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ABSTRACTS BOOK





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ABSTRACTS BOOK

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ABSTRACTS

Synthesis of hydrocerussite hexagonal disk and its applications in battery anode

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Abstract

A rapid, low temperature and additive-free hydrothermal process was firstly developed to synthesize hydrocerussite ($\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$) hexagonal disk. The products were characterized by XRD, SEM and TEM. Single-phase $\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$ hexagonal disk was obtained at 180 °C hydrothermal temperature with around 4 μm in diameter. The precursor suspension pH was critical for the product particles composition and morphologies. The crystal growth direction in hexagonal disk was indexed as (102) plane from HRTEM, and the growth mechanism for hexagonal disk was proposed. Hydrocerussite ring, as a new member in hydrocerussite family, was also successfully prepared by controlling the pH value at 10. The obtained hydrocerussite product was applied for the lab-scale lead-acid battery anode and discharged a high capacity of 144 $\text{mAh}\cdot\text{g}^{-1}$ at constant current 50 $\text{mA}\cdot\text{g}^{-1}$, which suggests that $\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$ can be applied for energy storage devices.

Key words: hydrocerussite, hydrothermal, hexagonal disk, ring, lead-acid battery.

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Optimization of CNC Turning for Aluminum alloy using Simulated Annealing Method

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Abstract

Surface roughness is a main parameter in computer numerical control (CNC) turning technology. The aim of this paper is to obtain an optimal parameters of turning process (cutting speed, spindle speed, feed rate and depth of cut) which results in an optimal of surface roughness for machining aluminum alloy ENAC43400 shaft (46×150mm).

The developed objective model is modeled using regression method then optimized by simulated annealing method in order to determine the best set of turning parameter values. This work conclude that simulated annealing method can be used for high precision modeling and estimation of turning parameters.

Key words: CNC turning, regression analysis, optimization, simulated annealing method.

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Effects of High Potential Cathodic Protection on Fusion Bond Epoxy Coated Steel

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Abstract

This paper describes experimental work investigating the effects of cathodic protection (CP) potentials on the disbondment of fusion bonded epoxy (FBE) coated steel samples. The objective of the work was to study the performance of FBE coated specimens with good and poor surface preparation and exposed to various applied CP potentials at 25 °C and 60 °C in aerated 3.5% NaCl solution.

Results of this work showed that coating surface preparation, temperature, applied potential and exposure time all play an important role in the resistance of FBE coating to cathodic disbondment. Cathodic disbondment tests showed satisfactory performance of FBE coating protected under CP conditions to a potential of -1200 mV (w.r.t. SCE) at 25 °C. Potentials more negative than -1200 mV (w.r.t. SCE) at 25 °C and more negative than -1000 mV (w.r.t. SCE) at 60 °C resulted in coating failure. Poor surface preparation also caused premature coating failure.

Key words: **Cathodic disbondment** - The failure of adhesion between a coating and a metallic surface that is directly attributable to the effects of cathodic protection current and is often initiated at a coating holiday.

Holiday - A defect in a protective coating at which bare metal is exposed.

Polarization - Change in the potential of an electrode as a result of current flow.

Current demand – Current required for cathodic protection to define the minimum potential required to suppress corrosion.

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The Dielectric Properties of (PVA-PEG-PVP-MgO) and (PVA-PEG-PVP-CoO) Biomaterials

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Abstract

In this paper, study of dielectric properties of two types of nanocomposites are (PVA-PEG-PVP-MgO) and (PVA-PEG-PVP-CoO) in frequency range (100 Hz- 5 MHz). The (PVA-PEG-PVP-MgO) and (PVA-PEG-PVP-CoO) nanocomposites have been prepared by casting technique. The dielectric parameters (dielectric constant, dielectric loss and A.C electrical conductivity) are increasing with the increase of concentrations of magnesium oxide and cobalt oxide nanoparticles. Also, the dielectric properties change with increasing of the frequency of applied electrical field.

Key words: nanocomposites, dielectric properties, electrical conductivity.

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Structural, Electronic and Optical Properties of Sodium Nitrate NaNO_3 : An ab initio Study

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Abstract

The structural, electronic and optical properties of sodium nitrate are investigated using the pseudo-potential plane wave (PP-PW) scheme in the frame of generalized gradient approximation (GGA). The geometrical parameters of the unit cell have been fully optimized and are in good agreement with the experimental data. The electronic structure shows that sodium nitrate has a band gap of 2.917 eV. The dielectric functions, reflective index, extinction coefficient, reflectivity and energy-loss spectrum are calculated. The optical properties of sodium nitrate are discussed based on the band structure calculations. The 2p states of the nitrate moiety play the major role in optical transitions as initial and final states. The absorption spectrum is localized in the ultraviolet range between 60 and 380 nm.

