

Vibronic Intensities in the Elpasolite type Systems.

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Abstract

A formal approach to deal with the vibronic intensity features in both absorption and emission is put forwarded with reference to the stoichiometric elpasolite type systems. We focus our attention upon both, the electronic and the vibration factors upon which the intensity may be derived from, as well as the details of the coupling between the internal and the external normal modes of vibrations. We introduce a generalized approach to rationalize on a quantitative basis the observed spectral intensity features in highly relativist features. Our models are intended to avoid any unnecessary parameterization and therefore to reduce the mathematical complications along with, the well known fact that the experimental basis set is always incomplete so that any supra parameterization of the vibronic intensity problems seems to be unrealistic. The advantages and disadvantages of our model calculation are illustrated with reference to several excitations in a number of elpasolites . New trends in the vibronic coupling theory are also discussed with reference to systems such as $\text{Cs}_2\text{NaSmCl}_6$, $\text{Cs}_2\text{NaEuCl}_6$ and $\text{Cs}_2\text{NaDyCl}_6$.

Structural, Electrical And Percolation Threshold Study Of Copper-LDPE Composites

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Abstract

We report on the preparation and characterization of conducting copper-low density polyethylene (LDPE) composites. In order to accomplish a polymer-copper composite, these project have investigated the structural and electrical properties of conducting polymer composite using copper powder aggregates. This research has used commercial thermoplastics and investigating the wetting behavior of the copper and polymer, and thus the electrical properties of these materials have been studied and optimized. The percolation threshold of the composite was derived and the properties around this value were measured and modeled. The composites were synthesized using spherical copper particles (Alfa Aesar, mean particle size: 200 - 300 nm) embedded in a polyethilene low density matrix (LDPE, Goodfellow, mean particle size: 1000 μm), using different volume concentrations of filler metal. All the samples were manufactured under inert atmosphere by means of pressure and temperature. The homogenized mixture was introduced in a mold at a pressure of 40 MPa at a temperature of 400 $^{\circ}\text{C}$, under inert atmosphere, during 10 minutes. The molecular weight analysis for the LDPE using Gel Permeation Chromatography (GPC) doesn't evidence modifications to the work temperature. SEM examination of the microestructure of copper-LDPE composite with 10%vol. of filler metal, have demonstrated the presence of infinite percolation bond between copper particles, distributed randomly into the polymeric matrix with and without contact between themselves forming a conducting paths into the polymer matrix. This behavior was observed in all the studied concentrations. The room temperature conductivity was measured using the two-probe technique with parallel silver contact. The ohmic behavior was checked in each sample. The experimental data fitted using theoretical model describes the conductivity in composites due to percolation of mobile carriers, in this way, the experimental results are in agreement with the theoretical law.

Evaluation of the back-scattering response of a textured population of complex particles.

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Abstract

To evaluate the potential of specific systems as US echogenic drug delivery particles, a simulation of the ultrasonic RF signal it performed on a population of two-body particles composed of an inner medium surrounded by a shell or membrane. This structure allows considering plain spheres, bare or coated, vesicles (liposomes), bubbles and contrast agents. The particles structure is defined by its outer radius, shell thickness, and by the compressibility and density of each component. The particles are randomly distributed in the specimen active volume center on the acoustic axis. Introducing a texture in the active volume allows evaluating the local effect of particle parameters on the acoustic response. The texture is defined as a fluctuation along the acoustic axis of a characteristic parameter: particle numerical density, the particle diameter or other. The actual model considers an incident harmonic plane wave pulse with a Gaussian envelope propagating along the Z-axis. The RF signal is calculated as the sum of back-scattering waves from all the particles in the active volume at the origin of the axis system. the calculation of the scattered wave amplitude will consider three main contributions: the scattering from a fixed rigid sphere, the oscillation of the particle in the acoustic wave displacement field and the pulsation of the compressible particle in the pressure field. Air bubbles dispersions and oil-in-water emulsions have been simulated. In these cases, textures have been generated for the particle density and size.

