the preparation of different hybrids.



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Dielectric Relaxation study of ionic liquid-montmorillonite nanocomposite. Effect of anion.

Mohamed Belhocine

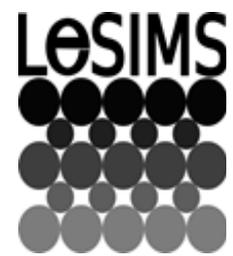
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Abstract: The aim of the present study is the effect of the anion on the electrical parameters in the case of montmorillonite intercalated with different ionic liquid. At first, the preparation of two new ionic liquids 3-methyl-1-(4-vinylbenzyl)-imidazol-3-ium sulfate and phosphate has been synthesis in the two-steps. For the first step, we change the previous synthetic route using 4-vinylbenzyl chloride as starting material, and with 1-methylimidazole to prepare the 3-methyl-1-(4-vinylbenzyl)-imidazol-3-ium chloride [VBMIM-Cl]. In the second stage, we have exchanged the anion Cl⁻ with HSO₄⁻ and H₂PO₄⁻. Our samples are characterized by ¹H NMR, ¹³C NMR and FT-IR. This clay montmorillonite has been intercalated by three ionic liquids [VBMIM-Cl], [VBMIM-HSO₄] and [VBMIM-H₂PO₄]. X-ray diffraction (XRD) shows an increase in the interlayer space for the modified montmorillonite comparing to the Na-Montmorillonite. In other hand, dielectric spectroscopy reveals that the choice of anion reacted with the ionic liquid has a very important effect on the electrical parameters (conductivity and permittivity).



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Study of the wear of alumina pellets developed for the optical glass grinding

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Institut d'optique et de mécanique de précision, university of Ferhat Abbas Sétif-1, Algeria

Abstract :

La technologie de rodage conventionnelle a été obtenue par un rodage abrasif lâche. Perte importante de temps et de grains dans l'utilisation de l'abrasif dans plusieurs applications [1-2]. Le procédé de finition abrasif délimité, connu sous le nom de broyage de granulés, est une technique qui permet le traitement de surface de composants optiques par l'élimination de défauts macro-géométriques et la préparation de surface pour l'étape de polissage. Plusieurs paramètres techniques peuvent influencer l'efficacité du fourrage et la qualité de surface obtenue [3], dans le cas de l'usure du grain abrasif formant les pastilles et les paramètres d'élaboration. Par conséquent, une étude de l'usure des grains abrasifs des pastilles et de l'influence des conditions de préparation sont nécessaires pour quantifier leur influence sur le processus de broyage. Dans cette étude, des granulés de broyage de grains abrasifs d'alumine ont été préparés avec différentes conditions. Après emploi des pastilles de broyage, les pastilles et leurs surfaces ont été étudiées. Plusieurs techniques de microscopie optique et de contrôle de surface ont été utilisées. Les résultats de la recherche sur les poudres abrasives subissent une faible usure pendant une phase de broyage. Les conditions de compactage et de compression peuvent provoquer une fracture des graines lors de l'élaboration des pastilles et affecter leur usure. Les résultats de la recherche sur les poudres abrasives subissent une faible usure pendant une phase de broyage. Les conditions de compactage et de compression peuvent provoquer une fracture des graines lors de l'élaboration des pastilles et affecter leur usure. Les résultats de la recherche sur les poudres abrasives subissent une faible usure pendant une phase de broyage. Les conditions de compactage et de compression peuvent provoquer une fracture des graines lors de l'élaboration des pastilles et affecter leur usure.



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Study and characterization of intercalated hydrothermal kaolinite

Naouel Hezil *University of Abbes Lghrou- Khenchela; Algeria*

Abstract:

This work aims in particular the characterization of a hydrothermal clay of eastern Algeria, intercalated by cationic surfactant (DTAC). The intercalation is intended to space the sheets (the interlayer space) of the material as far as possible and to widen the advantages of its basal distances, as well as to increase its hydrophobicity. The preliminary study of this material was made using several methods: X-ray diffraction characterization, scanning electron microscope analysis, ATG, ATD; chemical analysis and determination of specific surface area by BET analysis. The results obtained showed that this clay is of kaolinite type, and the surface area of natural kaolinite is $48,7\text{m}^2.\text{g}^{-1}$, The treatment of natural kaolin by the intercalation of cationic surfactant increased its specific surface of about 18 % ($63.72\text{m}^2.\text{g}^{-1}$). This characterization aims more particularly at the study of the structural and textural properties, which could allow an exploitation of this material in different fields of specific applications, given its availability and its great economic interest.



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The Estimation of the Hydrophobicity of Kaolinite by Adsorption of Surfactants

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Abstract:

The hydrophilic and hydrophobic components of the surface of the hydrothermal kaolinite has been characterized using adsorption of passively and negatively charged surfactants in aqueous solution. The hydrophilic and hydrophobic surface areas are inferred from the amount of probe molecule adsorbed and the structure of the adsorbed layer. The hydrophilic structure area of kaolinite is estimated from the adsorption of cationic surfactant: benzyl-demethyl-dodecyl-ammonium bromide (BDDAB). The adsorption of anionic surfactant; sodium dodecyl sulfate (SDS) onto kaolinite surface particles has been performed to assess their hydrophobic surface area. The area of the hydrophobic parts of kaolinite was found to be 37 m².g⁻¹. The sum of the hydrophilic (1.42 m².g⁻¹) and the hydrophobic surface gives 38.42 m².g⁻¹, a value which is only 21 % smaller than BET surface area (48,7m².g⁻¹).



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N-MWNT@MWNT Nanohybrid Synthesis using CCVD Technique

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Abstract: In this investigation, nitrogen-doped multi-wall carbon nanotubes “N-MWNTs” in nanohybrid new shape structural were prepared as a new catalyst support or new electrodes for energy storage using original way of partial doping focused on how to introduce the ammonium as nitrogen source during the CCVD doping process “partial doping mode”. Furthermore, the variations in this doping time were applied ranging from 30 min to 90 min of the total growth period depending to the doping mode (fixed to 120 min for in-situ and variable for out-situ mode reaching 180 min). A strong correlation between ammonia injection duration inside the growth and nitrogen concentration in the tube graphitic walls was observed between (0.15 at.% and 2.5 at.%) in form of outer waved walls with different coordination of carbon and/or oxygen as functional groups. These functionalized MWNTs were studied using High resolution TEM, FESEM, XPS, FTIR, BET, Thermal analysis and Raman spectroscopy in order to determine their structural characteristics, graphitization and crystallinity degree in quantitatively and qualitatively point of view. Consequently, we studied the effect of these partial N doping MWNTs as catalyst support on the deposited Pd nanoparticles size.

Keywords: Nanohybrid, Functionalization, N-Doped MWNTs, Nitrogen bonding, Catalysis, Environment.

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Design and analysis of a nano-photonic structure for different solid materials based on 2D photonic crystal ring resonator

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Abstract: In this work, we represent the study and design of a nano-photonic structure of a square array of two-dimensional photonic crystals. This structure is composed of dielectric rods immersed in the air. This study is based on the variation of the refractive index of three solid materials within an optical channel droplet filter (CDF) based on 2D photonic crystal ring resonator. We were able to obtain our numerical results with MATLAB and COMSOL software. These numerical results show the band diagram, the distribution of the refractive index and the mesh along the structure as well as the propagation of the electromagnetic wave at different refractive indices for Sodium aluminum hexafluoride (Na_3AlF_6), zirconium (ZrSiO_4) and Iodine (I_2) which have the following values: 1.338, 1.923 and 3.34 respectively. Knowing that, the refractive index of the rods (n), the radius of the rods (r) and the lattice constant (a) are three important parameters. In this work, we focus on the variation of the refractive index of the resonator core and we set the radius "r" of the rods at 205.625 nm and the lattice constant at 875 nm.



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Synthesis of bioceramic HAP from natural products

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Abstract:

In recent years, significant research effort has been devoted to developing powder of hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, HAP) because of its potential application in many interdisciplinary fields including chemistry, biology and medicine. The prepared hydroxyapatite, due to its identical structure of the natural bone, has good compatibility with the human organism, and is widely used in medical applications as an implant or as a coating on prosthesis. Currently, implantable phosphocalcic ceramics available on the market, such as stoichiometric phosphocalcic hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, is the main mineral constituent to human bones and teeth, the major departures in composition being a variable Ca/P mol ratio is 1.67. HA is not only a biocompatible, non-toxic, nonimmunogenic agent, non-inflammatory, but also bioactive. In this present work, we have synthesized the powder by chemical means by reacting the calcium hydroxide $[\text{Ca}(\text{OH})_2]$ with Phosphoric acid $[\text{H}_3\text{PO}_4]$. The physical parameters studied are granulometry, density, porosity and morphology of the phases obtained as well as the evolution of the microstructures with the change in the size of the grains and their appearance. The techniques used for the characterization of the synthesized powder are laser granulometry, XRD diffraction, IR infrared spectrometry, ATD analysis, ATG analysis and SEM scanning electron microscope.



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Formation of metastable solid solution in Al-C system using Mechanical alloying

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Abstract:

Synthesis alloys starting from elements with different density and undesirable interfacial reaction leads to be difficult using conventional technique. Where mechanical alloying technique resolve this limitation by an interesting advantage, which is the ability to synthesize supersaturated solid solution from immiscible elements at ambient temperature [1,2]. In the equilibrium processing methods, the system Al-C does not show any solid solubility, which means that carbon, is not soluble in aluminium [3]. In this work, an investigation of mechanical alloying (MA) on system Al-C was presented to force the dissolution. Using different techniques such as X-ray diffraction and scanning electron microscopy (SEM), it was proved that there were forcing of dissolution of carbon into aluminum by studying the specters for different milling time and by flowing the evolution during annealing in a differential scanning calorimeter, Furthermore, morphology of phases has been studied during milling time.



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The role of seed layer thickness on ZnO nanowires deposited by electrochemical method

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Abstract: Zinc oxide (ZnO) is a very important semiconductor with a direct wide band gap of (~ 3.37 eV) and large exciton binding energy (60 meV) at room temperature [1], ZnO has a wide range of structural morphologies of such as nanobelts, nanorods [2,3] and nanowires[4]. Due to its important characteristics, ZnO is an ideal material for various applications in future electronic and photonic devices, such as solar cells, light emitting diodes and photoconductive sensors [5]. In this study, we reported the growth of ZnO nanowires directly on (ITO) coated glass substrates by electrodeposition route from aqueous solution under different thicknesses of ZnO seed layer ranging from 0 nm to 150 nm. The variation of the electrochemical, structural and optical properties of the ZnO nanowires grown at different thicknesses of ZnO seed layer were investigated. The Mott-Schottky analysis demonstrate an n-type semiconductor character for all the samples with a carrier density varied between $4,27 \times 10^{-20}$ and $9,27 \times 10^{-20}$ cm⁻³ when the thickness of ZnO seed layer increases. From the electrochemical impedance spectroscopy (EIS), a low charge transfer resistance (R_{ct}) of 100,44 Ω was obtained. The XRD patterns indicated that ZnO nanowires crystallize in a hexagonal Würtzite structure along (002) crystallographic plane with a preferential orientation along c-axis and an average crystallite size ranging from 95.816 to 97.23 nm when the ZnO seed layer thickness increases. UV-Vis spectra showed a significant optical transmission (up to 70%), which increased with ZnO seed layer thickness. The energy band gap values (E_g) have been estimated to be between 3.3 and 3.13 eV.

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Annealing of pigmented low density polyethylene with titanium dioxide nanoparticles and its Influence on mechanical and thermal Properties

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Abstract: In the recent years, composites using nanoparticles (nanocomposites) have gained much attention and been intensively investigated owing to their remarkable enhanced properties including mechanical, optical, thermal properties and their wide spread, potential applications [1]. Different inorganic nanoparticles have been used to improve polymer properties, such as titanium dioxide (TiO₂), silicon dioxide (SiO₂) and aluminum trioxide (Al₂O₃). Polymer-based TiO₂ composites have been extensively studied in the literature in order to improve mechanical and thermal properties of the polymer [2]. In this work, effect of annealing process on the mechanical and thermal properties of pigmented Low density polyethylene with titanium dioxide nanoparticles was investigated. It shows that at lower annealing temperatures, the improvement of can be well correlated to the increased crystallinity induced by lamellar rearrangement for Low density polyethylene. By using differential scanning calorimetry (DSC) techniques we show that two kinds of endotherms arise in low density polyethylene (LDPE) pigmented with titanium dioxide nanoparticles annealed for two different annealing temperatures 60 and 110 °C respectively. Of particular importance is the endotherm II, which reflects the melting of the crystallites generated at the annealing temperature by the partial melting/recrystallization mechanism.

Keywords: Recrystallization / Annealing / pigmented LDPE / Titanium dioxide/ Mechanical properties/ DSC.

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Isosteric heat of water adsorption and desorption in homoionic alkali montmorillonites.

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Abstract: The aim of the present work is to study by means of thermodynamic measurements, i.e. isotherms of adsorption and desorption of water, and Infrared (IR) spectroscopy, the effect of the interlayer cations on the mechanism of adsorption-desorption of water in the case of a montmorillonite exchanged with alkali metals. The raw material is subjected to a purification treatment by using the sedimentation followed by cationic exchange. XRD at the dry state confirms that the treatment does not deteriorate the clay structure. The adsorption and desorption isotherms measured at various temperatures show that the nature of the interlayer, i.e. exchangeable, cation changes the adsorbed/desorbed amount of water molecules for a given water relative pressure. The total amount of water adsorbed in the higher water pressure domain as well as the net isosteric heat of adsorption calculated from the Clausius–Clapeyron method follows the cation sequence $\text{Li} > \text{Na} > \text{Rb} > \text{K}$. However the net isosteric heat of desorption follows a slightly different sequence $\text{Li} > \text{Na} > \text{K} > \text{Rb}$ and in agreement with the Hofmeister series. This discrepancy between the adsorption and desorption heat is due to the higher irreversibility of the K exchanged montmorillonite. The IR spectra recorded at room temperature and under a primary vacuum reveal, after normalization that the amounts of adsorbed water follow the same sequence as that of the heat of adsorption. They also reveal predominant confined contribution of ice-like water and liquid-like water.



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Crystallization kinetics of α -cordierite ceramic from MgO–Al₂O₃–SiO₂–TiO₂ glasses using DTA analysis

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Abstract:

The results of studies of crystallization kinetics of α -cordierite ceramics from MgO–Al₂O₃–SiO₂–TiO₂ glasses that are obtained via melt cooling using Differential thermal analysis (DTA), Thermogravimetric analysis (TG), X-ray diffraction (XRD) and scanning electron microscopy (SEM) are presented. DTA experiments were carried out on samples between room temperature and 1400 °C under argon gas flowing at a rate of 40 cm³/min. Heating rates of 10, 20, 30, 40, and 50 °C/min were used in this investigation. X-ray diffraction was used to characterize the phase transformations of the sintered powders. The average activation energy values for α -cordierite formation, using DTA results was measured under both isothermal (Johnson–Mehl–Avrami (JMA) theory using Ligeró method) and non-isothermal (using Kissinger, Boswell, and Ozawa methods) treatments were found to be equal to 845 and 720 kJ mol⁻¹, respectively. The growth morphology parameters n (Avrami parameter) were found to be almost equal to 1.5, using non-isothermal treatments, and equal to 1.5 using isothermal (Ligeró method) and m (the numerical factor) was 1.5 obtained by Matusita et al. equation. The growth morphology parameters n and m are both approximated as 1.5, which is an indication of a three dimensional growth from a constant number of nuclei and resulting in a polyhedron -like morphology controlled by diffusion.



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Kinetic parameters of crystalline phase prepared in raw kaolin/20 MgO obtained via melt cooling

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Abstract:

The aim of this work was to synthesis via melt cooling crystalline phase (cordierite ceramics) from compositions containing two Algerian kaolinite from east Algeria (kaolin (DD1) rich in Al₂O₃ and kaolin (KT) rich in SiO₂) and synthetic magnesium oxide MgO with relative weight ratios of 54/26/20. The samples were characterized by means of the following techniques: thermogravimetry (TG), differential thermal analysis (DTA), X-ray diffraction and dilatometry in order to analyze sintering behavior, identify phase transformations, and determine kinetic parameters. The average activation energy for cordierite formation determined using non-isothermal DTA (using Kissinger, Boswell, and Ozawa methods) was 717 kJ mol⁻¹. The value of coefficient of linear thermal expansion was close to 2×10⁻⁶ K⁻¹ for the temperature range from room temperature to 1000 °C. The kinetic parameters n and m had values close to 3. Bulk nucleation from a constant number of nuclei was the dominant mechanism in cordierite crystallization, indicating Three-dimensional growth and shows a polyhedron-like morphology controlled by interface reaction.

Keywords: Cordierite, Kinetic parameters, Avrami parameter, Activation energy.



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Effect of calcination temperature on wear resistance of nanosized alumina alpha for biomedical applications

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Abstract: Friction and wear problems in the prosthesis for substitution of hip joints have been widely studied [1–6]. The choice of the materials for the total hip prosthesis takes a many properties in consideration such as mechanical resistance, tribological proprieties [2-4]. Ceramics can be given a very high, scratch-resistant, low friction coefficient and high wear resistance. [3-8]. Many studies were investigated friction and wear resistance of hip prostheses [16-21]. Nanocrystalline ceramics are extensively being studied with the aim of improving their mechanical properties by reducing grain sizes [9] crack propagation resistance [3-10]. The structural evolution and tribological behavior of the nanostructured alumina Alpha (α -Al₂O₃) powder, formed by calcinations of gibbsite (Al₂(OH)₆) at different temperatures (100-1200 °C) were reported using X Ray diffraction, XPS, MEB and Type ball on Disk tribometer. XRD analysis indicates that the transformation sequence involves the formation of κ -Al₂O₃ as an intermediate phase between χ - and α -Al₂O₃. The crystallite size of treated alumina (α -Al₂O₃) is as small as 10 nm after calcinations at 1200°C. The sliding wear rate and wear coefficient of friction were lower in the nanocrystalline samples calcined at 1200 °C at same applied load (3, 6 or 10 N). The enhanced friction and wear resistance is endorsed to the finer microstructure, hardness of the sample calcined at 1200 °C



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Characterization of MgAl₂O₄ Spinel nano-powder

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Abstract: In the field of material sciences, nanostructured materials, and among them nanostructured ceramics, have grown considerably in recent years. Within a nanometric entity, the overall behavior of the material becomes increasingly important as grain size decreases. This confers on nano-materials properties potentially different from those of conventional materials. Spinel Mg Al₂O₄ is a technologically very attractive material. It has special properties such as: a high melting temperature (2135 °C), good thermal shock resistance, high mechanical strength (180 MPa), low thermal expansion coefficient and excellent chemical resistance. It presents very interesting optical properties, especially transparency, if it is sintered from pure nanopowder with in high density and nanometric grain size [1]. In this work, we have characterized three types of nano-powders spinel MgAl₂O₄. They are noted: S25 CRX 14, S25 CRX 12 and S30CR and are commercialized by Baikowski. We have used them to fabricate a transparent nanostructured ceramics by Spark Plasma Sintering (SPS). We have analyzed and characterized these powders by X-ray diffraction, XRF, FTIR and laser granulometry. The XRD spectra confirms that the commercial powders correspond to the spinel MgAl₂O₄. Chemical analysis by XRF shows that the S25 CRX 12 powder presents high purity chemical composition than S25 CRX 14 and S30 CR powders, which have low amounts of sulfur. In addition, the particle size analysis shows that the powders having a fine distribution with an average grain size of less than 1.4 μm.



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Microstructural and structural study of the ball-milled Ni₈₀Cr₂₀ alloy

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Abstract:

Nanostructured Ni₈₀-Cr₂₀ powder mixtures was prepared from elemental Ni and Cr using a high energy ball mill (Fritsh P7) under an argon atmosphere. Microstructural and structural properties were followed by X-ray diffraction . The structural evolution and phase transformation were investigated by X-ray diffraction (XRD) by means of Siemens D501 diffractometer in a ($\theta-2\theta$) Bragg Brentano geometry using Cu K α radiation ($\lambda = 0.154056$ nm). Microstructural and structural parameters (crystallite size, $\langle L \rangle$ root-mean square strain, $\langle \sigma^2 \rangle^{1/2}$, phases percentage, lattice parameters) were deduced from Rietveld refinement of the XRD patterns by using the MAUD program which is based on the Rietveld method combined with Fourier analysis and well adapted for broadened diffraction peaks. After 24 h of milling, the Rietveld refinement of X-ray diffraction pattern reveals the coexistence of disordered Cr(Ni) and Ni(Cr) solid solutions. The crystallite size reduction down the nanometer scale is accompanied by the introduction of internal strains. The mixing kinetics of the elemental powders can be described by an Avrami parameter.



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The Effects of Concentration, Size, and Orientation on the Hardness of Nanoparticles in material.

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Abstract:

The inclusion of nanoparticles in a material is a common strategy to improve mechanical properties such as Young's modulus or hardness. In most cases, the degree of improvement depends on the distribution and size of nanoparticles as well as the process condition. In order to investigate the effects of nanoparticles on the mechanical properties of a material, a nanoindentation finite element analysis is carried out. In this study, different concentration, size, and shape (spherical, elliptical) of nanoparticles were included in material and the mechanical property (hardness) is calculated based on a finite element analysis. The results indicate that for a given concentration, copper with larger but less in quantity spherical nanoparticles of carbon has higher hardness than that in smaller but more dense counterpart. Meanwhile, large concentration of nanoparticle leads to higher hardness due to more population of nanoparticles. The orientation of elliptical nanoparticle also affects the hardness which means for nonspherical nanoparticle, the orientation is another factor that influences the hardness. The hardness enhancement mechanism for concentration, size and orientation is interpreted by the residual stress as well as projection area for particle inclusion which can be extended to other kind of inclusion.



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Preparation and characterization of biodegradable polymeric microparticles loaded by metformine.

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Abstract: Nanotechnology today is applied in several fields and areas of sciences because of its significant benefits in terms of improving the performance in many fields including medical and dental. In medical field like pharmaceutical sciences, nanotechnology is utilized with the objectives of developing new nano-delivery systems [1]. The treatment of diabetes type 2 with metformine (a high hydrophilic drug) is not effective because of its low bioavailability requires high dose frequencies which is causing side effects [2]. These limitations require the development of new delivery systems to encapsulate metformine in biodegradable polymers such as polyesters. This work focuses on the preparation and characterization of polymeric microspheres based on poly lactic acid (PLA) loaded metformine. Double emulsion solvent evaporation was used for their preparation and several techniques were used for the characterization such as Scanning electron microscopy (SEM), DSC and XRD. From XRD and DSC analysis, amorphous state of metformine in PLA microparticles was observed due to the dispersion of the metformine in PLA matrix. The drug release was established in simulated gastric and intestinal medium (pH 1,2 and 6,8 respectively) at 37°C of temperature and the metformine concentration was analyzed using HPLC method . The results demonstrated that the encapsulation of metformine in PLA polymer provide a promising system for prolonged release of metformine.