Key words: Ab initio, sodium nitrate, electronic structure, optical properties.

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Development of new Ti-Mo-Fe alloys as biomaterial

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Abstract

Titanium and some of its alloys are known as being the most biocompatible metallic materials due to their high strength, low modulus, and high corrosion resistance in biological media. Besides other important material features, the corrosion parameters and corrosion products are responsible for limiting the biocompatibility of metallic materials, and can produce undesirable reactions in implant-adjacent and/or more distant tissues. Electrochemical corrosion behaviors of novel beta titanium alloys, Ti-4.7Mo-4.5Fe, Ti-3Mo-0.5Fe and Ti-2Mo-0.5Fe were characterized in naturally aerated Ringer's solution at room temperature compared with currently used biomedical titanium alloy, Ti-6Al-4V. The corrosion resistance of titanium alloys were investigated through open circuit potential (OCP), potentiodynamic polarization measurements and optical microscope (OM). A high corrosion resistance was obtained for all alloys due to the stable passive film formed on their surfaces. The new present alloys are promising metallic biomaterials for the future, owing to their very low elastic modulus and good corrosion resistance capabilities.

Key words: titanium alloys, passive film, corrosion resistance, electrochemical potentiodynamic.

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Characterization of GaN nanostructures by electron beam techniques

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Abstract

Cathodoluminescence (CL) is an important technique based on the light emitted from a specimen (semiconductor) in response to electron-beam irradiation. The light emitted is the results of radiative recombination of the electron-hole pairs. In the last few years the technology of group III nitride epitaxy has shown great progress on modern materials and electronic devices as well as on high electron mobility transistors (HEMTs), Light emitting diodes (LED) and photovoltaic solar cell, etc.

The characterization of GaN nanostructures (e.g. quantum wells) by an electron beam technique (e.g. cathodoluminescence) needs a reliable simulation models because there are several phenomena associated with matter-electron beam interaction. In this paper, we present our hybrid model based on Monte Carlo and molecular dynamics methods. This model describes the electron beam interaction with the quantum wells of GaN and Al_xGa_{1-x}N. According to results, the electron beam can modify the material properties at nano scales due to the electron beam heating, that depends on electron beam parameters (accelerating voltage, primary current and scanning duration). The influence of some material parameters also is studied.

Key words:

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Preparation of (PVA-PEG-PVP-MgO, CoO) Nanocomposites and Study their Optical Properties

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Abstract

Nanocomposites have many applications such: optical integrated circuits, sensors, coatings, medical devices.. etc. So, this paper aims to preparation of new type (PVA-PEG-PVP- MgO, CoO) nanocomposites to production new nanocomposites use in many. applications. The nanocomposites were prepared by using casting technique. The polymers was mixed with different weight percentages are (PVA0.90-PEG0.05-PVP0.05). The nanomaterials (MgO and CoO) were added to polymers composites with concentrations are (0, 2, 4 and 6) wt.%. The results show that the absorbance (A) of nanocomposites is increased with increase of concentrations of magnesium oxide and cobalt oxide nanoparticles. The optical constants (absorption coefficient (α), extinction coefficient (k), refractive index (n), real and imaginary dielectric constants (ϵ_1 and ϵ_2)) of nanocomposites are increasing with the increase of the weight percentages of magnesium oxide and cobalt oxide nanoparticles. The energy gap (E_g) of (PVA-PEG-PVP) decreases with the increase of the weight percentages of magnesium oxide and cobalt oxide nanoparticles.

Key words: Nanocomposites, Optical Properties, Magnesium Oxide, Cobalt Oxide.

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SURFACE FILM PROPERTIES AND THEIR ROLE IN THE STRESS CORROSION CRACKING OF STEELS

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Abstract

Electrochemical techniques and scanning electron microscopy (SEM) were used to grow films on steel and study some of their properties. Polarization curve measurements were performed on Cr-Mo alloy steel specimens in carbonate/bicarbonate solutions at 25 C° 75 C°. It was found that stress corrosion cracking was most likely to occur between -660 and -750 mV (SCE). The films grown at -700, -725 and -750 mV (SCE) were completely passive, but the film grown at -800 mV was not. The films formed at 75 C° at different potentials had different morphologies according to the SEM analysis of air-dried samples.