Mesostructures obtained by Self Assembly Processes. From multifunctional porous materials to ordered nanocomposites

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Abstract

Mesostructured materials can be synthesised by the combination of sol-gel chemistry and self-assembly. A striking example is the synthesis of supramolecularly templated mesoporous oxides (MPO), which can be produced and processed as powders or films, displaying a great variety of mesostructures with controlled pore size, wall thickness, wall composition, pore system symmetry. Once these structures have been designed and constructed, their surface can be further modified with organic functions, obtained either by one-pot or post-grafting methods, which lead to multifunctional materials. The regular pore size and surface control also makes the pore systems ideal candidates for nanoparticle (NP) templates, leading to NP@MPO composites, which can be tailored to combine the properties of two kinds of nanometric size elements, which are in intimate contact through an extended interface, all combined in a robust matrix. In this work, we present examples of multifunctional mesoporous films, created by adding organic functions to MP silica or transition metal oxides (TMO, such as TiO₂ or ZrO₂). Organic molecules bearing grafting (phosphate, phosphonate, diolate, carboxylate...) and functional (hydrophobic, ionic, metallophilic) groups are used to perform functionalisation. Grafting kinetics have been followed in order to assess pore accessibility and to optimise function incorporation. Diffusion is relatively quick for thin films or small particles; however, mass transport seems to be limiting function uptake in particles larger than 1-2mm. Leaching experiments show that phosphate are better anchoring groups than diolate or carboxylate. Multilayered films with compositional or pore size differences are also presented. Cation adsorption into the pore systems of these films has been monitored, and metal uptake has been found dependent on the pH and surface chemistry of the host oxide. Reducing conditions (chemical or electrochemical) have been employed to generate Au, Ag, Fe or Cu metallic particles within the pores, generating robust nanocomposites with interesting properties.

Eutactic stars in Nature

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Abstract

An eutactic star is a set of M vectors in R^n ($M > n$) that are projections of M orthogonal vectors in R^M . In this work, we show that this concept turns out to be important when the need for handling redundant vector sets arises. We present new characterizations of eutactic stars, suitable for applications in crystallography and some biological problems. In particular, we apply our results to describe and parameterize polyhedral truncations, to the construction of generalized reciprocal sets and to study the geometry and function of the five ambulacral petals of plane irregular echinoids.

Biom mineralization Associated to Sulfated Polymers: A Source for Bio-inspired Materials

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Abstract

Biom mineralization leads to the formation of inorganic crystals with unique, ordered, sculptured shapes that are regulated by specific macromolecules. This process has been a source of inspiration for exploring novel approaches to the fabrication of inorganic-based surfaces and interfaces. Among those macromolecules, sulfated polymers, referred to as proteoglycans, have received not enough attention, although it is increasing evidence of their widespread occurrence in biominerals. Here we examine the available information on the nature, distribution and possible role of sulfated polymers in biom mineralization, and highlight new directions to stimulate further research activities.

Tetranuclear Copper(II) complexes: Structural

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Abstract

Since higher nuclearity copper(II) complexes are of current interest as model of copper metalloenzymes and inorganic materials. Special attention has been drawn to tetranuclear μ_4 -oxo bridged copper (II) complexes of general formula $[\text{Cu}_4\text{OCl}_6\text{L}_4]$ (L= Lewis-base ligand)

In this complexes the copper (II) atoms are configured in a tetrahedron around the μ_4 -bridging central oxygen. Each one of the four copper atoms is bridged by μ_2 -halides. In this work we describe the synthesis, and X-ray crystal structure of μ_4 -oxo-bridged copper (II) complexes with 2-methylimidazole and pyridine-N-oxide ligands.

Science And Technology Of Multifunctional Thin Films And Interfaces: A Vision To Nanoscience And Nanotechnology

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Abstract

A new paradigm is occurring in the science and technology of multifunctional thin films and interfaces and new phenomena sustained in film-based nanostructures. These materials are opening the way to revolutionary nanoscience and nanotechnology. In this talk, the science and technology of two classes of thin film materials will be reviewed as examples of the broad materials paradigm currently underway. In addition to fundamental and applied science reviewed here, this talk will include a vision for the application of multifunctional films to the fabrication of micro and nanostructures that will enable a whole new generation of revolutionary micro and nanodevices.