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Effect of sintering temperature on tribological behaviour of β -type Ti-15Mo alloy

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Abstract: Titanium alloys are widely employed in the area of orthopaedics due to their superior corrosion resistance, biocompatibility, and high strength-to-weight ratio [1-4]. For this application, low Young modulus biomaterials are desired to diminish the stress shielding phenomenon that occurs at the bone-implant interface. Non-toxic β -stabilizers such as Mo, Sn, Ta, Nb, Zr, etc. are used as alloying elements to achieve new β -type titanium alloys with low elastic modulus [5] such as Ti-15Mo, Ti-11.5Mo-6Zr-2Fe, Ti-24Nb-4Zr-7.8Sn and Ti-36Nb-2Ta-3Zr [6]. In the present research, the Hot Isostatically Pressed (HiPed) Binary titanium alloy (Ti-15Mo) samples are prepared by subjecting them to different sintering temperatures ranging from 800 to 1100 °C, The morphological changes and structural evolution were investigated. Wear tests were conducted using a ball-on-plate type Oscillating tribometer, under different applied loads of 2, 8, and 16 N respectively. The morphological characterization indicated that the mean pore, and crystallite size continuously decreases with increasing sintering temperature to reach the lowest value of 4 and 29 nm at 1100 °C, respectively. The relative density of the 1100 °C sintered sample is as high as 97.0 %. Moreover, the higher sintering temperatures lead to the higher relative density and the greater hardness and young modulus of the sample. Both the friction coefficient and wear rate were lower in the samples sintered at 1100 °C This improvement in friction and wear resistance is attributed to the grain refinement and closed porosity. The Ti-15Mo sintered at 1100°C showed good tribological performance under all test conditions.



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The effect of molybdenum content on structural, mechanical and tribological properties of HIPed β - type titanium alloys for orthopedic applications

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Abstract: Orthopedic implants are being increasingly used to replace or repair damaged bone tissue [1]. Ti-alloys are commonly used as an ideal biomaterial in medical devices such as dental, and orthopedic applications due to their enhanced biocompatibility, high corrosion resistance, high strength-to-weight ratio, low density, and superior mechanical properties [2 – 4]. Aiming to develop alloys with good properties for orthopedic applications, the focus of the present research is to evaluate the effect of Mo at.% content on structural, mechanical and tribological properties of hot isostatically pressed β - type Ti-XMo (X = 0, 4, 12, 16, 20 at.%) alloys. The structural evolution, mechanical properties and tribological behavior of the nanostructured Ti-XMo alloys were evaluated using X-Ray diffraction, Scanning Electron microscope and ball on disk tribometer. The wear tests were carried out in accordance with the ASTM G 99, ASTM G 133–95 and ISO 7148-1:2012, standards under different applied loads of 2, 8 and 16 N respectively. Experimental results indicated that structural evolution and morphological changes of the milled alloys were sensitive to their molybdenum (Mo) content. The morphological characterization showed that the crystallite size and the particle size decrease with increasing Mo content (at. %) reaching the lowest values of 27 and 26 nm in the case of Ti-15Mo and Ti-20Mo, respectively. The coefficient of friction and wear rate were lower in the binary titanium alloys with 15 and 20 at. % Mo content. This improvement in wear and friction resistance is attributed to the closed porosity and grain refinement for binary Ti-alloys with 15 and 20 Mo.



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Effect of Kr-implantation on the nano-bubbles formation in SiO₂

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Abstract :

SiO₂/Si samples with thickness of 300 nm are implanted with Kr at 220 keV and with a dose of 5×10^{16} at/cm². The maximum concentration of Kr at ΔR_p is taken to be 6×10^{21} Kr/cm³ much less than the limit of solubility of Kr (6.03×10^{22} Kr/cm³). MET outcomes reveal the formation of nano-bubbles having diameters of about 13 nm along with a homogeneous distribution over a range of 220 nm. Such homogeneity is confirmed by RBS spectroscopy. IR spectroscopy shows that the implantation leads to breaking the so-called bridging bonds in Q³-type tetrahedrons and Q⁴ species. Furthermore, it is possible to quantify various effects of Kr implantation in silica and show that the most probable process during the implantation is governed by the reaction '. The presence of E' contributes strongly to the formation of nano-bubbles leading to the reduction of the silica permittivity from 4 down to 2.8.



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Effects of Halloysite Nanotubes on Physico-Mechanical Properties of Polyamide-11 Bionanocomposites

Nadjet Dehouche

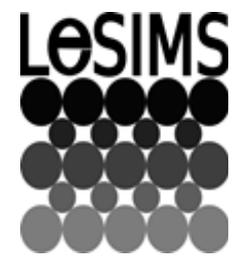
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Abstract: Halloysite nanotubes (HNT), which are a mineral clay, have recently attracted a great deal of interest in the field of nanocomposite materials due to their tubular structure with a lumen and peculiar properties [1] such as biocompatibility, good thermal stability and reinforcement. Despite these advantages, there are however, a few works reported on the use of HNT as filler in polyamides [2]. Therefore, the objective of the paper was to investigate the effects of HNT on morphology, thermal, viscoelastic and mechanical properties of polyamide 11(PA-11) bionanocomposites at filler content of 5 wt.%. The samples were prepared by melt compounding through twin screw extruder. HNT were mined directly from Djebel Debbagh deposit (eastern Algeria). The morphological results obtained by SEM and WAXD showed that HNT were homogeneously dispersed in PA-11 matrix, although the presence of small aggregates was observed. DSC data indicated that the presence of HNT in PA-11 enhanced the crystallization process of the bionanocomposite samples. Furthermore, Young's modulus and tensile strength were improved, in line with the increase of storage modulus evidenced by Dynamic Mechanical Analysis. Rheological curves of the nanocomposite samples exhibited a Newtonian behavior with increasing of shear storage modulus and complex viscosity compared with the neat PA-11. The resulted improvement in the physical properties of PA-11/HNT could be attributed to strong interactions between the mineral filler and the polymer matrix [2,3].



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Correlation between the structural and optical properties of KCl:CuO single crystal

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Abstract:

The aim of this work is the incorporation of nanocrystallites of CuO in the matrix host matrix KCl. In this case, we have used Czochralski (CZ) technic to elaborate a KCl: Chou (1 weight %) single crystal, the obtained crystal was cleaved parallel to the plan (100). The characterization by X ray diffraction proved the presence of Cu monoclinic phase, furthermore the considerable broad of peaks relative to the gets material (CuO) indicate that the crystalline of Chou have a nano regime size. As a complement analysis, the Raman spectrometer was used, where the vibration mode Cu-O (Ag, Bg1, Bg2) of monoclinic phase is present. In other side, the optical properties were investigated using UV-visible absorption measurements and photoluminescence (PL) the hole results indicate that the band gap of the KCl:CuO crystal is 434 nm (2.85 eV), and it shows a significant amount of blue-shift ($\Delta E_g = 1 \text{ eV}$) in the band gap energy of CuO, which is due to the quantum confinement effect exerted by the CuO nanocrystals. In addition, the PL spectrum of the KCl:CuO shows a broad emission band centered at around 438 nm, which is consistent with the absorption measurement.



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Effect of Nb at.% content on friction on tribological behaviour of nanobiomaterials Ti-Nb alloys .

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Abstract: Aiming to develop alloys with good properties for orthopedic applications, the focus of the present research is to evaluate the effect of Nb at.% content on structural, mechanical and tribological properties of hot isostatically pressed β - type Ti-XNb (X = 0, 4, 12, 16, 20 at.%) alloys. The structural evolution, mechanical properties and tribological behavior of the nanostructured Ti-XNb alloys were evaluated using X-Ray diffraction, Scanning Electron microscope and ball on disk tribometer. The wear tests were carried out in accordance with the ASTM G 99, ASTM G 133-95 and ISO 7148-1:2012, standards under different applied loads of 2, 8 and 16 N respectively.

Experimental results indicated that structural evolution and morphological changes of the milled alloys were sensitive to their Niobium (Nb) content. The morphological characterization showed that the crystallite size and the particle size decrease with increasing Nb content (at. %) reaching the lowest values of 28 and 30 nm in the case of Ti-15Nb and Ti-20Nb, respectively. The coefficient of friction and wear rate were lower in the binary titanium alloys with 15 and 20 at. % Nb content. This improvement in wear and friction resistance is attributed to the closed porosity and grain refinement for binary Ti- alloys with 15 and 20 Nb.

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Study of thermal and dielectric properties of LDPE/Al₂O₃ Nanocomposites

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Abstract:

Since the last ten years, the polymeric nanocomposites have gained rapidly increasing interest through combinations of desirable properties they exhibit. In this context the present study aims to study the effect of alumina on properties of nanocomposites LDPE / Al₂O₃. The filler was treated by dry co-mixing method and the various formulations were prepared by melt at various charge rates ranging from 0.5, 1 to 2%. Thermogravimetric analysis showed that the alumina has significantly improved the thermal stability of the composite by delaying the degradation. Measuring the electric conductivity shows that the electric conductivity increases with the content of alumina with an optimum at a charging rate of 1 %.



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Solid base catalysed 5-HMF oxidation to 2,5-FDCA over Au/hydrotalcites

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Abstract:

5-Hydroxymethylfurfural (HMF) is an organic compound derived in particular from sugars such as fructose and glucose. It consists of a furan heterocycle and has two functional groups, one aldehyde and the other alcoholic. The oxidation of 5-HMF is a very important reaction; it leads to the formation of many compounds considered as platform molecules with commercial and technical potential very interesting. Among these compounds, there is 2,5-furan dicarboxylic acid (FDCA), which results from the oxidation of the functions aldehyde and primary alcohol of 5-HMF in carboxylic acid functions. We have studied the oxidation of HMF in FDCA in liquid phase on catalysts based on gold nanoparticles supported on hydrotalcites of MgAl type, prepared by deposition-precipitation. Different Mg / Al ratios were used for the preparation of the support. After being assured of the support inactivity alone in the oxidation of HMF at 90 ° C, we studied the properties of the 2% Au / hydrotalcite catalysts. These catalysts allowed us to obtain excellent conversion and selectivity with better activity obtained on the hydrotalcite-supported gold catalyst prepared with an Mg / Al ratio of 2. The catalysts were characterized by DRX, BET and TGA.



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The synthesis and characterization of Mg-Al and Ce-Doped hydrotalcite – supported gold nanoparticles for catalytic applications

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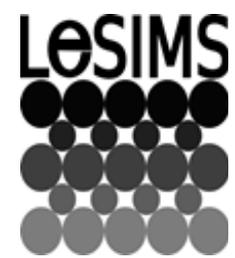
Abstract:

Efficient basic hydrotalcites (HTs) supported gold nanoparticles (AuNP) catalysts have been prepared and characterized by XRD, BET, TGA. The catalysts have been developed for the synthesis of imines from alcohol and amine, catalyzed under mild ($T=98^{\circ}\text{C}$) and soluble base-free conditions. The catalytic performance can be finetuned for this reaction by simple adjustment of the Mg/Al atomic ratio, and the doping of Ce metal to HT support. The synthesis of imines benefits from the high basicity of HT and greatly improves the imines selectivity (Mg/Al=1:2 and HT/Ce=13:10). These catalysts not only benefits the oxidation of the starting alcohol but also the subsequent steps of the reaction. A control of the composition and ratio of support has been shown to yield optimum selectivity.



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Study of a filter for refractive index sensing

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Abstract:

All-optical sensors have attracted much attention in biological/ medical research, chemical safety, and environmental monitoring. The optical sensors principle of operation relies on variations of optical characters when properties of the surrounding media change [1, 2], a key performance indicator of the sensors is the ability to detect the small change of refractive index (RI). For resonant sensors, this ability is expressed in terms of quality (Q) factor and sensitivity (S) [3]. In this work we propose a novel refractive index optical sensor based on 2D photonic crystal filter structure. Whereas, the refractive index sensing is realized by introducing a resonant cavity in the photonic crystal structure. In order to acquire the high sensitivity and transmission and increase quality factor of this sensor, the geometric structure is modified. We begin our consideration by the study of an optical filter that is initially based on two waveguides sections (W1) and one linear cavity. By the increase of holes number between the cavity and the waveguide structure, and changed the holes sizes that are located at the cavity ends and the position of the fourth adjacent cavity holes, we demonstrate that the quality factor and the transmission efficiency gradually evaluates. Then, we infiltrated the holes nearby the resonant cavity being functionalized. We vary the number of holes (N= 10, 16, 26, 34, 40 holes) to study the mass sensitivity ($\Delta\lambda/N$) of the device as a function of the number of functionalized holes. In our sensor design we determine that the functionalized hole number is N=26. After that we filled the functionalized holes with a change in refractive index from $n=1.33$ to 1.338 with an interval $\Delta n=0.002$. The sensitivity can achieve 300 nm/RIU. All analyses are based on the finite difference time domain method (FDTD).

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Preparation and characterisation of nanoparticles of modified Biopolymers

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Abstract:

Recently, much attention has been focused on polymeric composite materials filled with nano-sized particles called nanocomposites. Starch nanoparticles (SNPs) are considered one of the most promising polymers for fabrication of polymer nanocomposites and degradable materials, due to their wide availability, biodegradability, impressive mechanical properties, and low permeability. Starch is a natural, renewable, and biodegradable polymer produced by many plants as a source of stored energy. It is the second most abundant biomass material in nature. In the native state, starch is insoluble in cold water and consists of granules have microscopic sizes with diameters ranging from 0.1 to 200 μm . In the present work the modification is done by the introduction of hydrophobic groups on the surface of the biopolymer which gives it amphiphilic properties. Amphiphilic modification is an effective method of improving the hydrophobicity of starch and has been attracting more researchers' interest. Amphiphilic polymers have a wide variety of applications, particularly in emulsification, encapsulation, films and coatings, and gel production. Native and modified starch nanoparticles having particle sizes of about 500 nm have been synthesized.



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Characterization of poly (lactic acid) /polycarbonate blends and nanocomposites after the reactions transesterification with samarium acetylacetonate

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Abstract:

The main objective of this study is to compatibilize the blend of poly (lactic acid) (PLA) and polycarbonate (PC) to promote PLA performances, particularly thermal and mechanical properties. Due to the polyester structure of the two polymers, the reactive compatibilization method was employed by promoting the transesterification reactions after adding 0.25 and 0.5% of samarium acetylacetonate (Sm-Acac) used as a catalyst. Concentrations of 1, 3 and 5% of an organophilic montmorillonite (MMT) were also incorporated into the mixtures with different PC contents. The rheological and thermal characterizations of the blends based on 0.5% of Sm-Acac showed the formation of a random copolymer. The incorporation of the nanofiller contributed to a noticeable improvement of the PC dispersion into the PLA matrix and caused significant variations on the thermo-rheological properties and the thermal stability of the systems with and without Sm-Acac [1,2].



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Green synthesis of Ag-Cu alloy nanoparticles using *Rosmarinus officinalis* plant extract and its antibacterial activity.

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Bejaia University; Algeria

Abstract:

Nanoparticles have received considerable attention in recent years due to their wide range of applications in various fields. Biosynthetic methods have emerged as a simple and viable alternative to chemically synthesized. The easy availability and the protocol applicable at room temperature and pressure are the core advantages while using plant extract as the biogenic agents for the synthesis of metal nanoparticles [1, 2]. In this study, we synthesized silver-copper (Ag-Cu) alloy nanoparticles by green voice using *Rosmarinus officinalis* plant extract at room temperature. During the syntheses, the reaction mixture shows increase in potential and decrease in solution pH. The formation of nanoparticles was confirmed using scanning electron microscopy (SEM) coupled with EDX, Thermogravimetric analysis (TG) and, using X-ray diffraction. SEM shows spherical shape of nanoparticles was obtained, XRD pattern shows face cubic center structure and the crystallite size was found to be about 33 nm. The antibacterial activity of Ag-Cu alloy nanoparticles was studied against four bacteria strains (*Escherichia coli*, *Staphylococcus aureus*, *Enterococcus faecalis* and *Pseudomonas aeruginosa*) by disc diffusion method, the result showed high activity obtained with a diameter of inhibition zone of 28mm against *E. faecalis*.



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Relationship between zeta potential measurement and the aggregation of micro and nano materials.

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Abstract:

In an ionic solution, particles with a net charge will have a layer of ions (of opposite charge) strongly bound to their surface; this is referred to as the Stern layer. A second diffuse outer layer is comprised of loosely associated ions. These two layers are collectively called the electrical double layer. As the particle moves a distinction is created between ions in the diffuse layer that move with the particle and ions that remain with the bulk dispersant. The electrostatic potential at this “slipping plane” boundary is called the zeta potential and is related to the surface charge of the particle. In the present work we study the relationship between the zeta potential of solutions containing micro and Nano particles of (pure ceria, pure silica, mixed silica) and the formations of colloids, the tested materials have been chosen in the purpose to cover a wide variety of zeta potential values which provides us the opportunity to focus only on the effect of the particles surface charges, the technique of particles size analysing indicates if there is any changing in the particles size distribution which provides evidence of the formation of colloids and aggregates, the findings of this study suggest that particles with zeta potentials greater than +30 mV or less than -30 mV are considered strongly cationic and anionic, respectively, in other terms particles with high zeta values are considered stable and tends not to form colloids and aggregates



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Effects of the charge rate and of the accounting agent on the theological and thermal properties of composites based on the low density polyethylene matrix

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Abstract:

Low density polyethylene nanocomposites/organophilic polyethylene terephthalate/monmorillonite nanocomposites were prepared by melt blending using a photograph [1]. A functionalized polyethylene maleic anhydride (PE-g-MA) was used as a compatibilizer in order scanning calorimetry (DSC) and rheological measurements . The effect of the concentration of PE-g-MA and the operating conditions was examined. It is shown that DSC showed a slight variation in crystallinity with fiber content, and the addition of MMT0 and PE-g-MA. The theological measurements show that the kneading torque is mainly conditioned by the level of fiber added to the formulation. The melt index of composites decreases with fiber levels, organophilic monmorillonite and the addition of PE -g-MA compatibilizer.



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Elaboration and Characterization of Nanopowders and Thin films

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Abstract:

Perovskite and thin films nanostructures represent an interesting research area in materials science and have been developing steady in recent years due to the desire to create increasingly efficient materials. The hydrothermal method is an alternative synthesis process developed to prepare nanoparticles. It is a low temperature and high reacting rates method that permit to get powdered materials in short times with uniform microstructure. Due to short time and temperature reactions, this technique allows to control unwanted grain growth and the final particle size. A Perovskite calcium titanate (CaTiO_3) nanoparticle with average diameters ranging of (500-900) nm has been synthesized by hydrothermal treatment process. These powders were grown using calcium chloride dihydrate [$\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$], TiO_2 (Anatase), and NaOH] as raw materials in deionized water on quartz substrates. The resulting high purity CaTiO_3 powder were characterized by different techniques: Dektak surface Profilometer, X-ray diffraction (XRD), (SEM), energy-dispersive X-ray spectroscopy (EDXS), confocal microscopy, (UV/vis/NIR) spectrophotometer, (SE) spectroscopic. The objective of the present work is to prepare and demonstrate the characterization of CaTiO_3 nano powder and thin film by hydrothermal method using Autoclave, deposited it on different substrates. The aim also includes studying the composition, structural, surface morphology and the optical properties of the transparent films. The results show this structure as a good candidate for transparent oxides (TCOs) in Perovskite solar cells.

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Electrochemical Measurements of PANI Nanofibers

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Abstract:

Polyaniline (PANI) has been considered as an important conducting polymer material for supercapacitor electrodes because of its reasonably good conductivity, facile synthesis and environmental stability. In this investigation, facile and low cost free template hydrothermal precipitation method was used to synthesize PANI nanofibers. The nano-PANI structural and morphological properties were characterized by different techniques, such as: X-ray diffraction (XRD), Fourier transform infrared (FTIR), Raman spectroscopy and field emission scanning electron microscopy (FESEM). In addition, electrochemical measurements of these PANI nano-fibers were carried out using three electrode system in 6M KOH aqueous electrolyte. The electrochemical results depicted excellent electrochemical performance and exceptionally notable specific capacitance of about 1304 F/g at 5 mV/s.

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Free vibration analysis of carbon nanotube-reinforced composite plates resting on elastic foundation

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Abstract:

In this work we investigate dynamic behavior of carbon nanotube-reinforced composite (CNTRC) plates resting on the Pasternak elastic foundation including shear layer and Winkler springs. The plates are reinforced by single-walled carbon nanotubes with different distributions of uni-axially aligned reinforcement material. Exact solutions obtained from closed-form formulation based on higher order shear deformation plate theory. An accuracy of the present solutions is validated numerically by comparisons with some available results in the literature. Various significant parameters of carbon nanotube volume fraction, spring constant factors, plate thickness and aspect ratios, etc. are taken into investigation. According to the numerical results, it is revealed natural frequency increases as the increment of the factors for every type of plate.

FUNCTIONAL MATERIALS



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The form of the balancing coefficients of the surfaces mixture model for an ellipsoidal indenter

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Abstract:

In this article we chose to use an indenter having an ellipsoidal geometrical form, which, we used the model of the surfaces mixture, to separate the contributions of substrate and film on the composite covered material hardness. We have considered the coefficients a, b of the model as ratios of ecliptics surfaces. It represents the projections of the prints at the horizontal plans. We prove that the coating hardness present the contribution of the substrate and the film hardness. This work contained; firstly, a general mathematical concept about forms of the ellipsoid are highlighted, then, the expression of the Hardness of covered material is established. Secondly, expressions forms of balancing coefficients of the law of the surfaces mixture of the ellipsoid indenters are determined as a function of the depth or the diameter of imprint and indenters dimensions. Finally, the film hardness of coating material is expressed.



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Simulation of coated soda lime glass erosion

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Abstract: In the present work; we carried out a study about the erosion of the soda lime glass coated with a layer of the acrylic varnish. The results show that a maximum of the rate of erosion is recorded for the angle 25° . Which is typical in ductile materials. The comparison between the theoretical curves and the experimental curves, showed a dispersion due to the large number of parameters which included during the phenomenon of erosion. In the literature, and in spite of the complexity of the phenomenon of erosion, works ended in analytical models. The models of erosion are designed, first of all, by means of the calculation of the volume of material extracted during the impact of a single particle. The removed total volume is calculated by adding the volumes removed by all the particles. The obtained expression is generally a relation between the extracted volume and the various parameters of flow and the particles which are involved in the process. One or several empirical parameters stemming from experiments are generally introduced to correct the value calculated by the affected volume [1]. In this work, we used a theoretical model [2], to predict the rate of erosion of glasses taken on during the sanding. We notice that the maximal damage is observed in 25° for both curves. But he ya a difference in the value of the maximum of the rate of recorded erosion. It is obvious that mass loss increases according to the mass of the thrown particles, the dispersal between the theoretical and experimental curves can be due to parameters involvements during sanding (form and size of particles, speed of impact ...). During the process of erosion, the speed of the erosive particles plays an important role.



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Damage mechanisms under tension shear loading in friction stir spot welding of Aluminium alloy and Galvanized Steel

Mekri Hichem

Abstract:

This study investigates the fracture and damage of a single lap friction stir spot welding assembly formed from thin sheets of aluminum alloy 6061-T5 and galvanized steel. For fixed process parameters, two configurations are taken into account for the analysis of the global mechanical behaviour of the link. An experimental approach was carried out in order to analyse the sequence of damage mechanisms using acoustic emission and measurement of fields by digital image correlation techniques simultaneously [1]. The acoustic emission technique allows the monitoring of the evolution of acoustic activities. The digital image correlation technique confirms the damage scenarios after the treatment of strain field at any point near the fastener and especially between the exit hole and the shoulder footprint. The coupling of those two techniques allows identifying characteristic points and a breakdown of the load displacement curve in phases.