Key words:

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A Nonlinear Material Model for Fibrous Composite Materials and Its Effect on In-Plane Lamina Stresses

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Abstract

The composite material using a macro-scale approach is dealt with as a homogeneous continuum using averaged apparent properties. The corresponding mechanical properties of an orthotropic composite lamina are specified as: E_1 , E_2 , G_{12} and ν_{12} where the subscripts 1 and 2 indicate the principal material directions. Direct investigation of these properties can be obtained experimentally from the various corresponding uniaxial tests.

A group of failure envelopes were obtained for several fiber-orientation angles ($\Theta=30, 45$ and 60 -degrees), in order to study the effect of shear stress (τ_{xy}) variation on failure behavior of a well-known type of a composite material namely; Boron-epoxy Narmco 5505. Representative figures were selected to show such effect accounting for material nonlinearity exerted on failure behavior of unidirectional fibrous composite laminates. An energy-based nonlinear material model was adopted to predict the mechanical properties of a unidirectional composite lamina. A compatible failure criterion for nonlinear composite materials was utilized which incorporates the material response into the failure model. The resulting failure envelopes were compared for all the cases.

Key words: Nonlinear model, composite material, shear stress, failure envelope, fiber-orientation

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The effects of acid and thermal treatment on the characterizations of Iran natural diatomite

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Abstract

The characterizations of natural diatomite from Birjand deposit (Iran) were studied such as chemical compositions, specific surface area, total pore volume, pore size distribution and XRD. The diatomite that was treated only with sulfuric acid displayed a larger surface area, expanded total pore volume and increased pore size in comparison with both washed natural diatomite with deionized water (D-H₂O) and the diatomite treated with sulfuric acid then calcinated at 550°C (D-H₂SO₄+550). The specific surface area and total pore volume were increased 46.63% and 71.40%, respectively. The results showed that the diatomite samples were composed of cristobalite, quartz and feldspar phases. Acid treatment and then calcination at 550°C changed the Si/Al ratio and grew the crystallite size. BJH with DFT analysis showed that the diatomite samples had very disordered micro/mesoporous pore networks. The pore size distribution of the diatomite samples were from 1.4–100 nm. The isotherm of the samples were type IV and showed a long hysteresis loop that resembled the H3 type on the basis of the IUPAC classification. Therefore, the diatomite that was treated only with 3M H₂SO₄ can be to serve as a catalyst support or an adsorbent.

Key words: Iran natural diatomite, acid treatment, X-ray diffraction, crystallite size determination, scanning electron microscopy

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Synthesis, Crystal and Electronic Structures of CdAl₄O₇

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Abstract

Cadmium aluminate (CdAl₄O₇) is synthesized by solid state reaction in the presence of cadmium oxide (CdO) and gamma-alumina (γ-Al₂O₃) at temperatures ranged of 800-1000 °C. The preparation parameters, such as sintering temperature and molar ratios of Cd/Al, are thoroughly investigated. X-ray diffraction (XRD) technique is employed to monitor the phase transformations occurred in the sintered CdO + γ-Al₂O₃ system. Experimental results show that the formation of cadmium aluminate(s) is highly influenced by the sintering temperature. A favored crystallographical temperature for the significant formation of CdAl₄O₇ is found to be 950 °C. Single phase of CdAl₄O₇ is obtained at 950 °C for 36 h and an identical sintering process is repeated to ensure the product quality. The crystalline degree and microstructural characteristic of the product is examined by HRTEM. CdAl₄O₇ is identified to be a single phase with monoclinic structure (space group C2/m). The crystal structure of CdAl₄O₇ is also solved and determined by Rietveld refinement analysis of collected XRD data. The obtained structural details may provide possibility and feasibility for the potential application of CdAl₄O₇. The electronic structures (band structure and density of states) are calculated by GGA-PBE based on density functional theory (DFT). The calculated electronic structures revealing semiconductor character of CdAl₄O₇ with a direct band gap of 3.0 eV.

Key words: Aluminate, Monoclinic, CdAl₄O₇, Crystal Structure, DFT, Band Structure, DOS

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Effect of saline environment on mechanical properties of adhesive joints

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Abstract

Water diffusion into composite adhesive joints was experimentally studied by means of gravimetric measurements in bond specimens. The main parameters controlling the diffusion in the bond components were obtained from water uptake experiments carried out in bulk specimens of fiber-reinforced composite and epoxy adhesive. The diffusion of water in bonds is a complex mechanism due to the heterogeneous microstructure of the composite and its interface with the adhesive. This process was simulated through micro scale models which represent the microstructure of the composite and of the adhesive joint. Structural adhesive joints are adequate for joining aluminum with nearly constant. In terms of fatigue strength, for 10⁵ cycles, a decrease about 25% and 39% occurred in specimens immersed during

Key words: Structural adhesives, degradation of adhesives, water, motor oil, flexion test.

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