Complex oxide thin films provide a new platform material for novel micro- and nano-electronics. Our group is working on the fundamental and applied science of ferroelectric and high-dielectric constant (k) oxides. The former provide the platform material for the new generation of non-volatile ferroelectric random access memories (FeRAMS) that will replace current DRAM and flash memories, while the second provide the solution to the problem faced by the CMOS technology of having to replace the SiO_2 gate in the new nanoelectronics, since the low k of SiO_2 requires a $\leq 10 \text{ \AA}$ thick film to maintain the capacitance of the CMOS gates, which will render the next generation of CMOS devices unworkable. A novel Ti-Al amorphous high- k dielectric under development in our lab will be discussed as an excellent candidate for the new generation of gate oxides. The same material plays a critical role as a diffusion barrier for the integration of ferroelectric thin films such as $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ with Si for the fabrication of FeRAMS. The science of complex oxide thin films is now evolving into the science of oxide nanostructures and the integration of multifunctional oxides such as ferroelectrics and magnetic layers and into nano-oxide-biointerfaces, which are opening new fields of research and device development.

Nanocarbon materials in different allotropic forms such as nanocrystalline diamond thin films, carbon nanotubes, and fullerenes represent another material paradigm opening new avenues into revolutionary micro and nano-science / technologies. The fundamental and applied science of a novel ultrananocrystalline diamond (UNCD) material in thin film form developed in our laboratory will be reviewed, including the view to novel Si-based microelectromechanical (MEMS) and nanoelectromechanical (NEMS) devices. UNCD exhibit a unique combination of mechanical, chemical, tribological, electron transport and emission properties, and biocompatible properties that provide the bases for a new generation of multifunctional micro and nanodevices in inorganic form as well as implantable biodevices and biosensors. A discussion will be presented on the microfabrication processes and characterization of mechanical,

tribological, electronic transport, and bio-compatible properties of UNCD films. Application of UNCD as hermetic corrosion resistant coating to enable an artificial retina to restore sight to people blinded by retina degeneration will be discussed as an example of application of UNCD to biodevices. The talk will finish with the presentation of a vision for the Center for Nanomaterials currently under development at Argonne National Laboratory, which will provide the platform for revolutionary nanoscience and nanotechnology.

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Synthesis and Characterization of Cyclophosphazenes Encapsulated in a Silica Matrix and their Analytical Applications

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Abstract

Hybrid organic - inorganic materials are expected to have different, eventually better properties, than either of the two separate components. They promise new applications in many fields such as optics, ionic, mechanic catalysis and ceramic membranes¹. On the other hand, polyphosphazenes are very interesting polymers, their properties depending both on the inorganic $\text{P}=\text{N}$ - backbone and on the characteristics of the substituent groups attached to the skeletal phosphorus of the phosphazene chain. Although some hybrid phosphazene- metal oxides containing covalent bonds have been prepared, to our best knowledge, no inclusion materials containing phosphazenes in silica have been reported. Here we report the first example of triorganocyclotriphosphazenes encapsulated in a silica matrix and its application to capture metal coordination compounds on an analytical scale.

The oligophosphazenes $\text{P}_3\text{N}_3[\text{N}(\text{CH}_3)(\text{CH}_2)_2\text{CN}]_6$ (1), $\text{P}_3\text{N}_3[\text{OC}_6\text{H}_4\text{CN}]_6$ (2) and $\text{P}_3\text{N}_3[\text{OC}_6\text{H}_4\text{CH}_2\text{CN}]_6$ (3) were prepared according to previously reported methods.²

The composite (1)/ $(\text{SiO}_2)_n$ (1a) was prepared by a sol gel process using TEOS (tetraethyl orthosilicate) as starting material of the SiO_2 network and the cyclic phosphazene $\text{P}_3\text{N}_3[\text{N}(\text{CH}_3)(\text{CH}_2)_2\text{CN}]_6$ which bears organic units. The siliceous sol was previously obtained via acid catalysis of $\text{Si}(\text{OC}_2\text{H}_5)_4$ and subsequently mixed with the phosphazene completely dissolved in methylene chloride in the appropriate quantities in order to obtain a 1:30 molar ratio (phosphazene: SiO_2).

The composites (2)/ $(\text{SiO}_2)_n$ (2a) and (3)/ $(\text{SiO}_2)_n$ (3a) were prepared by a similar procedure which was detailed for (1a). Since cyclophosphazene (2) was not very soluble in methylene chloride, the composite was not well compatibilized. Since the product obtained for the synthesis of the cyclophosphazene (3) is a reddish oil, which is very soluble in methylene chloride, a good compatibilization of the material was obtained. The spectroscopic data obtained for both materials were similar to those of the material (1a).