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The effects of boehmite addition on the reaction-sintering of hydroxyapatite and alumina composites

Samira Djouallah;

Université Ferhat Abbas Sétif-1

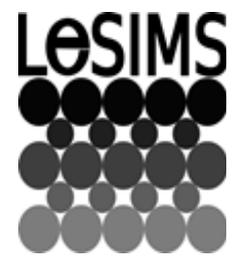
Abstract : In this work, the effects of boehmite addition on the reaction-sintering of hydroxyapatite and alumina composites were investigated. Hydroxyapatite (HAp) presents a very important bioceramics and has been widely applied as bone substitutes because of its excellent bioactive properties. However, the low mechanical properties of this bioceramics have been the main problem of the extensive use of this material. The addition of alumina, resulting from the boehmite transitions, to the hydroxyapatite has been carried out to improve the mechanical properties of sintered HAp. After ball-milling of seven compositions (0, 5, 10, 15, 20, 25 and 30 wt.% of Al₂O₃) for 5h, the reactions and phase transformations between hydroxyapatite and boehmite were studied using thermal techniques (DTA/TG), X-ray diffraction (XRD) and infrared spectroscopy (FT-IR). All samples were heated at different temperatures between 1000 and 1500°C for 2h and characterized by apparent density, open porosity measurements, XRD, FT-IR, micro-hardness and SEM analysis. The results showed the formation of different phases after high temperature. All mixture powders showed the formation of a number of alumina transitions through heat treatment. The mechanical properties of hydroxyapatite were enhanced by the addition of boehmite (alumina at high temperature). The mixture of hydroxyapatite and boehmite shows the partial decomposition of hydroxyapatite at high temperature.

Keywords: Hydroxyapatite; Bioceramics, Boehmite; Alumina transitions, composites.



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Buckling analyses of functionally graded material plate under mechanical loading

Benlahcene Fouad^{1,2}

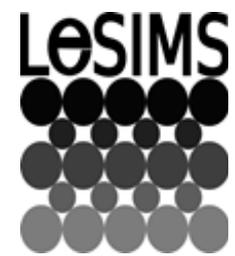
Abstract:

Functionally graded materials (FGM) have been designed and developed in many engineering parts that need to be super heat resistant, such as thermal barrier materials for text for this section, aerospace structural applications and fusion reactors. FGM material properties vary smoothly and continuously from one surface to the other. An analytical approach for mechanical stability analysis of functionally graded plate is presented. The equilibrium and stability equation are derived according to the first order shear deformation theory. These equations are solved for the functionally graded plate with variable thickness under different types of mechanical loading. The excellent accuracy of the present results with those available in the literature. Furthermore the effects of power of functionally graded material, parameter material, aspect ratio, loading types on the critical buckling load of the functionally graded rectangular plate are studied and discussed [1]. the realization of the plates in the different fields of use imposes a varied geometry the reason for which we are studying the varied thickness, even though thickness variation are rather rare in literature.



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Roughness influence on the adhesive power of optical glasses.

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Abstract:

The objective of this study is consisting with the measurement of the roughness of various optical materials by methods of diffusion. It is about an evaluation of the roughness of polished or rough surfaces according to the time of polishing of optical surfaces by the diffusion of the light by consideration of the hydrophobic or hydrophilic of the drop, deposited of various liquids on surfaces by measuring the contact angle via the technique of the drop sessile in order to determine the energy of surface and thus the adhesive power. The results showed the existence of a weak change in the optical properties of optical glasses. However, it was highlighted the great influence of the surface quality on the adhesive power at the time of the deposit of various liquids.



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Computational modelling of pipeline repaired with composite materials

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Abstract: With the invention of “manmade plastics” in the early 1900s, material science has rapidly advanced and is still racing forward with progress. These materials were quickly combined forming Fiber Reinforced Plastics or more generally, composites. Used primarily in aerospace and marine applications, composites have become an essential material in replacing traditional metals. Composites can be thinner and weigh less due to their high directional customization, unlike isometric metals. Eventually, composites matured to the point of being used as a quick and easy in-situ repair method for structural components. As composite repairs became more accepted in the piping industries, committees and standards arose to provide guidance for early composite designs. Due to the advancements in material sciences, composite materials have been used for the better part of the past 20 years to repair damaged piping and pressurized components in plants, refineries and pipelines. The use of composite materials has been accompanied by comprehensive research programs focused on the development and assessment of using composite technology for restoring the integrity to damaged piping and pressurized components. Of particular interest are composite repair standards such as ISO 24817 and ASME PCC-2 that provide technical guidance in how to properly design composite repair systems [1]. This work examine the mechanism using ABAQUS to create an accurate model of the material behavior to aid in the design before prototyping which is important because it not only decreases design costs but also the time to market release for the mechanism [2]. stress intensity factor is utilized as a fracture criterion for the investigation of a pipeline repaired with bonded composite wrap. The obtained results show that the presence of the bonded composite repair improve the residual lifespan of the pipeline.

key words : Composite materials, abaqus, pipeline, stress intensity factor

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Dynamic mechanical properties of Thermoplastic elastomers from blends of natural rubber /Polypropylene compatibilized by (ENR25 / PP-g-MA)

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Abstract: In this work we studied the compatibility of the blend based on Natural Rubber (NR) with Polypropylene (PP) to a proportion (70/30), the compatibilizing agent used is 25% of Epoxidized Natural Rubber (ENR25) with Maleic Anhydride grafted Polypropylene (PP-g-MA) at 2%, (ENR 25 / PP-g-MA) in various concentrations ranging from 5 to 15 Phr in a matrix based on NR / PP (70/30). The effect of compatibilizing agent on the Dynamic Mechanical Properties is investigated over a wide range of temperatures. The study of Dynamic Mechanical Properties allowed us to establish the following conclusions: The increase of the T_g transition temperature of the NR phase in the mixture NR / (ENR25 / PP-g-MA) / PP of 10 ° C., 9 ° C., 3 ° C at a concentration ranging from 5 to 15 Phr respectively and a disappearance of the β transition peak with respect to the NR/PP blend. This effect was attributed to the enhancement of the interaction that developed between the two polymers as a result of the compatibilizing agent (ENR 25 / PP-g-MA).

Keywords: Natural Rubber, Epoxidized Natural Rubber, Polypropylene, Maleic Anhydride Dynamic Mechanical Properties

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Mechanical characterization of thermoplastic elastomer blends based on natural rubber and low-density polyethylene

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Abstract: The tensile properties have been used to study to study the grafting effect of methyl acrylate (MA) on each compound of thermoplastic elastomer (TPE) based on natural rubber (NR) and low-density polyethylene (PE-LD). The blends were prepared via compounding of molten PE-LD-gr-MA with NR-gr-MA (30/70) in a Brabender plasticorder. Graft copolymers (PE-LD-gr-MA, NR-gr-MA) were prepared in solution using benzoyl peroxide as the initiator. The graft copolymers obtained after extraction of polymethyle acrylate (PMA) homopolymer with methanol for 24 h using a Soxhlet extractor were dried and then characterized by fourier-transform spectrometer (FTIR). The results of the modification of the blends showed an improvement of the tensile strength in (NR/ PE-LD-gr-MA) blends as well as the elongation at break in (NR-gr-MA/ NR) blends compared to the unmodified blend. Combination of both modifications of the polymers lead to medium properties of the TPE.

Keywords: natural rubber, low-density polyethylene, blend, methyl acrylate, mechanical properties

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Free vibration analysis of sandwich beams with viscoelastic core

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Abstract: In this work, we are interested in solving the problems of free vibrations of viscoelastic beams reinforced by composite layers whose Euler-Bernoulli theory is applied to sandwich composite faces and the Timoshenko theory at the viscoelastic core. The formulation of the equation of motion is realized by the virtual work method. The finite element method is used here to discretize the bending motion equation in order to obtain the eigenvalue problem corresponding to the linear vibrations of the composite beam with the viscoelastic material core. The difficulty of solving the eigenvalue problem due to the frequency dependence of the stiffness matrix leads us to use the numerical asymptotic method in order to obtain the damping modes and properties characterizing the viscoelastic sandwich beams. The results show the efficiency of our numerical algorithm under Matlab to solve the eigenvalues problem of sandwich beams with viscoelastic core. The results remain very acceptable for approximating the damping properties of different sandwiches with different laws of behavior. The optimal configurations for structures with viscoelastic materials are identified after studying the effects of their configuration parameters such as the viscoelastic loss factor, the fibres orientation of face layer and the thickness ratio on their damping properties.



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Reaction sintering of natural hydroxyapatite and aluminium slag

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Abstract:

Bio-ceramics based of Hydroxyapatite and tricalcium phosphate (a-TCP, b-TCP) are usually used as artificial implants in osseous substitution. These materials were imperatively used in biomedical since their composition is closer to that of the bone, as well as to properties of biocompatibility which make them particularly attractive. In this work, we prepared by reaction sintering different composites based of hydroxyapatite by using two different sources of hydroxyapatite such as: the natural phosphate from Djebelel-Onk (Tébessa, East of Algeria) and the bone bovine. Different experimental techniques, including density, porosity, DTA/TG, XRD and SEM techniques were used to analyze the formation and transformation of phases at different temperatures.



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Kinetic parameters of γ -Mg₁₇Al₁₂ phase dissolution from AZ91 alloy

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Abstract:

This study investigated the effect of aging on the precipitation and kinetics of dissolution of second phase Mg₁₇Al₁₂ in AZ91 magnesium alloy (Mg- 9 wt. % Al- 1 wt. % Zn), using X-ray diffraction, microhardness measurements and differential scanning calorimetric analysis (DSC). With the last instrument, the all samples were heated from room temperature to 400 °C, at heating rates of 10 to 30 °C/min. The results were supplemented by measuring the average of activation energies, using isothermal treatments by Johnson–Mehl–Avrami (JMA) methods and by non-isothermal treatments using Ozawa, Boswell, Kissinger, Augis and Bennett and Mahadevan methods were around 129,694 and 116.781 kJ/mol. the numerical factor m and the Avrami parameter n is estimated to be approximately equal to 1.211 and 1.152 respectively. This value corresponding that the bulk nucleation with varying number of nuclei was dominant in one-dimensional (needles) controlled by interface reaction.



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Activated carbon - polyurethane foam composite for oil spill cleanup

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Abstract:

This study aimed at synthesizing a new composite sorbent material using a polyurethane foam formulation. The prepared activated carbon/polyurethane foam composite is a novel and efficient sorbent combining an easy and low-cost manufacturing, a porous structure and a low resistance to filtration, and exhibits great potential in the field of aqueous phase adsorption and separation. A monolith foam was prepared having a macroporous structure and good mechanical properties and including powdered activated carbon in order to increase the capacity of sorption. The synthesized composite was used to remove crude oil which remains an environmental issue due to pollution by oil spill. The prepared material has enabled the recovery of 96% crude oil by absorption in the pores and can be partially regenerated by a compressive force [1]. This will allow the repeated use of this spongy material, which may be helpful for local economies.

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Effect of the Zircon and ZnO on the physical-chemical properties of opaque glazes for ceramic sanitary-ware

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Abstract: The effects of additions of Zircon and ZnO to traditional ceramic sanitary-ware glazes are examined. The glazes studies were prepared by traditional ceramic route and then thermally treated in an industrial tunnel kiln at temperature of 1250 °C. The crystalline phase, microstructural and morphological characteristics of the glazes were determined by X-ray diffraction, FTIR, Raman spectroscopy, Scanning Electron Microscopy (SEM) and thermal methods (DTA and TGA). The whiteness of the glazes obtained from instrument Micro color colorimeter data station. The flexural strength and Vickers microhardness were measured experimentally. Chemical durability of glazes in acid, basic and domestic aqueous solution media was investigated under laboratory conditions. The results showed that the Zircon was the main crystalline phases identified by X-ray diffraction, Raman spectroscopy and SEM investigations in the resulting glazes dissolved in the glassy matrix. On the basis of the results obtained, the optimal sample G5 with (15.75 wt. % Zircon and 1.25 wt. % ZnO) has a higher whiteness (up to 87 %), high flexural strength 55.06 MPa and high microhardness of Vickers 6.17 GPa. The chemical durability of the glazes is revealed to be acceptable for certain practical applications.

Keywords: Glaze; Ceramic sanitary-ware; Zircon; ZnO; Whiteness; Vickers Microhardness

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Bio-sourced composites made from Eucalyptus tannins

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Abstract: Increasingly high demand for composite materials is being recorded, creating a dilemma, especially for researchers. For some time now, a lot of work has been done on bio-sourced resins, derived from local plants such as eucalyptus in order to replace synthetic resins in the production of composites. Recently, there has been a growing interest in tannin resins for their low cost and also for their availability. Tannins are natural phenolic compounds, which have been extensively researched for the development of a wide range of industrial applications. In the first place the tannins are extracted (solid / liquid extraction) from the eucalyptus bark, optimization of the operating conditions proved necessary to determine the best extraction conditions giving the highest yields with the highest concentration in polyphenols (tannins), a complete characterization is carried out later (ATG, DSC, RAMAN, FTIR and DRX). Resins and foams based on phenol and furfuryl alcohol are synthesized with a progressive substitution of phenol (toxic product) by polyphenols (tannins) extracted from the eucalyptus bark, a 50/50 phenol / polyphenol substitution gave excellent results in terms of mechanical properties for the resins whereas for the foam we could have quite good properties desired with a ratio of 20/80, characterizations both chemical and mechanical (ATG, FTIR, RAMAN, DRX, study of the swelling rate, freezing time, friction test and TMA) are performed. Composite materials based on bio-sourced resins and foams are being developed to replace synthetic materials in different industrial sectors.



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Microstructural and mechanical properties of WC-Co alloy obtained by Sintering

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Abstract:

In this investigation, tungsten carbides alloy samples were prepared by mechanical alloying process and sintering technique. The binder used in this investigation is cobalt with different percentages. Several samples of standardized form are carried out by the technique of sintering at temperatures going up to 1420 °C. This experimental investigation revealed that the cobalt does not play only the part of insurer of the connection, the adherence of the grains of material, but it influences also considerably the microstructural, mechanical resistance, and the properties obtained from carbide like the flexural strength, hardness and density.



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Contribution to the improvement of the quality of continuous casting steels at Sider El-Hadjar - Annaba

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Abstract:

Continuous casting is the process between steel making and rolling. It consists of turning liquid steel into slabs, blooms, or billets. The molten steel comes into contact with the mold, it will solidify and the first phases of the steel will form.

This study confirms the need to check the quality of steel and the parameters of continuous casting such as; the casting speed, the extraction rate, the oscillation of the mold and the lubrication during primary cooling at the mold, the purpose of which is to produce a thermal model which is an important task allowing the prediction of the profiles of temperature on the different sides and edges of the product, in order to optimize the crust of the steel.



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FTIR, XRD and SEM investigations of phase evolution in mixtures of kaolin and aluminum

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Abstract:

In this study, we investigate mullite containing ceramics prepared from kaolin-aluminum mixtures. The kaolin was milled and then mixed with aluminum powder. The mixed powders were then activated by a high-energy ball milling at different times (1, 10, 20 and 40h). The measurements were performed on cylindrical samples sintered at temperatures ranging from 1100 to 1400 °C. In order to understand the mullitization process and structure formation a series of analyses were carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy. The results showed the formation of silicon and small amount of nacrite after 20h of milling at room temperature, the mullite phase can be formed at a temperature as low as 1300 °C, and The mixture of kaolin and aluminum milled for 40h show the formation of kyanite (Al_2SiO_5) at 1300 °C. The mechanical treatment enhances the formation and sintering of mullite.



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Synthesis, characterization of a metal organic framework: MIL-53 (Fe) and adsorption mechanisms of methylene blue dye onto MIL-53 (Fe) from aqueous solutions

Medjdoubi Zohra, Hamacha Rachida
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Abstract:

In this work, the metal organic frameworks MIL-53 (Fe), was synthesized and the adsorption interaction between this MOF and methylene blue (MB) in an aqueous solution was studied. The sample was characterized by XRD, IR, TGA, SEM, PZC, and BET methods. The effects of the parameters such as pH of solution, contact time, initial concentration, adsorbent dosage, and temperature on the adsorption capacity were investigated for the determination of the best fit adsorption kinetics, adsorption isotherm, and adsorption thermodynamics. It was found that the adsorption kinetics obeyed the pseudo-second-order kinetic model. The Langmuir and Freundlich adsorption isotherm models were also investigated. The results of the adsorption thermodynamics revealed that the adsorption of MB by selected MOF was a spontaneous and exothermic process. The MOFs structure leads to high adsorption capacities for MB.



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Numerical simulation for dielectric permittivity of a composite (Resin-Titanate-Carbon Black) in X band

Amina Bounar

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Abstract :

Recognizing the importance of an adequate characterization of the materials composites and consequently their development, the present study aims to contribute for the numerical determination of dielectric permittivity using a material composite made with Epoxy Resin (RE), Carbon Black (CB), and Magnesium Titanate (MT), this kind of composite is very solicited for applications and miniaturization of the components circuits (cavities, antennas, substrates, etc.) in hyperfrequency electronics. The dielectric parameters can be deduced from the scattering parameters by using electromagnetic three-dimensional simulation. For this, the technique used involves placing the samples in a microwave TEM-mode fixture and exciting the sample with an electromagnetic field. The boundaries of the materials under test are defined and afterwards the S parameters ($S_{21}(t)$ and $S_{11}(t)$) can be accurately known. By appropriately interpreting $S_{21}(t)$ and $S_{11}(t)$, one is able to determine the real and imaginary parts of ϵ as a function of frequency. We used the Nicolson-Ross-Weir mathematical model to retrieve the constitutional parameters (dielectric parameters).



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Characterization of cemented carbide containing 11% mass cobalt elaborated by hot isostatic pressing

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Abstract: Hot isostatic pressing (HIP) is known to be a process which permits to elaborate totally dense cemented carbide with perfect homogenous structure. It also offers the possibility to totally consolidate the powders mixtures WC-Co without reaching the fusion temperature of the binding cobalt. The HIP process was used in this work to produce three cemented carbide simples with 11% mass cobalt. The temperatures of treatment are 1350°C to 1400°C. The pressure of HIP cycle used is 1950 Bars.. The conditioning of powders mixtures of tungsten carbide and cobalt is realized in a titanium and mild steel containers. Within the context of this work we studied the reactivity of the material of the container with the components of mixtures of base powders densified by HIP. Observations by scanning electronic microscope revealed that the hipped sample obtained, is composed of a cobalt and tungsten carbide dispersed homogeneously. However, there is an inhomogenous distribution of both WC and Co phases at the interface steel container-compressed. Analysis by X-ray diffraction and energy dispersion reveals zones very rich in iron at the interface steel container-compressed. This results in the formation of mixed carbides FeW₃C, which generates an alteration of mechanical properties in zones close to the container. The transmission electron microscopy observations show that the WC-Co interfaces appear without any secondary phases and are parallel to the single crystallography planes of the WC lattice. On the other hand, the interfaces WC-WC appear in a form of a strong thin soldered joints of cobalt between a tungsten carbide grains. The densification by hot isostatic pressing induces a specific microstructure which is different of that observed in tungsten carbides elaborate by sintering. This change allows an improvement in the hardness of the products elaborated by the HIP process. It is noted that the improvement in mechanical properties is weakened by the use of steel container to encapsulate the powder mixtures of tungsten carbide and cobalt.



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Optical Transmission Improvement of Eroded Glass : Effects of the Projection's Speed and the Deposited Thin Layers of SiO₂.

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Abstract: To improve the surface state of eroded glass and restore its properties, a deposition of thin layers of metallic oxide basis (SiO₂) elaborated by sol-gel technique is conducted. The work is achieved in two stages: Firstly, samples of soda-lime glass are sandblasted with different projected sand masses M_p , varying the velocity V of the particles and maintaining the impact angle constant ($\alpha = 90^\circ$). The objective is to get different surface states. The second stage is devoted to the deposition of thin layers of SiO₂ on these eroded samples in order to repair the sandblasting defects and to improve the optical transmission (OT). The results show that after sandblasting, there is a strong increase of the roughness leading to an important falls of OT. At the raw state the OT is 91.5% at $\lambda = 550\text{nm}$. In the severe conditions tests of erosion ($M_p = 200\text{ g}$ and $V = 30\text{ m/s}$), the OT decreases to 56.45%. The deposition of silica layer basis colloidal SiO₂ nanoparticles by dip-coating permit to reduce the roughness of the sandblasted samples bringing a satisfactory improvement to OT. In the case of the speeds of 20 m/s and 25 m/s, the OT increases toward $89\% \pm 1\%$. In the case where $V = 30\text{ m/s}$, the deposition of two layers of silica allows to get a good correction of the greatly damaged surface state. The measures of OT show that the values know a better progression. Besides, the microscopic observations reveal a good restoration of the surface and confirm the brought improvements.



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Elaboration, optical and crystallographic structure studies of new organic-inorganic material

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Abstract: The materials design with new physical or chemical properties, in particular mechanical, electrical and optical are a major theme in materials science [1-4]. Nowadays, most of the hybrid materials that have already entered the market are elaborated and processed by using conventional soft based routes developed in the eighties. Organic-inorganic hybrid materials have been investigated for their interesting and important properties. The present organic-inorganic materials was elaborated by reaction of melamine with phosphoric acid. The crystal structure was determined by single-crystal X-ray diffraction, and it was characterized by UV-Vis, FT-IR, FT-Raman. X-ray single-crystal diffraction analysis revealed that the network is related by electrostatic interaction and hydrogen bonds, developing three-dimensional supramolecular structure. The TGA/DTA technique proves that the materials is stable over 250°C. The UV-Vis spectrum shows that the crystal has a good optical transmittance in the entire visible region with lower cutoff wavelength of 255 nm, offering to the material to be UV protector.

Keywords : hybrid materials, SXRD, Thermal stability, Ionic materials.

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The effect of mechanical activation on the reaction between natural phosphate and aluminum powder

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Abstract:

In order to fabricate cheaper porous hydroxyapatite we worked on the opportunity to use Algerian phosphate and aluminum metal powder. Hydroxyapatite (Hap) is a bioceramics due to its similar composition to bone substitutes because of its excellent bioactive properties which was used on widely applied [1] especially a very well-known in the medical field [2] However, the low mechanical properties of this material have been the major problem of the extensive use of this bioceramics. Aluminum metal powder was used to obtain reinforced hydroxyapatite composites materials with alumina. The alumina phases resulting from the oxidation of aluminum powder at high temperature. The powder mixtures were performed in a Fritsch planetary ball-mill (pulverisette 6). The reactions and phase transformations between hydroxyapatite and aluminum powder were studied using thermal techniques (DTA/TG), X-ray diffraction (XRD) and infrared spectroscopy (FT-IR). All samples were heated at different temperatures and characterized by apparent density, open porosity measurements, XRD and SEM analysis. The results showed the formation of different phases at room temperature. The mixture powder milled showed the formation of different phases during heat treatment. Porosity was shown to be increased with temperature increasing and controlled by the reaction between phosphate and aluminum metal powder.

Keywords: Hydroxyapatite; Bioceramics, Aluminium powder, thermal.



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The use of clay as a support for drugs in polymeric matrix

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Abstract :

Over the past few years, particular interest has been paid towards the fabrication of new Drug Delivery Systems (DDS) to specifically deliver the therapeutic agents to target sites [1, 2]. This technology offers great advantages over conventional DDS such as low toxicity, wide therapeutic window, minimized side effects, ideal drug efficacy and releasing drugs in a sustained rate [3]. Multifarious carrier systems can be formed with the help of montmorillonite (Mt) to deliver drug effectively. Controlled release of drugs from bio-composites made up of polymer and montmorillonite has been studied extensively since last few years. We choose in this work to speak about two bio-composites systems which are: Montmorillonite Ibuprofen/Carboxymethylcellulose noted: (MtIb/CMC) and montmorillonite Diclofenac/Carboxymethyl cellulose noted: (MtDS/CMC). We first intercalated the drugs onto Mt galleries and then added polymer in solution to obtain final systems. The new polymer/(clay-drug) bio-composites were characterized by FT-IR, XRD, DSC and TGA techniques. Both the XRD and differential scanning calorimetric (DSC) studies revealed that the intercalation of the drugs between the clay layers induced their amorphization . A study of the release of both drugs from the synthesized biocomposites in simulated intestinal fluid (pH 7.4) was investigated.