These materials were fully characterized by elemental analysis, IR, ^{13}C , ^{31}P and ^{29}Si MAS NMR Spectroscopy, TG/DSC, SEM and TEM microscopy.

Considering the good coordinative properties of the nitrile groups present in the composites (1a), (2a) and (3a) the potential use of these encapsulated phosphazenes to retain metal complexes has been tested in this work. The encapsulated phosphazenes (1a) and (3a), have shown to be excellent solid phases for the retention of chromophore cationic complexes making it possible to evaluate the analytical signal directly by spectrophotometry or derivative spectrophotometry. The compound TPTZ (2,4,6-tripyridyl-1,3,5-triazine) was used as chromogenic reagent to form the blue complex Fe(II)-TPTZ at pH= 5.0.

The encapsulated cyclophosphazenes (1a) and (3a) serve as good solid phase retainers of cationic complexes. It is possible the determination of metal complexes at trace levels (ng/mL) with these new materials.

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Consolidation of the productive process of INGEPOL to assure the competitiveness the product developed from recycled polypropylene.

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Abstract

KEY WORDS: processes, polypropylene, recycled, extrusion, innovation, construction, General Efficiency of the Equipment (EGE).

EXPOSITION OF THE PROBLEM

INGEPOL S.A. is a company created with the idea to give him to application and use to the plastic remainders, specially and agricultural industrial, domestic remainders of polypropylene. It has developed elements that previously have made in materials like wood, concrete and steel, and we have replaced them by recycled polypropylene 100

It has developed to products of use in the sectors agricultural, industrial and construction, elaborating elements such as wood teeth, teeth for walls, bridges, covers and ring of sewage system, covers inspection boxes of energy and telephone. Additionally of all those products that can be elaborated by means of the joint of these elements, as it is the peatonal bridge , tables, banks, walls, floors, among others.

Therefore INGEPOL S.A. has come producing these elements under low parameters of productivity, since we are exploring in a field that has not been worked with the suitable technology at national level observing that those that it has worked not have done it efficiently had mainly to the lack of technical knowledge; on the other hand the mixtures of materials used by the company, being different from the standards, do not have technical information that it allows to a suitable design and adaptation of the processes and the equipment. Then aspects arise to which it is not had technical information sufficient, that it allows the suitable development of the process, to improve the productivity, with which to be able commercial ensure success of the developed innovations. The present situation is characterized by a low index of global efficiency of the equipment and by a high percentage of added internal rejections to the consequent extension of the times of delivery.

KEY ASPECTS WITH KNOWLEDGE DEFICIENCY

- i. Classification and selection of raw materials.
- ii. Intermediate processes that they must be put under to adapt them to the uses in products.
- iii. Mixtures that are due to make with the different types from polypropylene and in some cases with additions of other materials.
- iv. Parameters of process for the mixtures and their extrusion, to make them compatible with the added materials.
- v. Temperatures and their profile of work for the mixtures during the process and during strip of products. I saw.

vi. Design of molds as far as material, geometry and manoeuvrability, and the adjustment of necessary equipment

vii. Standardization of the characteristics of the product: properties physical - mechanical associated to the performance

GENERAL MISSION

To consolidate the productive process of INGEPOL to assure the competitiveness the product developed from recycled polypropylene.

WAITED FOR RESULTS OF THE PROJECT

i. Registry of suppliers available and described by capacity of delivery of raw material.

ii. Optimization of the physical and human resource in the production: Produced tons/Month/hr-man 15

iii. Increase in the efficiency of the production of the equipment: General efficiency of the Equipment Installed by improvements in the equipment design and process. 25

iv. To diminish the variability in the mechanical properties physical of products: Units produced and rejected/Total produced units. 20

v. Socialization of the results of the investigation and portafolio of INGEPOL products: Key y/empresas people for the business of INGEPOL contacted with received information 200

IDENTIFICATION OF THE PROPOSE INNOVATION

i. Product development with polypropylene recycling.

ii. Conventional product replacement of wood, and concrete steel and.

iii. Product development for the construction and the industry

Poster "Shape Instability in Neurites: Changing the elastic properties of the axon"

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Abstract

We investigated the shape instability in PC-12 neurites by means of the presence of specific drugs to modify the internal structure of the axon; shape instability appears after the depolymerization of microtubules or actin network. Studying in-situ the elongation or shrinking of the axon using a laminar flow to impose a well controlled hydrostatic pressure over it and measuring the bending during the instability development, showing evidence about the modification of the elastic properties of the axon.