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Mechanical properties of Co-Ag coatings prepared by electrodeposition

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Abstract : Electrodeposited Co-Ag coatings are considered as suitable materials to use in magnetic sensors, storage devices and electrocatalysis because of their interesting properties such as giant magnetoresistance (GMR) effect, high corrosion resistance and remarkable electrocatalytic activity. In the present work, Co-Ag thin films have been prepared by potentiostatic deposition on Cu substrate from mixed sulphate chloride baths. Different molar ratios of electrolyte components Co/Ag were used in order to study the influence of bath composition on the micro hardness, roughness and the crystalline structure of the deposited films. The obtained films were characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), micro hardness and roughness measurements. The structural analysis of the Co-Ag thin films revealed the presence of FCC-Ag, HCP-Co and FCC-Co Bragg peaks. The morphological analysis of the deposits shows a uniform and compact surface. The increase of the Co/Ag molar ratio in the electrolytic bath improves both the microhardness and the roughness of the electrodeposited coatings, especially for the high values of the Co/Ag molar ratio (>8:1). This improvement is mainly related to the gradual incorporation of cobalt atoms into the deposited film and the decrease of the crystallite size.

Keywords: Co-Ag Thin Films, Electrodeposition, Structure, Microhardness, Roughness.

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Synthesis of new functional materials by a montmorillonite clay called Maghnite-H+ (Algerian MMT).

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Abstract :

A new green technique to synthesize functional materials biocompatible poly (ethylene glycol) dimethacrylates (PEGDM) is suggested based on use of chemically modified clay (Maghnite-H+) as heterogeneous, cost-effective, environmentally friendly catalyst for synthesis of poly(ethylene glycol)dimethacrylates (PEGDM) under gentle conditions. Poly (ethylene glycol)s of various molecular masses (M_n) 1000 to 8000 g/mol) were reacted with methacrylic anhydride to form PEGDMs. Maghnite clay, obtained from Tlemcen Algeria, was investigated to remove heavy metal ion from wastewater. Maghnite-H+ is an ion-exchanged montmorillonite prepared by treatment with sulfuric acid, which leads to increased interplanar spacing due to intercalation of acid protons between sheets, a crystalline change clearly seen in the X-ray diffraction (XRD) spectrum. The catalyst removed from the reaction mixture simply by filtration could be regenerated and reused. Combined analyses of infrared (IR) and 1H and ^{13}C nuclear magnetic resonance (NMR) confirmed the formation of prepolymers of high purity. The catalyst was characterized by X-ray diffraction and FTIR spectroscopy.



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Valorization of aluminum industry waste for use in grinding of optical glass

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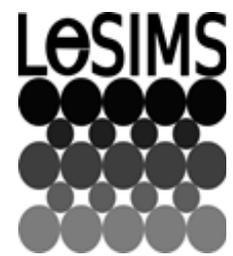
Abstract:

Recently, the recovery of industrial waste for sustainable development has attracted international attention. Aluminum production produces a significant amount of waste. In this perspective, several works have access to the recycling and re-using of this Industrial by-product [1] [2]. In the East of Algeria, ALGAL M'SILA, is the main industry for producing aluminium profile. During its transformation processing, there is a huge of aluminium slag production. That's why, we have suggested to valorize this industrial waste. The aim of this work is to extract the aluminium dioxide for this material and reuse it as abrasive grains. We have rinsed the waste for extraction the excess of salt. After that the samples were chemically et thermally treated from 1000°C to 1300°C. At the end of each treatment step a physic-chemical characterization was conducted. Then, the obtained powder was used for glass grinding. The obtained results, are very satisfying, we have found a decrease in the mass loss in the glass samples after the grinding process. We also noticed a clear decrease of the samples' surface roughness.



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Experimental analysis of Mechanical behavior in bending of composites sandwich structures Aluminum-Aramid Fibers.

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Abstract: Composite sandwich structures are a very good compromise between lightness, strength and rigidity. The mechanical performance of composite sandwich material depends on the mechanical properties of skins [1], those of the core [2], as well as the connection between the skins and the core. Today, sandwich structures are common in the aerospace, shipbuilding, railroad, civil engineering and many other industrial sectors. Several studies have been carried out on the use of Aramid Fiber [3] as a material constituting the core and continue on this material in order to control the bending behavior in specific environments and structural applications, the mechanical properties of composite sandwich structures can be severely impaired. Therefore, given the long-term use of sandwich materials as structural elements, research on bending behavior is of paramount importance. It is therefore imperative to know the behavior of these structures by bending, as well as the influence of the various defects (indentation, delamination, artificial notches) on the damage and the degradation of the materials sandwich structures [4]. The objective of this work is to study the mechanical behavior in 3-point bending in static and the damage of honeycomb composite sandwich structures. The purpose of the study is to determine: the essential mechanical characteristics (stiffness in bending, in shear, maximum stress in bending, the deformation arrow, etc.), the effect of the orientation of the cells of the core, the effect of the distance between support and the effect of the density of the core and reveal the different modes of damage resulting in the total degradation of the sandwich. Experimental tests in three-point bending were carried out on specimens for the different distances between supports (100,120, .. .400 mm) and density of the core (48, 80, 128 and 144 Kg / m³) and by varying the configuration of the cells of the core (L, W). The analysis of all the results showed that the sandwich composite Aluminum - Aramid fibers behaves like fragile materials. Microscopic observations of the tested specimens showed that the damage resulted in buckling followed by shearing of the walls of the sandwich cells, and a localized indentation in the level of the load application for all the distances between supports and for the L and W configurations of the sandwich core.

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Impacts of rich alumina clay added on the properties of a Tunisian kaolinitic clay in refractory silica-alumina bricks

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Abstract: Kaolinitic clay (A) from the Sidi Bader quarry (north-west Tunisia) was selected in order to be evaluated in silica-alumina refractories manufacturing, in the framework of a general prospection evaluating the suitability of some Tunisian clays. A rich alumina commercial clay (B) was added to the main mixture composed of the (A) clay in chamotte grog form, to improve its physical and pyroscopic aptitude. The chemical composition of the raw materials shows the relatively higher SiO₂ content (61.9 %) and the relatively lower Al₂O₃ content (23.6 %) of the (A) clay versus the (B) clay with (49.4 %) of SiO₂ and (33.4 %) of Al₂O₃. The mineralogical composition consists mainly of kaolinite associated with quartz, illite and anatase underline the possibility of the (A) clay to be valorized in low alumina fireclay refractory materials manufacturing (LF10 Group) according to the ISO 10081-1. The refractory specimens were sintered at 1350 °C for 2 hours, elaborated using two mixtures, Mixture M1 composed of (A) clay in chamotte grog and crude form and Mixture M2 composed of (A) clay in chamotte grog and a rich alumina clay (B) in crude form, were characterized by their bulk density, open porosity, linear shrinkage, compressive strength, scanning electron microscope (SEM) micrographs, XRD analysis and refractoriness under load. Specimens with (B) clay added are more resistible in terms of compressive strength (44 MPa) versus those without (B) Clay added (35.7MPa), whereas they exhibit approximately the same properties; bulk density (2.02 g/cm³), open porosity (18-19%) and linear shrinkage (2%). The mineralogical composition consists mainly on three major components: mullite, cristobalite and amorphous phases. The SEM micrographs show mullite particles, and a micro porous structure confirming the physical and mineralogical properties. All the obtained results are promising and comply with standards.



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Tribological behavior study of a hydroxyapatite deposit (HAP, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$) on a Ti-6Al-4V alloy substrate

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Abstract: This work aims at the tribological study of a hydroxyapatite deposit (HAP, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$) on a Ti-6Al-4V alloy substrate, HAP is used as a coating in the industry biomedical for several decades for dental and orthopedic implants. It appears to be the most suitable ceramic material for the construction of artificial bone tissue due to its excellent biocompatibility properties. Unfortunately, the mechanical characteristics of pure ceramics of hydroxyapatite are bad. Medical applications are limited to small implants not mechanically loaded. Titanium and its alloys are extensively used in implantation and are known as biomaterials of choice because of their excellent mechanical properties and their moduli of elasticity which makes them compatible with bone structures [1, 2, 3] Hydroxyapatite is used as a coating on titanium alloys to facilitate the grafting of the implant with the bone tissue because it represents the first mineral constituent of the bone [4]. In this work, test samples obtained by plasma projection were studied. After microstructural observation in optical and scanning microscopy, surface roughness and hardness were measured. A rotational wear test was used to measure the coefficient of friction μ and to quantify the loss of mass, which increases with the normal force applied. The hydroxyapatite coating exhibits better tribological behavior than the Ti-6-Al-4V alloy. Wear tracks analyzed by SEM show abrasive wear.

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Study of the effect of surface topography on the wear rate of a Co-Cr-W biomaterial developed by powder metallurgy

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Abstract: The manufacture of prosthetic implants by powder metallurgy allows the oste-integration of cells by promoting the presence of porosity, and thus, obtain new materials with better exploiting properties [1.2.3]. This work aims to study the effect of roughness on the wear rate of Cobalt-Chrome-Tungsten alloy-based biomaterials developed by powder metallurgy. After characterization of the samples by scanning electron microscopy (SEM), friction and wear tests with lubrication on the least porous series of samples were undertaken to determine their wear rates and friction coefficients according to their initial surface conditions. The analysis of the results obtained after sintering showed that porosity rates close to 4% were obtained, especially in alloys with high chemical heterogeneity. These results also showed that the evolution of the friction coefficient and the wear rate are dependent on several parameters such as hardness, surface topography and the third body



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Chemical finishing of optical materials

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Abstract :

With continuous development of optical technology, more and more optical components are used in complex system related to civil, military, space and other fields, so improving the ultra-precision grinding, lapping, and polishing are most critical factors. In this study, a comparison between chemical polishing by centrifugation (spin polishing) with the aid of HF based- solution and chemo-mechanical polishing (CMP) using acidic diamond slurry of two types of glasses (flint and crown) was investigated. Dissolution rate, roughness and optical transmission were analysed during this process, the results reveal that the process of chemical polishing by centrifugation is more effective than chemo-mechanical polishing (CMP) for its capacity to remove or reduce surface and subsurface defects (SSD); the results also show that the polishing time of the spin polishing technique is reduced. Implication of the results and future research directions are also presented in this work.



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Comparison study between K-geopolymer and (Na, K)-geopolymer based on calcined clay from Tamazert (north eastern Algerian)

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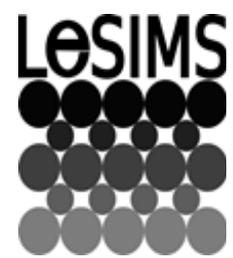
Abstract:

The term of geopolymer introduced in the 70s by the Professor Davidovits, defines a class of materials obtained by the reaction between aluminosilicate powder and an alkaline solution [1]. Basically, these materials were developed as alternatives to organic polymers. The first applications are therefore found in the field of shipbuilding, resins, protection of wooden structures, adhesives resistant to high temperatures, refractory [2]. Geopolymers are currently of considerable interest because of their good thermal [3], chemical [4] and mechanical properties [2] and their potential for use as a green cementitious binder. The geopolymer are based on the amorphous nature of these materials and the coordination numbers of silicon and aluminum. The aim of this work is the comparison between two geopolymers: K-geopolymer and (Na, K)-geopolymer based on calcined clay at 750°C from Tamazert (north eastern Algerian) activated with alkaline potassium silicate solution and mixed sodium and potassium silicate solution respectively and curing at 70°C. The results carried out by infrared spectroscopy during the K-geopolymer formation process shows the observation of the displacement of the band located at 980 cm⁻¹ which proves the reorganization of network and consequently the polymerization. It was demonstrated that mechanical properties by compressive strength of (Na,K)-geopolymer are higher than that recorded for K- geopolymer which are respectively 40 MPa and 16 MPa what allows their use in the field of construction.



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An economic process to fabricate resistant anorthite using kaolin and calcite: CaF₂ addition effect on sintering and mechanical properties

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Abstract: Anorthite (CaO·Al₂O₃·2SiO₂) was obtained by solid state reaction, using a modified milling system (MMS). Based on a preliminary work, the new selected composition was 80 and 20 wt% of kaolin (DD2 type) and CaO and containing different contents of CaF₂ (0, 0.5, 1.5 and 3 wt%). The sintering temperatures of mixtures were between 700 and 1000 °C. Optimizing the main parameters controlling anorthite production (MMS and CaF₂ additions) may lead to better anorthite materials. Subsequently, the obtained phases in the elaborated samples were investigated by X-ray diffraction, Raman spectroscopy and scanning electron microscopy analysis. A bulk density of about 2.70 g.cm⁻³ of the theoretical was reached for samples containing 0.5 wt% CaF₂ sintered at 800°C for 1 h. Excellent mechanical and properties: The three-point flexural strength (3PFS), Vickers micro hardness (VMH) and apparent porosity of samples containing 0.5 wt% CaF₂ sintered at 800°C were 260 MPa, 9.7 GPa and 3%, respectively.

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Improvement mechanical properties by exposure to hot isostatic pressing of α -Al₂O₃ ceramics at different times for total hip arthroplasty (THA)

Bouzid Hannachi

Abstract:

This study was focused on the experimental investigations about mechanical characteristics and tribo-logical mechanisms of nanometric alpha- alumina for biomedical application. A ball milling Al₂O₃ powder was carried out in order to produce nanostructured α -Al₂O₃, The structural evolution and mor-phological changes of powder particles during ball milling were studied by X-ray diffractometry and scanning electron microscopy analysis Furthermore the crystallite size of the sample decreased to 25 nm after ball milling for 24 h. Morphological studies of powder particles indicated that the powder particle size continuously decreases with increasing milling time. Hardness and elastic modulus values of pow-der particles were measured by nanoindentation method. A oscillating tribometer testing machine was used to test the friction and wear behavior, The sliding wear rate and wear coefficient of friction were lower in the nanocrystalline samples milled at 24h at same applied load. The finer microstructure of the sample milled for 24 h is believed to be responsible for improved wear resistance.



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Elaboration of a cellular glass

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Abstract:

Cell glass samples are elaborated from recovered glass from vehicles windshields and calcium carbonate. The aim is to promote them in the building sector as insulating materials and to contribute to the environment protection. The protocol adopted is as follows: the glass is first ground to a fine powder to a size less than 100 microns, then it is mixed with a variable content of calcium carbonate for 30 min in a kneader. The thermal cycle includes heating at high temperature (800, 850 and 900) ° C for 15 min, followed by cooling in the oven to room temperature. The results show that the best composition of thermal and sound insulation is obtained with the content 1% CaCO₃. The porosity level is of 90%.

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Functionalized Activated Carbon by Ionic Liquids, A Structure, Spectroscopic and Thermal study

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Abstract: During the last decade, the chemistry of ionic liquids has garnered spectacular interest from the scientific community. Currently, however, only a few of Algerian laboratories are working on these compounds, most of them using conventional methods. The present research work aims to determine and understanding the structural, spectroscopic and thermal properties of new functionalized activated carbon (FACILs) by ionic liquids (ILs), the structure of incorporated ionic liquids based on mono (IL) and dicationic (DILs) imidazolium cation and containing bromide, hexafluorophosphate, and bis[(trifluoromethyl)sulfonyl]imide as anions. Firstly; the obtained ionic liquids is characterized by ¹H-NMR, ¹³C-NMR, ¹⁹F, ³¹P-NMR and FT-IR spectroscopy. In order to confirm the insertion of these mono and dicationic ILs on the pore structure and surface chemistry of functionalized activated carbons (FACILs), their structures have been characterized using X-ray diffraction (XRD) analysis, the results indicate that the obtained functionalized activated carbons are disordered and leads to orientation of the crystalline planes. In the second stage and for a better understanding of their thermal proprieties, the subsequent decomposition and degradation process of produced activated carbons were investigated. Moreover, vibrational spectroscopy studies were conducted by infrared (IR), Raman (FT-Raman) spectroscopy. Hence, the mechanism of interaction between ionic liquids and activated carbon has been discussed in detail. These results seem to be promising regarding to the potential application of these modified materials as adsorbents or for the melt processing.

Keywords: ionic liquids functionalized activated carbons; vibrational spectra; thermal stability; XDR measurements.

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Porous and/or functionalized MCM-41 by DEHPA for solid phase extraction of lithium from chloride medium

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Abstract :

This study is a continuity of our research works on the water treatment by the recovery of pollutants, such as heavy metals, by nanoporous and/or functional materials [1-3], which can be used then for further applications in the industry. The synthesis of neutral mesostructured and/or impregnated MCM-41 by acid ligand (DEHPA) was realized. The so prepared solids were characterized by various physico-chemical techniques namely: X-rays diffraction, adsorption of nitrogen in 77°K and infrared spectroscopy. The quantity of the trapped ligand was determined by UV-VISIBLE analysis and calcination. These materials were used for the recovery of Li(I) by solid-liquid extraction method. Various factors were been studied namely: the pH, the kinetics of extraction and the capacity of retention of the metallic cation in solids, while maintaining constant the ionic strength of the aqueous solution. The metallic cation is extracted at acid pH values. The extraction yield was determined by spectrophotometric analysis.



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Disorder effect on optical properties of chiral structures, single crystal X-ray diffraction and DFT calculations

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Abstract : Two chiral molecular structures were synthesized via the base-catalyzed Pudovik chemical reaction [1]. with one hydrogen of the first structure is substituted by a para-methoxy in the second one. The Single crystal X-Ray Diffraction analyzes reveal that the structures crystallize into a same system with the same space group mono-clinic P24/n symmetry, with 3D chiral helical along Z axis, the difference caused by the adding of radical is an increasing of disorder and increase the filling rate of unit cell. In addition, those molecular structures retain its molecular chirality and even the chirality of crystal lattices, for it, the polarimetry measurement is used in the focus to measure and compare the rotating power of visible light polarization , the particular chirality of the two structures can found good applications in the optics. Moreover, The UV-Visible absorption spectrum shows that those materials exhibit a good optical transmission in the visible domain, and strong absorption in middle ultraviolet, this characteristic can offer to the materials a possibility to be UV protector on glasses. Finally, the comparison of physic-chemical and thermodynamic parameters such as ionization potential (I), electronegativity (A), hardness (s), softness (h), electronegativity (c) and electrophilicity index (u), are also carried out The using theoretical DFT (B3LYP method and 631G (p, d) basis sets) [2].



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Synthesis and Characterization of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ (CCTO) Powders and Ceramics by Solid State Reaction

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Abstract:

Recently, the perovskite-based oxide $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ (CCTO) has attracted much attention of researchers in scientific fields due to its exceptional dielectric properties, This ceramic is one of such the material that displays giant dielectric constant, (≈ 12000) at 1 kHz in the temperature range of 100 to 400 K [1, 2]. In this work we report the preparation of the ceramic of CCTO by the traditional solid-state reaction method [3]. Highly pure CaCO_3 , CuO and TiO_2 , as starting materials, were weighed out in stoichiometric proportions, ball-milled in alcohol for 9h, dried and then calcined at 1100C for 6h; the calcined powders were compacted at 520 MPa and then were sintered at various sintering temperatures. The crystalline structure of the calcined powder and of the sintered samples was characterized by X-ray diffraction (XRD). The morphology of the ceramics was observed using scanning electron microscopy (SEM). The relative bulk densities of the sintered pellets measured by the Archimedes method. The dielectric constant and loss were also studied in the medium-frequency range.



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Effect of glucose on electrochemical behavior of cobalt chromium alloy elaborated by powder metallurgy technique

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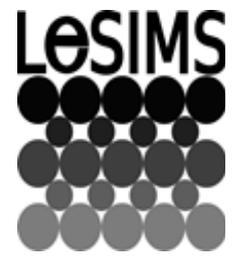
Abstract:

Cobalt-based alloys are widely used in biomedical applications. Various compositions of Co-Cr alloys were produced by powder metallurgy route. This study investigates the morphological aspect and electrochemical behavior of these Co-Cr alloys in comparison with a Fe-Cr-Co casting alloy. The application of this technique aims to have interesting mechanical properties, following the reduction of the elastic modulus in such a way to have a mechanical behavior similar to that of the bone, [1, 2, 3], and which allows a good distribution of the mechanical load between the two materials. Influence of Nickel and Tungsten has also been taken in consideration. The Co-Cr-Ni powder was mixed and compacted in the form of pellets using uniaxial press and then sintered in a vacuum furnace. The dispersive energy X-ray spectroscopy (EDS) test is used for elemental analysis of each sample. The obtained results showed that sample with Co₇₀Cr₂₀Ni₀W₁₀ composition presents the best densification and the best electrochemical behavior either in saline solution or in saline and glucosed solution.



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Study of heterogeneous joints welded by Friction stir spot welding case: Aluminum / Steel

Mekri Hichem Hichem

Abstract:

The present study is part of a Ph.D. thesis on Friction Stir Spot Welding (FSSW) heterogeneous spot welding of a bimetallic configuration of an aluminum alloy 6061-T5 (Al) and galvanized steel. The purpose of this investigation is to optimize the FSSW welding parameters for improving the mechanical properties of welded structures. Preliminary work targeted the determination of macrostructural and mechanical properties. At this level, the influence of the penetration distance and the speed of rotation was analyzed via monotonic tensile tests and micro-hardness. Thus, the morphology of welded joints was highlighted in order to better understand the material flow during the FSSW process of a multi material.



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Physicochemical properties of oak acorn starch physically modified by heat moisture treatment (HMT)

Mounira Boukhelkhal

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Abstract:

In this work, the effect of heat moisture treatment on the physicochemical properties of oak acorn starch has been studied. Heat moisture treatment was performed by microwave (HMT-Mw), hot air oven (HMT-Hao) and autoclave (HMT-Ac) with starch samples conditioned at 25% moisture (p / p). The solubility of the three modified starches increased, with values of 18, 20 and 34% for HMT-Ac, HMT-Hao and HMT-Mw respectively. The swelling power also increased for HMT-Hao and HMT-Mw about 16g/g, but it was lower for HMT-Ac (11g/g) than native starch. The amylose content of the modified starches HMT-Mw and HMT-Hao increased while that of HMT-Ac decreased. HMT modification of acorn starch causes a decrease in its intrinsic viscosity and molecular weight. In the FT-IR analysis, no effect was observed on the molecular composition (functional groups) after physical modification. X-ray diffraction study presents a B-type of acorn native starch which changed to A-type after heat moisture treatment by Mw, Ac and Hao. However, differences were observed in pics intensities and crystallinity was increased by HMT.



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Functional hybrid materials based on pillared clay/biopolymers: Synthesis, characterizations and environmental applications

Leila Chabane

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Abstract:

Functional hybrid materials derived from pillared clays are substances of increasing interest based on both structural characteristics and functional applications, including environmental uses. This study introduces a recent example of clays derivative useful as adsorbents for environmental applications such as the removal of dyes pollutants. Others materials considered here are related to the biopolymers: sodium alginate and polyvinyl alcohol. A major property of alginate is its ability of forming gel by cross-linking of alginate molecules in the presence of divalent cations. Polyvinyl alcohol is use as reinforcing agents in alginate chains to make the functional hybrid materials stiffer. Obtained functional hybrid materials were characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM). FTIR spectra confirmed that pillared clays particles were successfully incorporated into the sodium alginate gel. SEM images show a regular morphology with a porous surface of functional hybrid materials. The exam of X-ray diffractograms of different samples shows the presence of the interactions between the biopolymers with the hydroxyl groups of pillared clays. These interactions of hydrogen, electrostatic and / or intermolecular types favor the creation of numerous points of contact between the silicate chains and those of the biopolymers used. That confirms the results obtained by the SEM and FTIR methods. Functional hybrid materials were used as adsorbent of dyes from aqueous solution under different operating conditions. Adsorption study results indicate that adsorption on functional hybrid materials remains an efficient method for removing dyes from aqueous solutions with adsorption efficiency greater than 50 %.



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The effect of Sb_2O_3 content on the microstructure and electrical properties of $(\text{Mn}_2\text{O}_3, \text{V}_2\text{O}_3)/\text{ZnO}$ varistor materials

Kharchouche Façal

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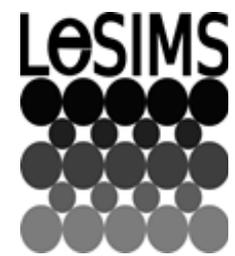
Abstract :

The microstructure and electrical properties of $\text{ZnO}-(\text{Mn}_2\text{O}_3, \text{V}_2\text{O}_3)$ -based varistor ceramics doped with Sb_2O_3 content sintered at 1000°C were investigated. The study deals with the 0 and 0.1 mol% Sb_2O_3 doped $\text{ZnO}-(\text{Mn}_2\text{O}_3, \text{V}_2\text{O}_3)$ Based varistor containing 0.5 mol% of V_2O_3 , 0.5mol% of Mn_2O_3 and 99mol% of ZnO has been manufactured by conventional ceramic procedure. Different, characterization technique such as X-ray diffraction (XRD), scanning electron microscopy (SEM) equipped with energy dispersive X-ray (EDX) have been used. Microstructure and electrical characteristic have been analyzed as a function of the Sb_2O_3 content and sintering temperature. Various oxides and, solide solutions such as Hexagonal $\text{Zn}_3(\text{VO}_4)_2$ and Sb_2ZnO_4 have been formed. The results from the experiments showed that the microstructure and electrical properties of the samples varied with the increase content of Sb_2O_3 . Optimal values for the electrical characteristics of the varistor ceramics were obtained when we increase content of Sb_2O_3 . Grain size, the dielectric constant and relative density, decrease when Sb_2O_3 content increases whereas, non-linearity coefficient, the dielectric loss and breakdown voltage increased with increase content of Sb_2O_3 .



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Synthesis and Structural characterization of tin Gadolinium Pyrochlore $Gd_{2-x}Sr_xSn_2O_7$ ($0 \leq x \leq 0.5$) solid-oxide fuel cells (SOFC)

Fatima Fati Melit

Université de Jijel; Algeria

Abstract :

Materials with the pyrochlore lattice structure have attracted much recent attention due to their wide applications in ceramic thermal barrier coatings , high-permittivity dielectrics, potential solid electrolytes in solid-oxide fuel cells , and immobilization hosts of actinides in nuclear waste Pyrochlores oxides are oxides of general formula $A_2B_2O_7$; the site A may be occupied by Na, Ca, Sr, Mn, La, etc.; site B can be occupied by Nb, Ta, Ti, Sn and O.. They are named after mineral pyrochlore (NaCa) (NbTa) OBF / (OH). The ideal $A_2B_2O_7$ pyrochlore structure is commonly described as a derivative of the fluorite structure where the scheduling of type A and B cations at two sites results in a doubling of the unit cell to about 10.5 Å. The oxide can be written $A_2B_2O_6O'$ with cubic coordination space group Fd-3m. The work described in this paper is devoted to the synthesis and characterization of a pyrochlore structure based on Gadolinium (Gd_2O_3) and tin (SnO_2) oxides of general formula $Gd_2Sn_2O_7$, substituted by Sr at the site Gd . Their structures were determined from X-ray powder diffraction using Rietveld analysis. All the compositions present the space group Fd-3m. The substitution of Gd by Sr in the $Gd_2Sn_2O_7$ compound causes a variation of the cell parameters.



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Study of the effect of surface topography on the wear rate of a Co-Cr-W biomaterial developed by powder metallurgy

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³ *Water and Environment Laboratory (LEE).université Hassiba Benbouali, Chlef.*

Abstract:

The manufacture of prosthetic implants by powder metallurgy allows the osto-integration of cells by promoting the presence of porosity, and thus, obtain new materials with better exploiting properties [1.2.3]. This work aims to study the effect of roughness on the wear rate of Cobalt-Chrome-Tungsten alloy-based biomaterials developed by powder metallurgy. After characterization of the samples by scanning electron microscopy (SEM), friction and wear tests with lubrication on the least porous series of samples were undertaken to determine their wear rates and friction coefficients according to their initial surface conditions. The analysis of the results obtained after sintering showed that porosity rates close to 4% were obtained, especially in alloys with high chemical heterogeneity. These results also showed that the evolution of the friction coefficient and the wear rate are dependent on several parameters such as hardness, surface topography and the third body



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Wave propagation investigation of thick P-FGM plates using A Novel four variables refined plate theory

Boukhari Ahmed

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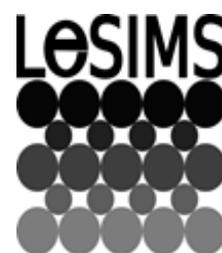
Abstract: An efficient shear deformation theory is developed for wave propagation analysis of an infinite functionally graded plate in the presence of thermal environments. By dividing the transverse displacement into bending and shear parts, the number of unknowns and governing equations of the present theory is reduced, and hence, makes it simple to use. The thermal effects and temperature-dependent material properties are both taken into account. The temperature field is assumed to be a uniform distribution over the plate surface and varied in the thickness direction only. Material properties are assumed to be temperature-dependent, and graded in the thickness direction according to a simple power law distribution in terms of the volume fractions of the constituents. The governing equations of the wave propagation in the functionally graded plate are derived by employing the Hamilton's principle and the physical neutral surface concept. There is no stretching–bending coupling effect in the neutral surface-based formulation, and consequently, the governing equations and boundary conditions of functionally graded plates based on neutral surface have the simple forms as those of isotropic plates. The analytic dispersion relation of the functionally graded plate is obtained by solving an eigenvalue problem. The effects of the volume fraction distributions and temperature on wave propagation of functionally graded plate are discussed in detail. It can be concluded that the present theory is not only accurate but also simple in predicting the wave propagation characteristics in the functionally graded plate. The results carried out can be used in the ultrasonic inspection techniques and structural health monitoring.

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Pressure effect on the structural, electronic and magnetic properties of the $\text{CoX}'\text{MnSi}$ ($X' = \text{Ru, Rh}$) Heusler alloys

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Abstract: The present work explores the structural, electronic and magnetic properties of the $\text{CoX}'\text{MnSi}$ ($X' = \text{Ru, Rh}$) Heusler alloys under pressure by using first-principles calculations in the framework of density functional theory. The exchange-correlation effect was treated through the generalized gradient approximation taking into account the two spin states. Geometric optimizations were carried out for pressures ranging between -8 GPa and 25 GPa. Calculated values of the equilibrium parameter a are in good agreement with the available theoretical findings. Calculated bulk modulus B values for the two studied materials were larger than 238 GPa, indicating that $\text{CoX}'\text{MnSi}$ compounds are resistant to volume changes. Electronic properties were investigated by computing the energy band dispersions and density of states diagrams. Analysis of the obtained results reveals that these two studied materials are half-metallic ferromagnets. Pressure effect results in a significant variation of the spin polarization. Calculated values of the magnetic moments of CoRuMnSi and CoRhMnSi are typically integers; $4 \mu_B$ and $5 \mu_B$, respectively, in agreement with Slater-Pauling rule. It is found that $\text{CoX}'\text{MnSi}$ half-ferromagnetism character can be maintained for pressures ranging between -8 GPa and 25 GPa, indicating their potential candidates for future spintronic applications.

Keywords: Heusler alloys, First-principles calculations, Electronic properties, magnetic properties.

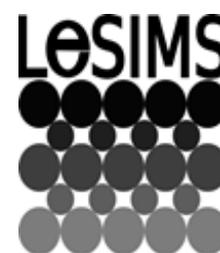
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Ab initio calculation of fundamental properties of $\text{Ca}_x\text{Mg}_{1-x}\text{A}$ (A = Se and Te) alloys in the rock-salt structure

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Abstract: We employed the density-functional perturbation theory (DFPT) within the generalized gradient approximation (GGA) and the virtual-crystal approximation (VCA) to study the effect of composition on the structure, stability, energy gaps, electron effective mass, born effective charge, optical and acoustical phonon frequencies and static and high dielectric constants of the rock-salt $\text{Ca}_x\text{Mg}_{1-x}\text{Se}$ and $\text{Ca}_x\text{Mg}_{1-x}\text{Te}$ alloys. The computed equilibrium lattice constant and bulk modulus show an important deviation from the linear concentration. From the Voigt-Reuss-Hill approximation, $\text{Ca}_x\text{Mg}_{1-x}\text{Se}$ and $\text{Ca}_x\text{Mg}_{1-x}\text{Te}$ present lower stiffness and lateral expansion. For Ca content ranging between 0.25-0.75, the elastic constants, energy gaps, electron effective mass and born effective charge are predictions. The elastic constants and computed phonon dispersion curves indicate that these alloys are mechanically stable.

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Structural, electronic and magnetic properties of $\text{Cr}_{x-1}\text{Ba}_x\text{P}$ alloy (with $x=0, 0.25, 0.5, 0.75, 1$)

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Abstract:

On the basis of ab-initio calculations we have investigated the electronic and magnetic properties of $\text{Cr}_{1-x}\text{Ba}_x\text{P}$ alloy, our calculations suggest that as we dope BaP with Cr atoms and move towards $\text{Cr}_{1-x}\text{Ba}_x\text{P}$ where $x=0, 0.125, 0.25, 0.50,$ and 0.75 all alloy are HM-FM. Interestingly $\text{Cr}_{0.25}\text{Ba}_{0.75}\text{P}$ is a HM-AFM otherwise ‘fully compensated ferrimagnet’, this alloy should be of special interest for applications since it creates no external stray field and thus exhibit minimal energy losses. In addition, the robustness of half-metallicity with respect to the variation of lattice constants of $\text{Cr}_{1-x}\text{Ba}_x\text{P}$ is also discussed; moreover ferrimagnetism co-exists with the half-metallicity, resulting in the desired fully compensated half-metallic ferrimagnetism, for a wide range of lattice constants. Furthermore we found that this new HMFCF is stable according to its small formation energy



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Structural stability and electronic properties of silver halides (Ag-VII) ternaries and superlattices

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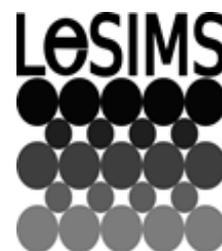
Abstract:

We have investigated the structural and electronic properties of AgCl and AgBr binary compounds, their ternaries $\text{AgCl}_x\text{Br}_{1-x}$ and superlattices $(\text{AgCl})_n/(\text{AgBr})_n$ for specific cases of $x=0.25, 0.5$ and 0.75 and $n=1, 2,$ and 3 by using first principles with full potential linear muffin-tin orbital (FP-LMTO) method, in the framework of the density functional theory (DFT) within the local density approximation (LDA). The ground-state properties are determined in the cubic phase Rocksalt and zinc-blend for comparison. Calculation of the electronic properties in the Rocksalt (B_1) phase shows that ternaries have a semiconductor behavior with an indirect band gap while the superlattices have a metallic behavior. In the Zinc-blend (B_3) phase, results show that our superlattices exhibit a semiconductor behavior with a direct gap for the three configurations mentioned above.



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Hydrogen Storage via Sodium Borohydride

Ghellab Torkia

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Abstract :

A comprehensive study of structure, phase stability and electronic properties of $NaBH_4$ light-metal hydrides is presented by carrying out first-principles calculations within density-functional theory using the full-potential linear augmented plane wave (*FP-LAPW*) method. The exchange–correlation potential is treated within the *LDA* [1] and *GGA* [2] to calculate the total energy, Furthermore, the Engel–Vosko (*EV-GGA*) [3] approach is employed to compute the electronic properties. The phases α , β and γ of $NaBH_4$ hydrides are investigated, the phase transition from β to high-pressure γ phase is determined for $NaBH_4$ compound and is accompanied by a 1% volume decrease. The materials under consideration are classified as wide band-gap compounds. From the analysis of the structures at different phases, it is deduced that the hydrides show strong covalent interaction between *B* and *H* in the $[BH_4]^-$ anions and ionic bonding character between $[BH_4]^-$ and Na^+ for $NaBH_4$.



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The electronic structure of the hydrides

Zoulikha Charifi

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Abstract :

The structural and electronic properties of the Hydrides have been studied using the full potential linearized augmented plane wave approach (FP-LAPW) based on the density functional theory (DFT). We employed the local density approximation (LDA) and generalized gradient approximation (GGA) for the exchange-correlation potential, however for the electronic properties we used mBJ approximation. The obtained results are in agreement with the available experimental and theoretical data. The study of the electronic structure of the compounds has been carried through the calculation of the band structure, total and partial electronic density of states diagrams. The calculation showed the existence of an energy gap for the hydrides under consideration with a considerable improvement for the band structure using the mBJ approximation comparatively to the GGA and LDA approximation. New copolymer involving poly (9-vinylcarbazole) and Poly(9,9-dioctylfluorene-alt-benzothiadiazole) (F8BT) for optoelectronic devices: Synthesis, characterization and modeling



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Optical and Nonlinear Optical Properties of $\text{Ln}(\text{Tp})_2$ where $\text{Ln} = \text{La}, \dots, \text{Lu}$, and $\text{Tp} = \text{tris (pyrazolyl) borate}$: a DFT+TD-DFT Study

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Département de Chimie, faculté des sciences, université Ferhat Abbas Setif1

Abstract:

The molecular structure of (where, $\text{Ln} = \text{La}$ to Lu rare earths, and $\text{Tp} = \text{ring-unsubstituted tris (pyrazolyl) borate}$) complexes, is determined by DFT calculations at B3LYP/CEP-121G and PBE/TZP levels. The first order hyperpolarizability ($\chi^{(1)}$) and related properties (a , a_0 and D_a) of the title compounds are calculated by using B3LYP/CEP-121G in gas phase. The effect of solvent on nonlinear optical (NLO) response has been studied using DFT-CPCM model. Time dependent density functional theory (TD-DFT) and Slater's transition state (TS) have also been used to calculate the optical absorption spectrum of the lanthanide complexes in gas phase. For the first time, our results demonstrate that the NLO activity enhancement is much more related to the direct contribution of $5d_x$ electrons, dipole moment and non-centrosymmetry of complexes to the first order hyperpolarizability than to the f orbital filling.



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Electronic and optical properties of the alkali metal tellurides: First principles study

Souadia Zohra

Abstract : In this work, we have systematically calculated the structural, electronic and optical properties of M_2Te compounds (M: Li, Na, K and Rb) using the full-potential linearized augmented plane wave (FP-LAPW) in the framework of density functional theory (DFT) as implemented in the WIEN2k code [1]. Exchange-correlation effect was modeled using the generalized gradient approximation (GGA-PBEsol) [2] and the Tran-Blaha modified Beck-Johnson potential (TB-mBJ) [3]. Calculated equilibrium lattice parameters are in very good agreement with the available experimental data. Analysis of the calculated band structures using TB-mBJ shows that the studied compounds are wide energy band gap semiconductors. It is found that the spin-orbit coupling reduces the band gap width. Frequency-dependence of the optical functions, including dielectric function, refractive index, extinction coefficient, absorption coefficient, reflectivity and energy loss function was explored. The critical points in the optical spectra are assigned to the interband transitions according to the calculated band structures.

Keywords: Alkali metal tellurides; First-principles calculations; Spin-Orbit coupling; Electronic structure; Optical functions.

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Structural and Thermodynamic properties of the Zintl phase $KAsn$, first principles investigation.

Abla Guechi

Institute of Optics and Precision Mechanics, Algeria

Abstract:

In recent decades, a large number of inorganic compounds have been synthesized and their study has given much information about structure-property relationships in the field of semiconductor cluster or Zintl compounds. The structures and properties associated with main group intermetallics found in the boundary region between metals and non-metals have generated interest within the solid state community. The term “Zintl phase” refers to a class of compounds and is used to recognize contributions to the field of solid-state inorganic chemistry by E. Zintl. Zintl phases were initially defined as a subgroup of intermetallic phases where the anions or anionic network could be considered formally to be valence satisfied. These compounds are made up of electropositive elements from groups 1 and 2 that, in a formal sense, donate their electrons to the electronegative elements from groups 13, 14, and 15, which use them to form the correct number of bonds such that each element has a filled shell. using the pseudopotential plane wave approach based on density functional theory (DFT) method within the generalized gradient approximation developed by Wu–Cohen (GGA-WC), the structural and thermodynamic properties of the Zintl phase $KAsn$ have been presented. The calculated lattice constants agree reasonably with the available experimental and other theoretical data. The effect of high pressure on the structural parameters has been shown. Through quasi-harmonic approximation in rang 0-20 GPa and 0-1000K, the thermal effect on the heat capacity C_v , free energy, and Debye temperature has been performed.



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Mechanical and thermodynamic properties of Zr-Fe: First Principle investigation

Farouk Mebtouche

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Abstract: In the core of Nuclear Power Plant (NPP) reactors, Zirconium alloys have been widely used as the fuel-rod cladding material. However, during nuclear power plant operation they suffer some important weaknesses which lately leads to minimize the ageing and the nuclear safety of the NPP. One the other hand, some alloys are required to achieve good mechanical and thermal properties of the Zirconium. These alloys are all alloying with a certain amount of Fe. Zr-Fe system has received much attention in the past decades, it has been examined the existing phase diagrams of Zr-Fe [1-2]. Lumley et al [3] has confirmed that Fe atoms occupy octahedral interstitial (O) sites and proven also that the formation energy for intermetallic phase of Zr₂Fe is metastable. The effect of Fe impurity on mechanical properties of the cladding material is remarkable, which can improve and achieve good mechanical properties in term of hardness and compressibility; the volume expansion and thermal expansion are obviously changed at height temperature. These variations are related to the iron impurity where it was put in the octahedral interstitial site of Zr Supercell (2x2x2).

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First principles study of the structural and dynamical properties of lithium vanadate.

Mohamed Khedidji

Université des sciences et de la technologie Houari Boumediene, Alger, Algeria.

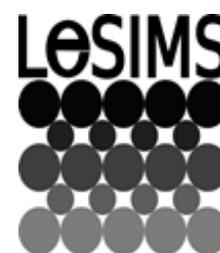
Abstract:

Due to the high mobility of Li^+ cations and the unidimensionnal character of its structure, LiVO_3 appears as an important ferroelectric material which has been studied intensively in the past years. It belongs to the recently discovered hyperferroelectrics [3], which are a new class of proper ferroelectrics with persistent polarization. This characteristic makes them extremely important to designing modern devices since, by forming interface with other functional materials such as semiconductors, strongly-correlated oxides, or multiferroics [2]. Here, we performed the first-principles simulations using the ABINIT software package [1], on hypothetical rhombohedral R3-c phase of LiVO_3 . The born effective charges, optical dielectric tensor and phonons frequencies are computed thanks to density functional perturbation theory (DFPT). The full relaxed structure is in good agreement with the experimental data. The calculated effective charges of Vanadium and Oxygen ions are anomalously large compared to their nominal values, similar to ABO_3 perovskite oxides. We found four unstable TO modes at center of the brillouin zone, which, after their condensation lead to more stable phases of low symmetry. Finely, we investigated the energy landscape around the R3-c paraelectric phase of LiVO_3 .



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MBJ-LDA calculations of electronics properties of nitride based III-V compounds

Belkacem Karima, Beldi Lilia, Bouhafs Bachir

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Abstract: The group-III nitride semiconductors represent a very unique material system with many outstanding features such as wide tunable band gap (6.2 eV for AlN, 3.4 eV for GaN, and 0.7 eV for InN)[1] [2] , high mechanical and thermal stability, and excellent electro-optical properties. The ground state electronic structure of wurtzite AlN, GaN, and InN has been calculated using full-relativistic all-electron full-potential linearized-augmented plane-wave method. Several DFT exchange-correlation functional[3], including the recently proposed a Modified Becke-Johnson generalised gradient approximation (MBJ-GGA)[4] have been used. In our current work, we focus on the role played by MBJ-GGA functional on the band structures and the density of states. We find that the MBJ-GGA improves the accuracy of the energy gap and the semi core d states levels. This new functional slightly outperforms both the local density approximation (LDA) and the generalized gradient approximation (GGA) overall as to energy gaps, and valence band widths. We find also that the MBJ-GGA induced modifications of the band structure are significant, but limited to the energy gaps, while leaving all other features identical to LDA and GGA calculations. Our theoretical results can be used to predict group III-nitride nanostructures.

Keywords: Density functional theory, Local density approximation, Generalized gradient approximation, MBJ, Electronic structure, Nitrides.

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Electronic and optical properties of the alkali metal tellurides: First principles study

Souadia Souadia, Bouhemadou Abdelmajid

Abstract: In this work, we have systematically calculated the structural, electronic and optical properties of M_2Te compounds (M: Li, Na, K and Rb) using the full-potential linearized augmented plane wave (FP-LAPW) in the framework of density functional theory (DFT) as implemented in the WIEN2k code [1]. Exchange-correlation effect was modeled using the generalized gradient approximation (GGA-PBEsol) [2] and the Tran-Blaha modified Becke-Johnson potential (TB-mBJ) [3]. Calculated equilibrium lattice parameters are in very good agreement with the available experimental data. Analysis of the calculated band structures using TB-mBJ shows that the studied compounds are wide energy band gap semiconductors. It is found that the spin-orbit coupling reduces the band gap width. Frequency-dependence of the optical functions, including dielectric function, refractive index, extinction coefficient, absorption coefficient, reflectivity and energy loss function was explored. The critical points in the optical spectra are assigned to the interband transitions according to the calculated band structures.

Keywords: Alkali metal tellurides; First-principles calculations; Spin-Orbit coupling; Electronic structure; Optical functions.

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Characterization of Nickel Based Metallic Superconducting Materials

Benmalem Yasmina

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Abstract: We report in this work, a theoretical study of electronic and transport (thermoelectric) properties of some superconductor nickel-based antiperovskite XNi_3 ($X =$, Zn, Ag) using first-principles calculations with the full-potential linearized augmented plane wave (FPLAPW)[1] method based on the density functional theory (DFT) as implemented in the WIEN2k[2] package. Electronic properties are calculated and show that the studied materials are of metallic type which is in good agreement with experimental data. The Seebeck coefficient, thermal conductivity, electrical conductivity[23-3] and figure of merit were reported. The results obtained show that the zinc (Zn) and silver (Ag) materials are characterized by a high value of the figure of merit [30-4]at room temperature (300 K) which is respectively 0.86 and 1.02 in a p-type region.. The electric conductivity values are almost invariant with the temperature except for the case of $AgNi_3$ compound in which it increases with T slightly. So, the superconducting materials based on silver and zinc are the best for the thermoelectric applications at room temperature due to the very important value of the factor of merit and the Seebeck coefficient obtained.

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Insight into Magnetic and Optoelectronic Properties of Sr₂CrYO₆ Double perovskite compound: Half-Metallic and Ferromagnetic Behavior

Haid Slimane Slimane;

Mostaganem University; Algeria

Abstract:

The effects of spin polarization on the structure, magnetic, and optoelectronic properties of Cr-based double perovskites Sr₂CrYO₆ has been studied by using the full-potential linearized augmented plane-wave method (FP-LAPW)[1], based on the density functional theory (DFT) as implemented in the Wien2k code[2], within the generalized gradient approximation (GGA), GGA + U, and GGA plus Trans-Blaha-modified Becke–Johnson (TB-mBJ) as the exchange correlation[3.4]. Our results show a half-metallic ferromagnetic ground state for this material. From the electronic properties, it is found that Sr₂CrYO₆ has a direct band gap at (Γ - Γ) direction. Furthermore, we have computed the optic properties which are investigated for the first time. Consequently, the magnetic, optoelectronic properties show these compounds are promising for high technological applications, namely spintronic materials.



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Synthesis, Nonlinear optics properties of new thin films of schiff bases ligands containing o-tolidine.

Samihha Arroudj

Université Abbas Laghrour Khenchla, Algeria

Abstract :

This paper explores the synthesis, structure characterization and nonlinear optics properties of new schiff bases. These compounds were obtained by condensation of o-tolidine with salicylaldehyde and cinnamaldehyde. The obtained ligands were characterized by UV, 1H and NMR. Their third order NLO properties were measured using the third harmonic generation technique on thin films at 1064 nm [1]. The electric dipole moment (μ), the polarizability (α) and the first hyperpolarizability (β) were calculated using the density functional B3LYP method with the lanl2dz basis set. For the results, the title compound shows nonzero β value revealing second order NLO behaviour.

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First principles simulation of properties of arsenic doped by transition metal atoms As_{10-n}Mn (n= 0-10, M= Mn, Ni) clusters.

Safer Sofiane

University of Bejaia, Algeria.

Abstract :

Cluster containing a few to thousand of atoms consist an intermediate form between individual atoms and bulk materials [1-2]. Over the past decades, the binary clusters have received considerable attention, as arsenic and transitions metal elements are important for industry and environment [3]. It is important to understand the physical and chemical properties of pure arsenic clusters and their interactions with transition metal elements [4]. In this work, we report the structures, electronic and magnetic properties of As_{10-n}Mn (n= 0-10, M= Mn and Ni) clusters. We have used the density functional theory (DFT) with generalized gradient approximation functional (GGA) and pseudo-potential implemented in the SIESTA program, to investigate All of this properties. We find that the binding energies increase with the increasing of Ni atoms in the As_{10-n}Ni clusters and they decrease when the number of Mn atoms increase in the As_{10-n}Mn clusters .This means that the Ni atoms enhance the stability of this atomic systems and the stability of each system depends on the number of atoms of the dominating species in the clusters. The HOMO-LUMO gaps gradually decrease with some local oscillations as the cluster size increases. This may indicate that the metallic characteristics of As_{10-n}Mn clusters are enhanced by the doping M (M= Mn and Ni) atom. The magnetic properties depend on the number and positions of M atoms. Indeed, we find that the magnetic moment increase quickly with the number of atoms in the system in the case of As_{10-n}Mn. In the case of As_{10-n}Ni, the total spin magnetic moment is not immediately influenced by the As caging. We have also examined the vertical electron affinity (VEA) and vertical ionization potential (VIP) for all As_{10-n}Mn (n= 0-10, M= Mn and Ni) clusters. We find that there VEA show a decreasing tendency with the increasing cluster size. It indicates that the clusters As_{10-n}Mn will need more energy to capture electrons. We have also observed that the VIP decreases slowly with the increasing of cluster size. This indicates that the different As_{10-n}Mn clusters tend to show a high metallic character which implies that these clusters can more easily lose one electron comparatively to the clusters of smaller size.



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Ab-initio investigation of the Pt-Sn binary system

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Abstract:

The aim of the present work, based on ab-initio calculations, is to investigate the relative stabilities of the different compounds involved in the (Pt-Sn) system. Having our calculations performed at 0K, We will be mainly focusing on the determination of the ground state line of this system. Our calculations were based on density functional theory (DFT) as implanted in the Vasp Code [1]. We used the projector augmented-wave (PAW) method, which is an all-electrons technique within the frozen core approximation. Only generalized-gradient approximation (GGA) was considered. A study of convergence has been done for the plane-wave cutoff energy and allowed us to fix the Ecut at 520eV. The formation enthalpies of the compounds were obtained through the following equation: $H_f(\text{Pt}_p\text{Sn}_q) = E_{\text{tot}}(\text{Pt}_p\text{Sn}_q) - (E_{\text{fcc}}(\text{Pt}) + q E_{\text{BCT}}(\text{Sn}))$, Where $H_f(\text{Pt}_p\text{Sn}_q)$ is the enthalpy of formation of the compound Pt_pSn_q , $E_{\text{tot}}(\text{Pt}_p\text{Sn}_q)$, $E_{\text{fcc}}(\text{Pt})$ and $E_{\text{BCT}}(\text{Sn})$ are the ground state total energies (per atom) of the compound Pt_pSn_q and its constituents Pt and Sn, respectively, in fcc and BCT structure.

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First-Principles Study of Structural, elastic and electronic properties of FeMP (M = Ti, Zr, Hf) compounds

Amel Tanto

Development of New Materials and Their Characteristics, University Ferhat Abbas of Setif 1, Algeria, Algeria.

Abstract:

First principles calculations are applied in the study of FeMP (M = Ti, Zr, Hf) compounds. We investigate the structural, elastic, mechanical and electronic properties by combining first-principles calculations with the CASTEP approach. For ideal polycrystalline FeMP (M = Ti, Zr, Hf) the shear modulus, Young's modulus, Poisson's ratio, elastic anisotropy indexes, Pugh's criterion, elastic wave velocities and Debye temperature are also calculated from the single crystal elastic constants. The shear anisotropic factors and anisotropy are obtained from the single crystal elastic constants. The Debye temperature is calculated from the average elastic wave velocity obtained from shear and bulk modulus as well as the integration of elastic wave velocities in different directions of the single crystal.



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Ab initio calculation of elastic properties of GaX (X = As, N, P and Sb) semiconducting Alloys.

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Abstract :

Elastic properties in general describes how well the system with stand deformation when exposed to an external force. The knowledge of the elastic properties is crucial for many applications. In this work, we present a study of the elastic properties of binary alloys: GaAs, GaN, GaP and GaSb. In our calculations we are using the Projector Augmented Wave (PAW) method within density functional theory (DFT). The exchange-correlation potential was treated using the generalized gradient correction (GGA). The elastic constants C_{ij} are predicted using the total energy variation versus strain technique. The polycrystalline elastic moduli, namely; shear modulus, Young's modulus, Poisson's ratio, sound velocities and Debye temperature are derived from the obtained single-crystal elastic constants. Ductility behaviour of these compounds is interpreted via the calculated elastic constants C_{ij} .



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DFT and TDDFT study of the structure and optical properties fluorene-based monomers

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Abstract :

Fluorene-based monomers have attracted significant attention due to the possibility of their applications in photovoltaic cells, electroluminescent displays, field effect transistors, plastic lasers, and optical sensors. Two novel monomers, 2,7-bis[(thien-2-yl)cyanovinyl]-9,9-dipentylfluorene (FPT) and 2,7-bis-[(2,3-dihydrothieno [3,4-b][1,4]dioxin-5-yl)cyanovinyl]-9,9-dipentylfluorene (FPE) are synthesized in Chemistry laboratory of Materials, University of Mentouri Brothers Constantine, Algeria. The properties such as optimized structural parameters, spectroscopic (FT-IR) of these two monomers were investigated experimentally as well theoretically using density functional theory calculations (DFT). The UV-visible spectra and excited state was calculated by B3LYP [1, 2] method of the TD-DFT [3] using 6-311G (d,p) basis set with GAUSSIAN 09 program. The experimental results were compared with theoretical results and fairly good agreement between experimental and theoretical results was obtained.



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Electron–phonon interaction in the binary supraconductor Lutetium carbide LuC_2 via first principle calculation

Souad Dirmi

University of M'sila, 28000 M'sila, Algeria

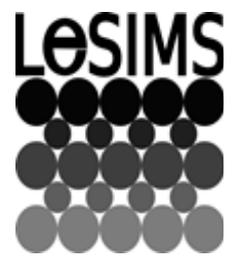
Abstract:

In this work, we have studied the Structural, electronic and superconducting properties of the intermetallic compound LuC_2 . All calculations were performed by the first-principles calculations using the plane wave pseudo potential (PP-PW) based on the density functional theory DFT and PDFT implemented in the QUANTUM ESPRESSO code, For the exchange correlation function we used the generalized gradient approximation GGA of Perdew–Burke–Ernzerhof (PBE). Our results are in agreement with the available experimental data. The obtained low value of electron phonon coupling parameter confirmed that LuC_2 is a weak coupling Bardeen-Copper-Schrieffer (BCS) superconductor.



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Structural and electronic properties of Lithium Niobate from ab initio calculations

Boukhtouta Moufida

Abstract :

The structural and electronic properties of lithium niobate (LiNbO_3) have been investigated using the full-potential linearized augmented plane wave scheme (FP-LAPW) [1]. in the generalized gradient approximation. By adopting the hexagonal unit cell for lithium niobate in its ferroelectric phase [2-3] and using the (PBE-GGA) as the exchange-correlation potential, the optimized equilibrium structural parameters (a and c) obtained are in good agreement with results found by other authors [4-7]. For the band structure and density of states, the calculated fundamental gap was found to be direct (Γ - Γ) of about 4.084 eV [8]. Unlike the mBJ approximation that has a remarkable influence on the energy of the gap, the spin-orbit coupling (SOC) has no great influence on this fundamental parameter.



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Electronic and optical properties of the LiZnX (X = P, As and Sb) filled-tetrahedral compounds

Allali Djamel

Faculty of Technology, University of Mohamed Boudiaf, 28000 M'sila, Algeria.

Abstract:

The structural, electronic and optical properties of the LiZnP, LiZnAs and LiZnSb filled-tetrahedral compounds were explored using the full-potential (Linearized) augmented plane-wave plus local orbitals method (FP-(L)APW+lo)). Calculated structural parameters, including the lattice constant (a), bulk modulus (B) and its pressure derivative (B'), for the considered compounds using both the local density (LDA) and generalized gradient approximations (GGA) are consistent with the available data in the scientific literature. As the density functional theory with the common LDA and GGA underestimates the band gap, we have used a newly developed functional that is able to accurately describe the electronic structure of semiconductors, namely the Tran–Blaha-modified Becke–Johnson potential. The three investigated compounds demonstrate semiconducting behavior with indirect band gap (Γ –X) ranging from about 1.41 to 1.90 eV. The charge-carrier effective masses were evaluated at the topmost valence band and at the bottommost conduction band. The evolution of the value and nature of the energy band gap under pressure effect was also investigated. Optical functions of the tile compounds, including the dielectric function, refractive index, extinction coefficient, reflectivity, absorption coefficient and electron energy-loss function, were calculated for the energy range 0-20eV. The origins of the peaks and structures in the optical spectra were determined in terms of the calculated energy band structures.



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Theoretical study of methane activation on the CuRu 25%(100) bimetallic surface.

Khettal Habib

Ferhat ABBAS Setif 1 University; Algeria

Abstract:

The fabrication of catalysts for methane activation is a scientific challenge especially economical cheaper catalysts. The goal of the present work is the use of the first principles calculations to study the methane, the methyl and the hydrogen interactions with the CuRu(100) bimetallic surface using periodic density functional theory (DFT) calculations. The dissociative adsorption energies of methane to CH_3+H were also studied. The interesting result of our study was the chemical interaction between the methane and the CuRu(100) surface. we have calculated the adsorption energy for different molecular orientations with 1, 2 or 3 H pointing to the surface. Whatever the site of adsorption of CH_4 . the results indicate that a chemical interaction is manifest with a most stable configuration is obtained for the top Ru site when 2 H atoms are directed to the surface. the adsorption energies being at best in the 150 meV range.



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Theoretical study of 1-formyl-3-phenyl-5-aryl-2-pyrazoline derivatives as corrosion inhibitors of steel in acidic medium

Ilhem Selatnia¹, Oday Khamaysa², Assia Sid³, Merzoug Benahmed⁴

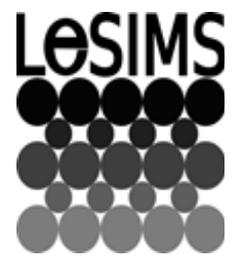
Abstract:

The inhibition reactivity of two synthesized pyrazoline derivatives namely: 1-Formyl-3-phenyl-5-(4-methylphenyl)-2-pyrazoline (P1) and 1-Formyl-3-phenyl-5-(4-chlorophenyl)-2-pyrazoline (P2), towards steel corrosion was studied by using quantum chemical calculations and molecular dynamics simulation (MD) to give more insights into the action mode of studied inhibitors. Several parameters such as EHOMO, ELUMO, energy gap (ΔE), fraction of electron transfers (ΔN) and Fukui index have been studied. Moreover, MD simulation is performed to simulate the best adsorption configuration of the investigated inhibitors on Fe (110) surface. Results indicate that the active sites of the molecules were mainly located on the pyrazoline ring and on the carbonyl group. The binding strength of the studied inhibitor molecules on Fe surface follows the order $P1 > P2$.



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Structural, electronic, optical, elastic and thermal properties of La_2GaN_3

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Abstract :

We report on results of first principle calculations on La_2GaN_3 . Equilibrium lattice parameters a , c , β and V were calculated, the results are in good agreement with experimental data. Elastic constants C_{ij} for single crystal; the deduced parameters bulk modulus B , shear modulus G , Young modulus E and the compressibility coefficients χ_a , χ_c , χ_v for polycrystalline aggregate were also presented. Bonding nature and bonds strength were discussed based on two points of view. Firstly, from the pressure effect on the structural parameters and the relative change of the bonds length. Secondly, from the electronic aspect based on the partial densities of states and the electronic charge distribution. La_2GaN_3 has an indirect band gap energy of 1.3 eV which decreases with increasing pressure. Thermodynamic properties such as Debye temperature θ_D , heat capacities (C_v and C_p) and expansion coefficient α_V were investigated based on the quasi-harmonic Debye model. Dielectric optical function, refractive index and absorption coefficient suggest that this compound is promising candidate for photovoltaic applications due to its high absorption of solar radiation in the visible range.



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Elastic and thermodynamic properties of the LiCdX (X = N, P, As and Sb) filled-tetrahedral compounds: An ab initio FP-LAPW study

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Abstract: The structural, elastic and thermodynamic properties of the LiCdN, LiCdP, LiCdAs and LiCdSb filled-tetrahedral compounds were investigated through ab initio full-potential linearized augmented plane wave calculations. Calculated structural parameters, including the lattice constant (a), bulk modulus (B) and its pressure derivative (B'), for the considered compounds using both the local density (LDA) and generalized gradient approximations (GGA) are in good agreement with the available experimental and theoretical data. The single crystal elastic constants were numerically estimated using total energy-strain approach with two different sets of distortions. The polycrystalline aggregate elastic parameters were calculated from the single crystal elastic constants via the Voigt–Reuss–Hill approximations. Mechanical stability, sound velocities, ductility/brittleness, elastic anisotropy, Debye temperature and pressure dependence of the elastic constants of the title compounds were also assessed. Temperature dependences of the lattice parameter, bulk modulus, volume thermal expansion coefficient, isochoric and isobaric heat capacity and Debye temperature in a wide temperature interval at some different fixed pressures were predicted through the quasi-harmonic Debye model.

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Linear and nonlinear optical properties of some phosphazenes

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Abstract:

Quantum chemistry methods are used to predict structure, linear and nonlinear optical properties for a series of phosphazenes compounds. Several studies show the efficiency of phosphazenes compounds type in nonlinear optical field [1-3]. Close structures have been obtained with some density functional theory functionals. The chosen level of theory was found to describe satisfactory the molecular structure (r. m. s. of the relative deviations). The study reveals that these organophosphazenes are a remarkably large first order NLO response. The results obtained from the traditional functional are in good accordance with those obtained by the corrected functional. The results will provide into the electronic properties of this important class of compounds.



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First principles calculation of structural, electronic, magnetic and optical properties of Mn-doped GaN in cubic phase

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Abstract:

Perfect GaN or Mn-doped GaN semiconductors are widely interesting systems for optoelectronics or spintronics applications. We have investigated the structural, electronic magnetic and optical properties of perfect GaN and Mn-doped GaN in cubic structure using a supercell of 64 atoms. First principles calculations based on density functional theory are performing by using the full potential linearized augmented plane wave method. The local spin density approximation (LSDA) were used as the exchange correlation potential to calculate the structural and electronic properties. In addition, the Tran-Blaha modified Becke-Johnson (TB-mBJ) was applied to give a better description of the band gap energies, magnetic moments and optical spectra. The results show that the system of Mn-doped GaN exhibits typical half-metallic properties in which Mn forms deep levels in the forbidden band and increases static dielectric constant. The total magnetic moment is mainly from the Mn atoms and the contributions from Ga and N are very small.



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Ab Initio Investigation of Structural, Electronic, and Magnetic Properties of Cr-Doped ZnS and ZnSe in Wurtzite Structure

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Abstract:

Using first-principles calculations with the full-potential linear muffin-tin orbital (FPLMTO) method, we investigated the structural, electronic, and magnetic properties of $Zn_{1-x}Cr_x$ (S, Se) diluted magnetic semiconductors (DMSs) in wurtzite structures with varying concentrations ($x = 0.0625$, $x = 0.125$) of Cr. The electronic properties indicated that $Zn_{1-x}Cr_x$ (S, Se), in all concentrations, exhibited half-metallic ferromagnetic (HMF) behaviour with a spin polarisation of 100%. The density of states showed a hybridisation between the p (S, Se) and 3d (Cr) states, which created an antibonding state in the gap that stabilised the ferromagnetic ground state linked to the double-exchange mechanism. Therefore, these compounds are highly likely candidates for spintronics applications.



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First principal DFT study of structural, electronic and magnetic properties of PdGen (n=1-11) clusters

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Abstract:

In this work we give a small view on the structural, electronic and magnetic properties of pure germanium clusters as well as effect of substituting one germanium atom by the palladium's one. Employing density functional theory[1] implemented in SIESTA code we focus on the relation between the binding energy and the size of the clusters. We find that the binding energy increases by increasing the clusters size which means that the system continues to gain energy during the growth process. For fixed cluster size, the binding energy decreases by substituting one germanium atom by the palladium's one. Looking now to the electronic properties, we find that the HOMO-LUMO gap basically decreases by increasing the size of the clusters. For a given cluster the substituting of one germanium atom by the palladium's one leads to decrease the HOMO-LUMO gap. Analysing the ionisation energy and the electronic affinity of different clusters, we show that they decrease and increase, respectively, by increasing the clusters size. The latter parameters allow to evaluate the chemical hardness of different clusters which shows that the size the biggest clusters are chemically less stable. In addition, the inclusion of silver atom leads to reduce this stability.



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First principles study of structural, elastic, electronic and optical properties of the nitridomagnesogalltes $\text{CaMg}_2\text{GaN}_3$

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Laboratoire d'Etudes des Surfaces et Interfaces des Matériaux Solides (LESIMS), Université Ferhat Abbas Sétif1, Algeria.

Abstract:

First principles calculations [1] were made to perform a study of the structural, elastic, electronic and optical properties of $\text{CaMg}_2\text{GaN}_3$ [2]. This compounds crystallize in the hexagonal type structure (space group $P63/mmc$). The obtained results for the lattice parameters a , c and V_0 are in satisfactory agreement with experimental ones. The deviation is less than 3% for the calculated equilibrium volume V_0 . Hexagonal symmetry possesses five independent elastic constants C_{11} , C_{33} , C_{44} , C_{12} and C_{13} , our results show that C_{11} (a -axis) is higher (stronger) than C_{33} (c -axis), which is confirmed by the lower contraction of a -axis against increasing pressure. The band structure reveals a narrow direct band gap energy ($\Gamma_v \rightarrow \Gamma_c$), partial densities of states and the electronic charge density distribution show a predominant covalent bonding in this compound. Optical properties demonstrate that these compounds are suitable candidates for optoelectronic devices. Phonon dispersion relation and vibrational stability were presented and discussed.



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High-pressure structural phase transition and the electronic properties of chalcogenoid praseodymium

Hakim Baaziz

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Abstract:

An ab initio study was performed using the full-potential linearized augmented plane wave method (FP-LAPW) within the framework of density functional theory (DFT), with both approximations: generalised gradient approximation GGA for the structural properties calculation and for the electronic and magnetic properties we have used both approximations GGA and mBJ (modified Becke -Johnson) to improve the results of the praseodymium chalcogenides family PrX ($\text{X}=\text{P}, \text{As}, \text{Bi}$) which have an technological interest in the spintronic field. The calculation has showed that PrX ($\text{X}=\text{P}, \text{As}, \text{Bi}$) compounds are stable in the Phase B1 (NaCl), and undergo a phase transition under hydrostatic pressure to CsCl (B2) phase and a transition of the phase B1 (NaCl) to the phase L10 (tétragonal). The electronic properties show that these materials are half-metals in the phase study B1 (NaCl). The magnetic moment is equal to $2\mu_B$.



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Stability and magnetic properties of Cr-substituted ScN from first principles

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Abstract:

Recently, many efforts have been focused to obtaining III-V dilute magnetic semiconductors (DMS) by doping semiconductors. Among these latter, nitride based diluted magnetic semiconductors are attracting increasing attention, such scandium nitride (ScN) doped with transition metal elements. We have studied the structural, electronic and magnetic properties of Rocksalt scandium nitride (ScN) and chromium doping Sc_{1-x}Cr_xN (with x=0.25). We used density functional theory (DFT) [1] framework as implemented in the projector augmented wave method (CP-PAW)[2]. The generalized gradient approximation (GGA)[3], as well as hybrid functional have been employed for the electronic exchange and correlation effects. The equilibrium structural parameters, density of states (DOS) and magnetic moment are analyzed and discussed.

Keywords: DFT, spintronic, magnetic semiconductors.

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Structural properties Refinement with the Whole Pattern Matching Method

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Abstract:

The object of this work is to study the structural properties of the $C_4H_6N_2$ compound such as: the lattice parameters, the space group; the integrated intensity.....; where we used the Whole Pattern Matching so called the Le Bail method, it is an effective way to determine these properties. Le Bail method is an extremely important method to confirm the results of indexing or to launch either a structure refinement or ab initio structure determination or to make a microstructural study. Several elements necessary to achieve the assigned task was utilized. In particular, a set of complementary software modules, and the X ray diffraction diagram of the $C_4H_6N_2$ compound in order to accomplish these objectives. So the results of the refinement of the Whole X ray diffraction diagram after several cycle; Show that the $C_4H_6N_2$ compound can crystallizes in the orthorhombic system with the following lattice parameters: $a = 9.7747 \text{ \AA}$ $b = 8.1893 \text{ \AA}$ $c = 6.2660 \text{ \AA}$ And $\alpha = \beta = \gamma = 90.000$ In the two possible space groups which are $P 21 21 21$ (19) and $P 2 2 2$ (16).



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Modeling of the effect of the void shape on effective elasticity modulus of porous materials

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Abstract :

The important physical and mechanical properties exhibited by porous materials have led to a vast range of industrial and engineering applications. Used as light-weight materials, catalyst carriers, electrodes, vibration and acoustic energy damping materials, impact energy absorption materials, they have aroused the interest of many researchers particularly over the last three decades. Mechanical and physical properties for the structural materials such as elasticity, plasticity and thermal conductivity have been largely investigated with the pore morphology as the main parameter of the studies; see [1] for the thermal conductivity and [2] for the plastic property. In this study, a numerical homogenization technique and morphological analysis based on the finite element method are used to compute mechanical properties of porous materials. This is achieved by considering two-dimensional matrix containing random distribution of identical non-overlapping circular or elliptical voids. Several microstructure configurations are considered by varying the voids morphology and the porosity of the matrix. The notion of the representative volume element (RVE) is used for numerical simulations in order to estimate the morphology effects of the voids on the effective elasticity modulus of the called Lotus-Type Porous Metals [3]. A confrontation of the obtained numerical results of the representative microstructures for different morphologies of voids and different properties with an analytical model and experimental data is performed. Finally, a formula improving the Boccaccini model is proposed to estimate effective elasticity modulus of porous metals taking into account the voids morphology [4].

Keywords: Numerical homogenization, lotus type porous metals, effective elasticity modulus, representative volume element.

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Structural, Elastic and magnetic properties of L10-XPt [X=Fe, Ni, Cr, Cu, Co, Mn]

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Abstract:

Materials with high magnetocrystalline anisotropy (MCA) have received considerable attention for ultra-high-density magnetic recording media fabrications. The structural, elastic and magnetic properties of XPt [X=Fe, Ni, Cr, Cu, Co, Mn] are studied using the density functional theory considering the L10 tetragonal phase. The calculations were performed in the framework of the DFT as implemented in VASP code. The ion-electron interaction was described by PAW pseudopotentials. For the exchange-correlation interaction, the Perdew, Burke and Ernzerhof (PBE) GGA approximation was used. From the calculated formation energy, we obtained the following stability order of CoPt < MnPt < FePt < CrPt < CuPt < NiPt. From the calculated elastic constants and moduli, we discussed the mechanical stability using the Born elastic stability criteria and inferred the brittle/ductile behavior from Pugh ratio, shear over bulk modulus G/B , and the Cauchy pressure proposed by Pettifor. All the alloys satisfy the stability criteria and are mechanically stable. Ductile behavior could be observed only for XPt [X= Cr, Co, Fe]. On the contrary, CrPt alloy is covalent or exhibit $G/B > 0.5$ leading to a brittle behavior and moderately for NiPt and MnPt. The Zener anisotropy factor is different from 1 indicating that these compounds are elastically anisotropic materials. A strong correlation is found between G and the Young modulus E , slightly above $G \sim 3/8 E$ widely found experimentally for polycrystalline metals.



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Half-Heusler compounds : novel materials for energy application

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Abstract:

In this work, first principle calculation of structural, electronic, magnetic and thermodynamic properties of the half-metallic [1] ferromagnetic Half-Heusler [2] compounds KSrC and RbSrC are presented. We have applied the full-potential linearized augmented plane waves plus local orbitals (FP-LAPW+lo) [3] method based on the density functional theory (DFT) [4-5]. For the exchange and correlation potential generalized-gradient approximation (GGA) is used [6]. We found that the KSrC and RbSrC in the ferromagnetic state are more favorable than the antiferromagnetic state and they exhibits half-metallic ferromagnetism, the computed equilibrium lattice parameters agree well with the available theoretical and experimental data. The calculated total magnetization of 1 μ B is in excellent agreement with recent experiments. We give also a comparison between the standard generalized gradient approximation (GGA) and the modified Becke–Johnson exchange potential approximation (mBJ–GGA) [7] on the electronic and magnetic properties.



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Spin-orbit effect on the electronic structure of MoSe₂/WSe₂ heterobilayer

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Abstract :

Investigating the electronic structures of the single-layer and heterobilayer of dichalcogenides MoSe₂ and WSe₂ we observe an unusual nature of their excitations. To do so, we used first-principles methods based on density-functional theory (DFT) [1,2] and many-body perturbation theory (MBPT - the GW approximation and the Bethe-Salpeter equation) [3,4] . The specific properties of the subunits, which play the role of building blocks in this van der Waals heterostructures are basically preserved. For example, the semiconducting character of the monolayers is maintained in the heterostructure and only the nature of the band gap was changed. Indeed, our calculations show clearly that the building blocks are direct semiconductor at K point of the Brillouin zone in the visible range while the heterostructure shows type -II band alignment with an indirect gap. Our results open up perspectives to create new low-dimensional materials with customized characteristics.



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N Doping Effect on the Structural, Optoelectronic properties of ZnO Using DFT Approach

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Abstract :

The present work is a theoretical study of the nitrogen (N) effect on structural and optoelectronic properties of zinc oxide (ZnO) wurtzite structure, using the density functional theory (DFT) which is developed to calculate the electronic states of solids containing huge numbers of electrons [1]. The band structure and Density of States (DOS) diagrams are plotted from the optimized equilibrium lattice parameters, an effective non-metal nitrogen approach is describe to modify the electronic properties of N doped ZnO shows best visible light absorption as compared to other doped models due to the band gap. The results confirmed that O acts preferential doping site in the crystal lattice. An appearance of a considerable electronic field in VBM revealing the p-type when nitrogen occupies the O site in ZnO with a little change in CBM. Additionally, the presence of impurity of N significantly decrease the transmittance of N doped ZnO which is expected to provide a new application of industrial optoelectronic and photovoltaic. Our calculations provide reasonable interpretation for the experimental findings.



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First principal calculations of properties of Cobalt doped Phosphorus clusters CoP_n (n = 1 - 24)

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Abstract : In this work, we have systematically investigated the equilibrium geometries, electronic and magnetic properties of P_{n+1} and CoP_n (n = 1-24) clusters by using the first principals density functional theory approach within the generalized gradient approximation (GGA) implemented in SIESTA simulation package. The relative stabilities have been studied in terms of the binding energies, the second-order difference of energies, the HOMO-LUMO gaps, the verticals ionization potentials and electronic affinities and the chemical hardness for all pure and doped structures. The obtained results show that the binding energies generally increase with the increasing of cluster size which indicating that the clusters continue to gain energy during the growth process. The evolution of the electronic structure can also be probed by calculating the characteristics of the energy gap between high occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The theoretical HOMO-LUMO gaps of the most stables CoP_n clusters are generally decreases as the cluster size increases. This indicates that the CoP_n clusters with large size seem to be approaching the gap closure characteristic of a metallic state which is enhanced by the doping Co atom. The clusters of CoP_n at size 5 and 8 exhibit high stabilities when compared to their neighboring clusters. The magnetic properties of CoP_n clusters are discussed according to the value of the total magnetic moment calculated for the lowest energies structure. The magnetic moment of CoP_n depend on the structure and symmetry of given clusters and on the position of Co atom and the number of his neighboring P atoms. We have also explored the vertical electron affinity (VEA) and the vertical ionization potential (VIP) of CoP_n clusters. We find that there are odd-even alternation in both AE and IP as a function of size of CoP_n clusters. This means that some CoP_n clusters have specific properties and they are more stables than the neighboring clusters.

Keywords: DFT, Phosphorus, Cobalt, clusters, structural properties, electronic properties, magnetic properties.



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Investigation of the optical interband transitions of the of Polymorphs RbPbI₃ and CsPbI₃: Implications for Main-Group Halide Perovskite Photovoltaics

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Abstract: Lead halide perovskites have attracted great interest because of rapid improvements in the efficiency of photovoltaics based on these materials. To predict new related functional materials, a good understanding of the correlations between crystal chemistry, electronic structure, and optoelectronic properties is required. First principles calculations by means of the potential linearized augmented plane wave method within generalized gradient approximation (GGA) were carried out for the electronic and optical properties of Main-Group halide compounds RbPbI₃ and CsPbI₃. They have cubic structure and show indirect band gap, the density of states and band gap pressure coefficients are given. On the other hand, an accurate calculation of linear optical functions like refraction index and both parts of dielectric function is performed. The assignment of the peaks and structures to the different interband transitions is analyzed in detail. The results are compared with previous calculations and experimental measurements, we show that our calculated values compare acceptably well with values reported in the literature.

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Structural, Elastic and Electronic properties of the AIX (X = N, P and As) in the B3 and B1 phases

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Abstract:

The structural, elastic and electronic properties under pressure effect of the AIX (X = N, P and As) compounds in the ZnS-type (B3) and NaCl-type (B1) structures were investigated using first-principles pseudopotential plane wave method based on density functional theory (DFT) with the LDA and GGA as implemented in the CASTEP code. Our results confirm that these compounds crystallize in the zinc-blende phase (B3) at ambient conditions and undergo a structural phase transition from the B3 phase to B1 phase under the effect of hydrostatic pressure. Computed single elastic constants increase linearly with increasing pressure and verify the generalized stability criteria. It is found that the hardness of the AIX (X = N, P and As) compounds decreases with increasing atomic number Z of the X element. Calculated electronic properties reveal that the three considered compounds in the B3 phase and the AlN compound in the B1 phase are indirect band gap () semiconductors, while the AlP and AlAs compounds in the B1 phase are metals. The nature of the fundamental band gap remainders unchanged under pressure effect. Calculated density of states reveals that these compounds possess a mixture of ionic and covalent bonding.



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Structural, elastic and electronic properties of CaSrTt ($\text{Tt}=\text{Si, Ge, Sn}$ and Pb)

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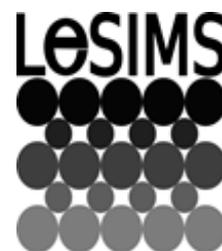
Abstract:

We present an ab initio study of the structural, elastic and electronic properties of CaSrTt ($\text{Tt}=\text{Si, Ge, Sn}$ and Pb) compounds. The calculations are based on the DFT theory with generalized gradient approximation (GGA) which is found to describe the properties of these materials rather well. In particular, the calculated lattice constants and equilibrium volumes are in good agreement with experiments with a deviation less than 0,67% for a ,2,74% for b and 1,7% for c for the equilibrium volume the deviation does not exceed 4,7% . Single crystal elastic stiffness's (C_{ij}) were calculated and the polycrystalline elastic moduli (B and G) were estimated according to Voigt, Reuss and Hill's approximations. Electronic band structure calculations suggest that these compounds are semiconductors, in agreement with literature data on their analogues.



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Effect of pressure and temperature on structural properties indium based compounds InX ($\text{X}=\text{As}, \text{Sb}, \text{P}$)

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Abstract:

In this Work, We present the results of a first-principles study of electronic and structural stability properties of indium compounds InX ($\text{X}=\text{As}, \text{Sb}, \text{P}$) for all three phase: Zinc-Blende (B3), Rock-Salt (B2) and CsCl (B1). We identify the stable phase and his parameter and we determinate the transition pressure for all structure and we investigate for the effect of temperature and pressure for the structural parameter. The computational method is based on the full-potential linearized augmented plane wave (FP-LAPW). The exchange and correlation energy is described in the local density approximation (LDA) using the Perdew–Wang parameterization including a generalized gradient approximation (GGA).



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Theoretical Study of the Metal Complexation Impact on the Antioxidant Activity of Curcumin and its Derivatives

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Abstract:

Novel metal complexes with curcumin and its derivatives, taken from literature with their proposed structures[1], were modeled in this work. Curcumin, known for its wide spectrum of biological and pharmacological activities, is very poorly bioavailable. In this context, numerous structural analogues of curcumin, including curcuminoids, have been synthesised and studied. Furthermore, complexation of curcumin and its derivatives with metals has gained attention in recent years for improvement of its stability. In order to gain a better insight into the molecular structure of the ligands and their metal complexes, geometric optimization and electronic properties analyses were performed using density functional theory (DFT). These calculations have been used to investigate reactivity properties and autoxidation mechanism. The simulation results are used to discuss the antioxidant behavior of the curcumin derivatives and their metal complexes, and to predict experimentally inaccessible properties which are not reported in the reference paper.

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Ab-initio study of structural, elastic, electronic and magnetic properties of LuR3 (R= Ru, Rh, Pd, Pt and Ir)

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Abstract:

We present results obtained from ab-initio calculations on LuR3 (R= Ru, Rh, Pd, Pt and Ir) compounds. our results of the lattice parameter a are in good agreement with experimental data, with deviations less than 1%. Single crystal elastic constants are calculated, then polycrystalline elastic moduli (bulk, shear and Young moduli, Poisson ration, anisotropy factor) are presented, LuIr3 has the highest elastic moduli. Based on Debye model, Debye temperature Θ_D is calculated from the sound velocities V_l , V_t and V_m . Band structure results show that the under study compounds are electrical conductors, the conduction mechanism is assured by R-d electrons. Different hybridization states are observed between R-d and Lu-d orbitals. The study of the charge density distribution and the population analysis shows the coexistence of ionic, covalent and metallic bonds.



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Theoretical study of 1, 3 bis (p-Fluorophényl)-5- Pentyl-1, 3, 5-Triazacyclohexane ligand and their complexes of formula CrCO_3 (TAC) and Cl_2M (TAC): (M= Fe, Ni, Zn) .

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Abstract:

Nitrogen heterocyclic compound represent an important class of ligands in transition metal coordination chemistry [1-2]. In particular Triazacyclohexanes ligands, wich have take since some years an immense interest both in organic chemistry and coordination chemistry [3-5]. Triazacyclohexanes adopt a chair conformation, with an axial diequatorial orientations (aee) for alkyl substituents (R3TAC) and an equatorial diaxial orientations (eaa) for aryl substituents (Ar3TAC). In this work, we are interested in studying the stability of 1, 3 bi (p-Fluorophenyl)-5- Pentyle-1, 3, 5-Triazacyclohexane ligand and studying their coordination with the transition metals of the first series : Cr, Fe, Ni and Zn(II).DFT [6] calculations with full geometry optimizations have been carried out, using the ADF[7] program, on a series of hypothetical complexes of the Cl_2M (TAC) (M = Fe, Ni, Zn) and $(\text{CO})_3\text{Cr}$ (TAC) type , (M = transition metal and TAC = Triazacyclohexane ligand). A rationalization of the bonding in hypothetical complexes is provided. Depending on the electron count and the nature of the metal, the Triazacyclohexane ligand can bind to the metal through the η^1 , η^2 and η^3 coordination mode. The Cr complexes prefers a closed-shell count (18-MVE), those of Fe, Ni and Zn prefers an open-shell count with: 16, 16 et 14 (MVE) respectively. Vibrational frequency calculations were performed on all the optimized geometries to verify that these structures are local minima on the potential energy surface.

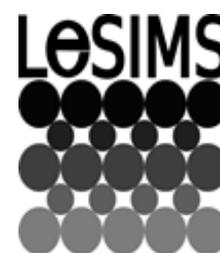
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Thermoelectric properties of the BaFAgCh (Ch = S, Se and Te) compounds

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Abstract:

Thermoelectricity, which is the direct conversion of heat into electricity, is the term that indicates the physical phenomena resulting from the motion of charge-carriers under the action of temperature gradient [1]. The electronic properties of the layered BaFAgCh (Ch = S, Se, Te) were investigated using the full potential linearized augmented plane wave (FP-LAPW) method [2] as implemented in the Wien2K code [3] with the TB-mBJ [4] functional to model the exchange-correlation potential. The FP-LAPW band structure and the semi-classical Boltzmann transport theory were used to study the charge-carrier concentration and temperature dependences of the thermoelectric parameters, including Seebeck coefficient, electrical conductivity, thermal conductivity and figure of merit [5]. The potential of the BaFAgCh (Ch = S, Se and Te) compounds as thermoelectric materials in the carrier concentration range $1 \times 10^{16} - 1 \times 10^{20} \text{ cm}^{-3}$ was assessed. The obtained results show that the values of the thermoelectric parameters for the p-type compounds are larger than that of the n-type ones. Seebeck coefficient value along the c-axis is found to be higher than its value in the ab-plan. However, electrical conductivity (σ), electronic thermal conductivity (κ) and figure of merit (ZT) are found to be higher in the ab-plan. This can be attributed to the fact that the charge carrier effective masses along the c-axis are larger than those in the ab-plan. The optimal charge carrier concentrations and temperatures that yield the maximum values of the figure of merit for the title compounds were calculated.



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Theoretical properties of semiconductor SnHfO₃ compound via DFT calculations

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Abstract:

In this work structural, electronic, elastic and magnetic properties of cubic SnHfO₃ material have been investigated using the gradient generalized approximation GGA [1] within the framework of Density Functional Theory (DFT) [2]. We have calculated the structural properties such as the equilibrium lattice constant, the bulk modulus and its pressure derivative and they are in good agreement with the available data. Additionally, the results show that our material is stable in non-magnetic phase via the ferro- magnetic one. Furthermore, to confirm the stability for material of title, the elastic properties have been studied in detail and it is concluded that SnHfO₃ is elastically stable. The magnetic moment is also discussed in our study; we find that the main contribution to the total magnetic moments comes from the oxygen atom, while the contributions of Sn and Hf atoms are very small. Finally, the electronic band structures reveal that this material exhibits a direct band gap (X-X) semiconductor by using GGA approximation.



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Structural, electronic and elastic properties of LaGaO₃- cubic

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Abstract:

Structural, electronic and elastic properties of LaGaO₃ cubic perovskite have been calculated using the full-potential linearized augmented plane wave (FP-LAPW) plus local orbital method which is based on the density functional theory (DFT) as implemented in WIEN2k code. In this approach the solid version GGA-PBESol of the generalized gradient approximation (GGA-PBE) was chosen to treat the exchange-correlation potential. Structural results such as the equilibrium lattice parameter, bulk modulus as well as the elastic results such as elastic constants and their related parameters especially Poisson's ratio, Young modulus, shear modulus we note that there is a good agreement of our calculations with experiment and theoretical available results. According to the value of B/G ratio, this compound has a ductile behavior.

Keywords: FP-LAPW, DFT, perovskite, elastic constants.

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Theoretical Study of Oxygen Vacancies Effect on the Spectroscopic Raman and IR Frequencies of SnO₂

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Abstract: In the last years, Tin dioxide SnO₂, present one of the most important materials because of their optical properties. This oxide present a large band gap energy of 3.6eV[5]. We define a several domains of application of SnO₂, for example, solar cells, detection of toxic gas, catalysis[1] ...etc. The rutile phase of tin dioxide (SnO₂) has a tetragonal structure with space group and two molecules per unit cell. Both experimentally and theoretically studies[1,2,4], proved that the presence of oxygen vacancies is responsible of amelioration of several properties, for example: magnetic; electronics and optical properties. For this reason, we focused our intention on the optical properties. The aim of this investigation is firstly, to calculate the RAMAN and IR frequencies of fundamental modes of vibrations at G point of the first Brillouin zone for SnO₂ rutile without and with oxygen vacancies. In the second stage, we compare our results with those obtained experimentally and theoretically in the literature. The comparison with fundamental optical modes of SnO₂: $G=A1g+A2g+B1g+B2g+Eg+A2u+2B1u+3Eu$ [2]. Where, the symmetrical modes A1g, B1g, B2g and Eg are Raman active modes, whereas, A2u and Eu modes are IR active modes. The modes A2g and B1u are neither Raman active nor IR active. Theoretical calculations of RAMAN and IR frequencies are released with CRYSTAL09[3] program, using SCF-LCAO with different Hamiltonians of periodic DFT approximation: hybrid B3LYP and a combination with non-local and local approximations: LDA, GGA and BPE. The creation of vacancies need a use of supercells of (2x2x2)_p, contain 48 atoms (16 Sn and 32 O).

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Vibrational Frequencies of SnO₂ (110) Surface: ab-initio calculations

Bouchelarem Naima

Abstract: SnO₂ (110) is one of the most thermodynamically stable surfaces[1] and it is one of a transparent materials, for these reasons, it has a wide applications in solar cells, catalysis, batteries and gas sensors [2-4]. The rutile SnO₂ has a tetragonal structure with space group ,when, the surface (110) of SnO₂ has a rectangular structure with C_{2v} symmetry group. Phonon modes calculations in harmonic approximation at the gamma (Γ) point in the first Brillouin zone were performed with CRYSTAL09 program [5], using density functional theory DFT at the B3LYP level [6,7] and effective core pseudopotential (ECP) basis sets with SLAB model. A different cells are considered from (1x1)p surface unit cell. To simulate the stoichiometric SnO₂ (110) surfaces and investigate the effect of size of cells on the optical properties we used one layer (1L), two (2L) and three layer (3L) of (1x1)p. Our aim is firstly, assign the vibrational frequencies observed for SnO₂ (110) surfaces. Then, determine relationship between the irreducible representation of D_{4h} and C_{2v} symmetry groups. Second, we study the effect of the size on the Raman and IR fundamental modes of vibrations of the surface SnO₂(110) and finally, compare our results with those obtained experimentally and theoretically. We find that the frequencies observed at 67.44, 278.5 and 641.17cm⁻¹ corresponds to A₁ surface modes are assigned to B_{1g}, E_{1u} (TO) and A_{1g} of bulk, respectively. Therefore, the surface frequencies at about 514.41cm⁻¹(A₁), 641.81cm⁻¹(B₁), 466.33(A₂) and 616.78(B₂)cm⁻¹ are assigned to the E_g, A_{2u} (TO), A_{2g} and E_{3u} (TO) fundamental modes of the bulk SnO₂, respectively.

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Geometries, stabilities, and electronic properties of Tin ($n=2-11$)

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Abstract:

The lowest energy structures of Titanium pure Tin are studied within ab initio calculations based on density functional theory DFT with generalized gradient approximation(GGA) and the first principles pseudopotential implemented in SIESTA method [1-2]. We interest to the small clusters in size range of 2 to 11 atoms. We found a number of new isomers, which are not previously reported. The atoms in more this clusters exhibit pronounced preference for residing on the surface. The binding energies increase with cluster size in this range, while the highest-occupied and lowest-unoccupied molecular orbital (HOMO-LUMO) gap decreases with the increase in cluster size.

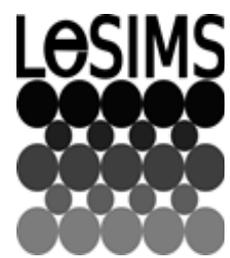
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DFT study of optoelectronic properties of CuGaTe₂ chalcopyrite compound for functional applications

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Abstract :

Due to their high absorption coefficients (10^5 cm^{-1}) in the visible range and their appropriate gap, the chalcopyrite semiconductor compounds of I-III-VI₂ and II-VI-V₂ families are promising candidates for photovoltaic's applications [1]. Also, thanks to the anisotropic characteristic of their linear optical properties ($E // oz$, $E \perp oz$), which confers on chalcopyrite materials a large amount of Optical Parametric Oscillator (OPO) and Second Harmonic Generation (SHG) [2], which gives great performance for lasers based on chalcopyrite compounds [3]. Among I-III-VI₂ chalcogenides, CuInSe₂ are extensively investigated [4]. Due to the very high cost and environmental concern of III-In system in addition to the high partial pressure of chalcogene VI-Se, the compound CuGaTe₂ stands as a potential candidate to be investigated in view of its application for functional materials. In order to demonstrate the potential of the proposed CuGaTe₂ compound for photovoltaic conversion, in WIEN2K code, within the framework of Density functional Theory (DFT) [5], using FP-LAPW approximation [6] and mBj [7] functional for exchange correlation energy, the optoelectronic properties, such as band gap (E_g), absorption coefficient ($\alpha(\omega)$) and photoconductivity ($\sigma(\omega)$) in the visible range have been reported, discussed and compared to the available literature data. To the best of our knowledge, for the first time using DFT method the degree of birefringence $\Delta n(\omega)$, which is a predetermining factor for laser performances [8] have been calculated using the relation $\Delta n = n_e - n_o$, where n_e and n_o is the extraordinary ($n(\omega)//oz$) and ordinary ($n(\omega)\perp oz$) refraction indices.

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Application of fractal model on the Self-compacting concrete formulation methods

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Abstract:

Self-compacting concrete has a more complex mix design compared to vibrated concrete. When looking into literature regarding self-compacting concrete, a wide range of materials can be noticed as well as a lot of different mix design approaches. This work aims investigate the different formulation of self-compacting concrete (SCC) using the fractal approach. Precisely, prove that the studied granular mixtures for each concrete followed a fractal distribution by tracing fractals lines ($N_{cum}=f(diam)$ in logarithmic coordinates) and deduction of fractal dimensions DF (The slopes of the adjusted straight lines).

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Theoretical study of electrical and thermal transport properties of Br doped Co₄Sb₁₂

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Abstract:

Co₄Sb₁₂ skutterudites is a popular group of thermoelectric materials (TEM) because they show low thermal conductivity with filled voids in their structure. To investigate the potential of filled Skutterudite as TEM; first principles calculations are performed on filled Co₄Sb₁₂ and Br is used as void filler. Calculations have been made using full potential Linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT). For exchange-correlation energy and corresponding potential, generalized gradient approximation (GGA) by Perdew–Burke–Ernzerhof (PBE) has been used. Our calculations shows that the BrCo₄Sb₁₂ is a semiconductor with small gap. Also an ab-initio calculations combined with classical Boltzmann transport equation under constant relaxation time approximation have been used to study transport properties of the material. We found that BrCo₄Sb₁₂ has large seebeck coefficient and low thermal conductivity.

Keywords: Thermoelectric materials (TEM), Seebeck coefficient and Thermal conductivity.



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Development of a wear-resistant steel

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Abstract:

In 1882, one of the first alloyed steels, manganese steel, which is composed of approximately 1.2% C and 12% Mn, was discovered by a metallurgist, Sir Robert Abbot Hadfield [1]. This alloy possesses properties such as high work hardening, high toughness, good ductility and wear resistance [2]. In the as-cast condition, Hadfield steel has a completely austenitic matrix with carbides, type Me_3C , precipitated at the grain boundaries. The existence of these carbides effectively improve the hardness of the steel and its resistance to wear but eventually weakens it. This requires a quenching heat treatment which allows the dissolution of these carbides. The aim of this work is to improve the hardness of Hadfield steel while keeping a good ductility in the heart of the material. The melting of this steel is carried out in an electric arc furnace. Two series of heat treatments were carried out, one at 1100°C and the other at 1050°C under a controlled heating rate. The holding times and temperatures of heat treatments were chosen in order to dissociate the maximum of carbides and obtain a homogeneous structure without enlargement of the austenitic grain. The microstructure of experimental steels were studied using optical microscopy (OM), scanning electron microscopy (SEM), energy dispersive spectrometer (EDS) and X-ray diffraction (XRD). The analysis by EDS shows that these carbides are of type $(Fe,Mn,Cr)_3C$. The microstructure of treated samples reveal two distinct phases for the two heat treatments applied, martensite and retained austenite. The variation of the temperature of heat treatment allowed a microstructural change of the alloy from where the interest of this study.



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Study of Thermodynamic and Electrochemical Degradation of Polymer Electrolyte Membrane Fuel Cell

Samia Latreche, Abd Essalam Badoud, Mabrouk Khemliche
Automatic Laboratory of Setif, Electrical Engineering Department, Faculty of Technology, University Ferhat Abbas - Setif1, Algeria.

Abstract:

In this paper, a new approach is proposed to evaluate the performance of a temperature of proton exchange membrane fuel cell (PEMFC) and to determine the lifetime of polymer electrolyte membrane (PEM). A fuel cell is a device of an energy conversion which takes some forms of fuel and converts it directly into electrical energy. There are numerous inevitable degradation phenomena occurring on various PEM fuel cell components. A prerequisite for optimal exploitation of these systems is assessment of their current. The problem of estimation is even more challenging due to the lack of accurate degradation models that incorporate the complex behaviour of a fuel cell as a whole. Therefore, the proposed research will focus predominantly on developing a bond graph model of solid oxide degradation for PEM fuel cells that can be evaluated online based on information that can be acquired without interrupting the normal operation of a system under test. In order to understand degradation of membrane and the effect of high temperature in fuel cell, a bond graph approach is developed. It is based on the integration of the thermodynamic and electrochemical phenomena taking place in the fuel cell. The thermal model is established from the fuel cell thermal energy balance. The model is implemented under SYMBOLS (System Modelling by Bond graph Language Simulation) software and validated for steady-state and dynamic modes alike.



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Control and Analysis of Piezoelectric Inertia Friction Actuators

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University Ferhat Abbas - Setif1, Algeria; Algeria*

Abstract:

The piezoelectric actuator is applied in a micro forging system which was designed specially by maximizing its structural rigidity to study size effects in micro forming. To generate accurate movement in micrometer/nanometer scale, a dynamical model of the piezoelectric actuator is in need. High accuracy of micro/nanometer scale manufacturing is required in the miniaturization of various applications such as high precision optical systems, and high accuracy positioning. The models for the Piezoelectric Inertia Friction Actuators (PIFAs) were used for the optimization of PIFA performance. In this paper, the critical challenges are first identified in control of PIFAs. Second, a general architecture of PIFAs is proposed to facilitate the analysis and classification of the literature regarding modeling and control of PIFAs. This general architecture covers all types of PIFAs and thus serves as a general conceptual model of PIFAs. The bond graph approach which considers the effect of multi-degree-of-freedom loading structures on the dynamics of the actuators is proposed in this paper. We try to fuse the new model with the bond graph control techniques, where the unknown parameters in the model are not needed to be identified. The control algorithm guarantees the stability of system. The challenges associated with the control problem are also discussed. The decoupled structure PIFA models have the advantages of being more accurate and flexible as compared to the decoupled ones. Among the existing hysteresis sub-models, for a tractable among of computation efforts, a contradiction between the capability of representing all hysteresis phenomena and maintaining model accuracy remains to be solved. The bond graph control is among the most promising ones as applied to PIFA positioning since when designed based on the decoupled structure PIFA models, it can completely reject the hysteresis and creep effects in theory. The bond graph control laws are usually simple and of a proportional type. The dynamic model is used mostly for the purpose of compensation, especially compensating for the hysteresis of the Piezoelectric Actuators material. Such a bond graph control is not quite robust and does not adequately address the highly uncertain dynamics of PIFAs.



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Removal of methylene blue dye from aqueous solutions by adsorption using a ziziphus jujuba stones treated with H₃PO₄

Abderraouf Guediri

Abstract:

Ziziphus jujuba stones treated with phosphoric acid H₃PO₄ was used as a biosorbent to remove methylene blue dye (MB) from aqueous solution under various operating conditions. The effect of the experimental parameters such as temperature (10-40 °C), pH (2-12), contact time (10-360 min), initial concentration (50-150 mg / l), salt, humic acid and Isoelectric point have been studied. The sorption kinetic uptake for MB by Ziziphus jujuba stones at various initial dye concentrations was analyzed by non-linear method using pseudo-first, pseudo-second, pseudo-nth order and intraparticle diffusion models. It was found that the pseudo-nth order kinetic model was the best applicable model to describe the sorption kinetic data. MB adsorption on biosorbent followed the linear Langmuir isotherm. The calculated values of ΔG_0 and ΔH_0 indicated the spontaneous and endothermic nature of the adsorption process.

Keywords: methylene blue, phosphoric acid, adsorption.

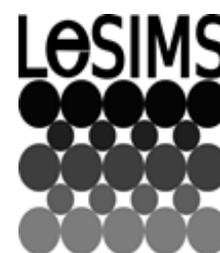
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Optimization and modeling of synthesis parameters of lanthanum trichloride using full factorial design analysis

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Abstract:

The lanthanide halides and their mixtures with alkali metal halides play a very important role in many modern technologies such as: metallic lanthanide or lanthanide-based alloy production [1], nuclear waste treatment, spent fuel recycling [2], and in the lighting industry [3] (high pressure discharge halide lamps). Such wide technological application of these compounds requires knowledge of their structural, physicochemical properties and in particular their thermodynamic properties. The study of these properties requires a high purity of these salts in order to have accurate data [4]. Therefore, good control of the different stages of synthesis and optimization of parameters that can affect the synthesis reaction is the preliminary step to cross [5,6]. The present work is focused on lanthanum trichloride LaCl_3 synthesis by sintering chlorinating of lanthanum oxide La_2O_3 with ammonium chloride NH_4Cl (under inert gas). It reports the influence of three synthesis parameters (temperature, contact time and chemical composition) on the reaction yield. The optimum conditions for synthesis of lanthanum trichloride were thus determined and discussed. A full factorial design was used in order to determine a mathematical model connecting these three factors with reaction yield and to gain insight into how the various factors interact and influence the response.

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Structural, vibrational and electronic properties of MoSe₂/ WSe₂ van der Waals heterobilayer

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Abstract:

2D materials such as graphene, hexagonal boron nitride (h-BN), and transition metal dichalcogenides (MoS₂, WSe₂, etc.) have a very high potential in the fields of energy (electro-catalysis, batteries, photovoltaic), electronics and optoelectronics. Beyond 2D materials considered individually, composite systems stacks of different layers, called van der Waals heterostructures are particularly attractive: They allow not only to modulate the properties of the materials, but also to further improve their performance. In this work, we report the structural, vibrational, and electronic properties of MoSe₂/WSe₂ heterobilayer obtained by a nanostructured combination of isolated MoSe₂ and WSe₂ monolayers. The calculations were carried out using density functional theory (DFT) [1,2] taking into account the effect of spin-orbit coupling. The phonon characteristics were calculated within density functional perturbation theory (DFPT)[3]. We found the bandgap of this vertical heterostructure to be smaller than the bandgaps of the subunits while its spin-orbit splitting is intermediate between those of the isolated layers. We also found the existence of three types of phonons, i.e., MoSe₂ -like phonons, WSe₂ -like phonons, and hybrid - like phonons. The hybrid phonons originated from the vibrations between the isolated monolayers.

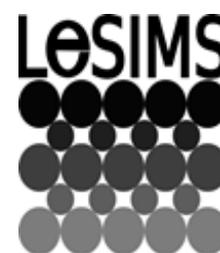
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First-principles study on the optoelectronic properties of inorganic perovskite $\text{RbxCs}_{1-x}\text{PbBr}_3$ for solar cell applications

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Abstract:

Recently, replacing or mixing organic molecules in the hybrid halide perovskites with the inorganic Cs or Rb cations has been reported to increase the material stability with the comparable solar cell performance. In this work, we systematically investigate the electronic and optical properties of all-inorganic alkali iodide perovskites $\text{RbxCs}_{1-x}\text{PbBr}_3$ using the first-principles virtual crystal approximation calculations. Our calculations show that as increasing the Cs content x , lattice constants, band gaps, exciton binding energies, and effective masses of charge carriers decrease following the quadratic (linear for effective masses) functions, while static dielectric constants increase following the quadratic function, indicating an enhancement of solar cell performance upon the Rb addition to CsPbBr_3 . When including the many-body interaction within the GW approximation and incorporating the spin-orbit coupling (SOC), we obtain more reliable band gap compared with experiment for CsPbBr_3 , highlighting the importance of using GW+SOC approach for the all-inorganic as well as organic-inorganic hybrid halide perovskite materials.

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First-principles investigation of the structural, electronic and optical properties of Ge-doped MgSiAs₂

Samir Cheddadi

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Abstract:

We report the results of studies on the structural, electronic and optical properties of MgSi_{1-x}Ge_xAs₂ ($x = 0, 0.25, 0.5, 0.75$ and 1) using density functional theory (DFT) based on the full-potential linear augmented plane wave (FP-LAPW) method. To treat the exchange-correlation potential for the total energy calculations, the generalized gradient approximation (WC-GGA) by Wu-Cohen was used. Additionally, the modified Becke Johnson (mBJ) potential approximation, which successfully corrects the band-gap problem, was used for the band structure calculations. The calculated lattice constants and band-gap values for these alloys are in good agreement with the available theoretical and experimental data. A decrease in the band gap is observed with an increasing Ge content. The dielectric function and absorption coefficient are calculated to investigate the optical properties. Electronic and optical properties reveal that these alloys should be very useful for applications in photonics, optoelectronics and optics.

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Structural, Elastic and Electronic properties of the AIX (X = N, P and As) in the B3 and B1 phases

Bedjaoui Abdelhak

Laboratory for Developing New Materials and their Characterization, University of Setif 1

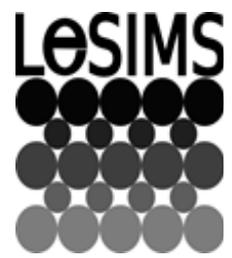
Abstract:

The structural, elastic and electronic properties under pressure effect of the AIX (X = N, P and As) compounds in the ZnS-type (B3) and NaCl-type (B1) structures were investigated using first-principles pseudopotential plane wave method based on density functional theory (DFT) with the LDA and GGA as implemented in the CASTEP code. Our results confirm that these compounds crystallize in the zinc-blende phase (B3) at ambient conditions and undergo a structural phase transition from the B3 phase to B1 phase under the effect of hydrostatic pressure. Computed single elastic constants increase linearly with increasing pressure and verify the generalized stability criteria. It is found that the hardness of the AIX (X = N, P and As) compounds decreases with increasing atomic number Z of the X element. Calculated electronic properties reveal that the three considered compounds in the B3 phase and the AlN compound in the B1 phase are indirect band gap () semiconductors, while the AlP and AlAs compounds in the B1 phase are metals. The nature of the fundamental band gap remains unchanged under pressure effect. Calculated density of states reveals that these compounds possess a mixture of ionic and covalent bonding.



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Isogeometric analysis of free vibration Timoshenko beams under various boundary conditions.

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Abstract

A isogeometric analysis method is applied to free vibration of Timoshenko beam in this paper. A theoretical study for the establishment of kinetic energy and strain energy of the beam, necessary to establish the equations of motion is made. Timoshenko beam theory is used to modelise the beam. the isogeometric analysis method using the B-spline function is applied to defined The model . Natural frequencies of the studied system are determined there after. A validation study is done, the results are compared with the results which are found in the literature. The influence the boundary conditions on the frequencies is considered.



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Absorption of cobalt (II) by materials and mesoporous coals of types SBA-15 and CMI-1

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Abstract:

Water pollution is one of the major concerns in terms of environment and therefore quality of life. The will to solve this general problem is marked by both a notion of time and type of pollutants released (heavy metals, hydrocarbon, dye ...). The retention of heavy metals is carried out in our study by adsorption on silicas and mesoporous coals, the characterization of these materials was carried out by X-ray diffraction, SEM and nitrogen adsorption-desorption (BET). The adsorbent properties of these materials are studied from kinetics and adsorption isotherms of cobalt II metal ions in aqueous solution using atomic absorption spectrometry. The modeling kinetics of the cobalt adsorption by the four materials in aqueous medium under optimal operating conditions is pseudo first order. The adsorption isotherms show that the Langmuir model is not applicable on the CMI-1 and SBA- materials, whereas these CMK-3 and CMK-3C coals follow this model. The Freundlich model is applicable on all four matrices.



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Numerical study for estimating time-dependent reliability of a corroding pipe to flange weld joint over its lifetime

Nahal Mourad

MCM Souk Aharas University ; Algeria

Abstract:

Failure probability of a corroding pipe to flange weld joint over its lifetime was investigated. A numerical model of a corroded weld joint connecting pipe to flange using finite element method was developed, and coupled with usual stress models. An empirical mechanical behavior model of the studied structure has been also proposed. Monte Carlo simulations, FORM and SORM methods have been applied for estimating reliability and failure probability under the both effects of corrosion and residual stress. A numerical case with high, moderate and low corrosion rates was conducted to determine the reliability of the welded connection pipe to flange. The founding results are analyzed and discussed for various corrosion rates. The obtaining result shows that the heat affected zone due to the welding process is very sensitive to corrosion effects. Hence, it is necessary to ensuring a rigorous inspection to ovoid human and environmental disasters.



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Ab-initio investigation of the Pt-Sn binary system

Dziri Fatima

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Abstract:

The aim of the present work, based on ab-initio calculations, is to investigate the relative stabilities of the different compounds involved in the (Pt-Sn) system. Having our calculations performed at 0K, We will be mainly focusing on the determination of the ground state line of this system. Our calculations were based on density functional theory (DFT) as implanted in the Vasp Code [1]. We used the projector augmented-wave (PAW) method, which is an all-electrons technique within the frozen core approximation. Only generalized-gradient approximation (GGA) was considered. A study of convergence has been done for the plane-wave cutoff energy and allowed us to fix the Ecut at 520eV. The formation enthalpies of the compounds were obtained through the following equation: $H_f(\text{Pt}_p\text{Sn}_q) = E_{\text{tot}}(\text{Pt}_p\text{Sn}_q) - (E_{\text{fcc}}(\text{Pt}) + q E_{\text{BCT}}(\text{Sn}))$, Where $H_f(\text{Pt}_p\text{Sn}_q)$ is the enthalpy of formation of the compound Pt_pSn_q , $E_{\text{tot}}(\text{Pt}_p\text{Sn}_q)$, $E_{\text{fcc}}(\text{Pt})$ and $E_{\text{BCT}}(\text{Sn})$ are the ground state total energies (per atom) of the compound Pt_pSn_q and its constituents Pt and Sn, respectively, in fcc and BCT structure.

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Electrochemical and theoretical insights of a new environmentally organic inhibitor for carbon steel corrosion in acidic media

Oday khamaysa

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Abstract:

The inhibition effect of new hydrazone derivative (Hyd-Iso) on the corrosion of carbon steel in 1 M HCl solution at 298K was studied practicing Potentiodynamic polarization and EIS methods. The obtained results showed that (Hyd-Iso) was an effective inhibitor in HCl medium. The inhibition efficiency, $\eta(\%)$, increased with the increase in concentration inhibitor. The activation dissolution thermodynamic parameters were calculated and discussed. Tafel curves reveal that (Hyd-Iso) behaves as a mixed-type inhibitor with cathodic predominance and obeyed Langmuir adsorption isotherm. With the aim of extracting the parameters of the electrochemical impedance spectroscopy an appropriate equivalent circuit model was offered. In addition, the mechanism of inhibition was also studied via DFT (Density functional theory) treatment of (Hyd-Iso) molecule.



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Modeling of the effect of the void shape on effective elasticity modulus of porous materials

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Abstract:

The important physical and mechanical properties exhibited by porous materials have led to a vast range of industrial and engineering applications. Used as light-weight materials, catalyst carriers, electrodes, vibration and acoustic energy damping materials, impact energy absorption materials, they have aroused the interest of many researchers particularly over the last three decades. Mechanical and physical properties for the structural materials such as elasticity, plasticity and thermal conductivity have been largely investigated with the pore morphology as the main parameter of the studies, see [1] for the thermal conductivity and [2] for the plastic property. In this study, a numerical homogenization technique and morphological analysis based on the finite element method are used to compute mechanical properties of porous materials. This is achieved by considering two-dimensional matrix containing random distribution of identical non-overlapping circular or elliptical voids. Several microstructure configurations are considered by varying the voids morphology and the porosity of the matrix. The notion of the representative volume element (RVE) is used for numerical simulations in order to estimate the morphology effects of the voids on the effective elasticity modulus of the called Lotus-Type Porous Metals [3]. A confrontation of the obtained numerical results of the representative microstructures for different morphologies of voids and different properties with an analytical model and experimental data is performed. Finally, a formula improving the Boccaccini model is proposed to estimate effective elasticity modulus of porous metals taking into account the voids morphology [4].



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Study of the quenching temperature effect on the thermal conductivity of poly (methyl methacrylate) (PMMA) pigmented with titanium dioxide (TiO₂)

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Abstract:

The objective of this work is to realize a numerical modeling of the thermal conductivity of a nano-composite material with polymer matrix: poly methyl methacrylate (PMMA) pigmented with titanium dioxide (TiO₂), and to compare the obtained results with theoretical prediction models and the experimental data as a function of the quenching temperature for TiO₂ fraction equals 3%. For this, a numerical study was conducted using the finite element method to predict the effective thermal conductivity of the nano-composite. In addition, a comparison with the results from the analytical models showed that the proposed numerical model is in good agreement with the analytical models of Hatta and Taya Hashin and Shtrikman for the contact resistance of 10⁻³. In the end the comparison of the numerical model to experimental results based on the quenching temperature shows that all quenching temperatures check the theoretical models of Hashin & Shtrikman and Hatta & Taya.



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The influence of void distribution on the mechanical behavior of materials by finite element

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Abstract:

The defects and in particular the pores play a determining role in the mechanical behavior of materials. However, their influence remains always badly understood. The nanoindentation is regarded as the technique most used to measure the properties of the thin or surface layers and the nanomaterial one. The goal of this work is to study by digital simulation using the software Abaqus, the influence of the presence of a pore in aluminum 6061 alloy during the nanoindentation. We have performed the simulations in 2D (axisymmetric) and in 3D, by using two types of indenter (spherical and Berkovich). We simulated the behavior of material in the absence and in the presence of a spherical pore according to its depth below the indenter. The obtained simulation results show that the presence of the pore in material led to the deterioration of its mechanical properties, such as the reduction in its hardness. In addition, this reduction is all the more important as the pore is closer to the surface of material. Finally, our results are in concord with former work.



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DC/RF performance of AlGaN/GaN underlap MOS-HEMT

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Abstract:

AlGaN/GaN metal oxide semiconductor high electron mobility transistors (MOSHEMTs) are very attractive for high power and high frequency and high temperature applications, with low gate leakage current. In this work we investigated the simulation of Hf₂O₂/AlGaN/GaN, Al₂O₃/AlGaN/GaN and TiO₂/AlGaN/GaN MOS-HEMTs, on sapphire substrates and the trapping effects of the devices using TCAD device simulation. Good simulation ID-VDS, ID-VGS, and gm-VGS plots of the passivated and unpassivated devices were obtained. Simulations have revealed in passivation case for Al₂O₃ as gate oxide, a very high drain current of 2.728A, peak Gm of 0.390 S, and a threshold potential VT of - 5.022 V. The peak values of fT and fmax, extracted from S-parameters, were found to be 299.91GHz and 194.53 GHz, respectively for highly scaled device. These results demonstrate the potential of AlGaN/GaN underlap MOS-HEMT for high power and high-frequency applications.



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Proton-Proton collision simulation in probing radiative neutrino mass models at high energy colliders LHC

Dounia Cherigui

Abstract:

Every second, over a billion neutrinos pass through your body, neutrino are by far the oddest of the fundamental particles, they are also the only electrically neutral lepton while the observation of neutrino oscillations for which the data can not be explained by massless neutrinos, the dark matter (DM), and the matter-antimatter asymmetry of the universe make in evidence one of the most popular mechanisms that generate small neutrino mass. Here we present one of the attractive way to induce naturally small neutrino mass, the KNT model proposed in [1], where neutrino mass are generated radiatively at three loop, our model extends the SM with two singlet charged scalars $S(1,2)$, and one singlet fermion, N , all having masses around the TeV scale, making it testable at collider experiments such as DM relic density [2]. In this work, we probe a class of neutrino mass models through the lepton flavor violating interactions of a singlet charged scalar, S at proton-proton collisions with 8 TeV and 14 TeV energies where this scalar produce neutrino missing energy. In our analysis we discuss the tripleton final state through magnetic and kinematic properties via different distributions by extracting relevant kinematical cut. Polarization and spin properties of opposite sign same flavor leptons signal, as well as the background free channel are studied here with the tau contribution which can enhance the signal/background ratio for center of mass energies 8 and 14 TeV. Some photonic characteristics are described in our model and different experimental constraints [3] are involving by considering two benchmark points, performed detailed analysis is presented while we use the 8 TeV LHC RUN-I data [4] to put constraints on this class of models and probe the model at 14 TeV.



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Monte Carlo Simulation of a GaInSb Based MESFET Transistor

Elouchdi Amine

Abstract:

The study of electron transport in submicron devices, constitute a good approach to determine the device ability to operate under hard conditions like temperature, electric field and frequency. In this paper, the electron transport characteristics of the Ga_{0.5}In_{0.5}Sb based MESFET are presented. The channel length is fixed to 65 nm. The characteristics are obtained using Monte Carlo Device Simulation based on the parallel resolution of the coupled Poisson-Boltzmann equations. The resolution of these equations allows calculating the electric field, energy, electron velocity and electrostatic potential distribution across the geometry of the device.

Keywords: Monte Carlo Device Simulation, III-V semiconductors, GaInSb material, Electronic Transport, MESFET Transistor

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Half metallic properties of the ternary XMnSe_2 ($X = \text{Rb}, \text{K}, \text{Cs}$) Chalcogenides compounds

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Abstract:

The electronic and magnetic properties of ternary compounds XMnSe_2 ($X = \text{Rb}, \text{K}, \text{Cs}$) were investigated by first-principles calculation based on full potential linearized augmented plane wave (FP-LAPW) method, implemented in the WIEN2k simulation package. The electron-exchange correlation is taken as generalized gradient approximation (GGA_PBE). The calculated total magnetic moment for both studied compounds is in good agreement with available experimental and theoretical results. The analysis of the electronic and magnetic properties using the total and partial density of state and band structure show that this ternary are spin polarised with half metallic band gap.

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