New Approach for the Detection of Metal Ions by Polymer Modified Electrodes

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Abstract

Contamination of the environment by trace metals represents a major current problem. It results in an ever-increasing demand for the determination of metal contaminants in environmental matrices (1). The electrochemical methods has long been recognized as one of the most sensitive methods for the determination of trace metals and is very suitable for the task of on-site and in situ analysis (2). The method was adapted for analysis with preconcentration by electrodeposition on mercury electrode (3). However, because of the toxicity of mercury, new alternative electrode materials are thus highly desired. One promising approach is the use chemically modified electrodes capable of preconcentrating target analytes from dilute solutions (4). One main advantage of this approach belongs to the ability of preconcentration at open circuit and, preconcentration can be extended to analytes that cannot be electroreductively deposited. Also, chemical preconcentration by complexation can provide a higher selectivity due to the selective co-ordination of a metal cation to a specific ligand. The use of functionalized polymers is an attractive way of preparing electrode materials for electroanalysis with preconcentration (5,6). We present now the application of poly(pyrrole malonic acid) P(Pyr-MA), poly(acrylic acid-co-styrene) P(AA-Sty), poly(acrylamide-co-4-vinylpyridine) P(Am-VPy) and poly(styrene-co-4-vinylpyridine) (PSt-VPy) film electrodes for the determination of copper and lead cations, using anodic stripping voltammetry and cyclic voltammetry. In the first case, the polymer film was prepared by electrochemical polymerization and the other ones were synthesized by radical polymerization and deposited by spin coating. Anodic stripping curves were recorded using square wave voltammetry (SWV) for P(Pyr-MA) modified electrodes, after 10 min preconcentration at open circuit in diluted copper(II) or lead(II) solutions (acetate buffer pH 4.4, 30 °C). The lowest concentration detected were 10^{-9} M for Cu²⁺ ions and 5×10^{-10} M for Pb²⁺ ions, which compares well with that already reported for other electrodes modified with complexing polymer films (6,7). The regeneration by soaking for a few seconds into an 1 mM EDTA solution indicates that the modified electrode showed remarkable stability and thus could be used several times without significant loss of complexing ability. Moreover, the reproducibility of the electrode response to copper and to lead was demonstrated by using several electrodes prepared in the same experimental conditions. Through different electrochemical techniques like CV, LSV, the complexing properties of the others polymeric materials have been investigated. The response of the film P(Am-VPy) in presence of Cu²⁺, shows a peak of stripping corresponding to Cu. One important aspect is that this peak decreases in intensity as the stripping cycles are repeated. This would indicates that the stability

of the complex is not very high. Moreover, the intensity of the peak depends on the thickness of the film, because decreasing such thickness, decreases the current of the peak. This may be attributed to the amount of the available functional site for the complexing process. The response of P(AA-Sty) film shows that the intensity of the current for the stripping peak is lower than for P(Am-VPy), but the shape is more symmetric. The response of the P(Sty-VPy) film indicates that the intensity of the peak is very similar to that of PAAV under the same conditions. This would suggest that there is a competence between the polymer functional groups. At the investigated pH, the pyridine groups are basically protonated and the carboxylic groups are as carboxylate groups. For the detection of Pb²⁺, the best results were found for the film prepared from P(AA-Sty). By comparison of different copolymer compositions, it was found that for P(Sty-VPy) as the content of styrene increases the moiety increases the stripping peak of the ion. This may be associated with the separation between pyridine groups as they are protonated, allowing a higher interaction between the metal ion and the aromatic ring. The polymeric electrode material that can be applied to the determination of trace metals. The practical utility of this approach relies on a reproducible one step synthesis of the electrode material, on low detection limits, and on the ability of the electrode surfaces to be regenerated without loss of sensitivity.

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Supramolecular Stabilization in Calixarene Frameworks

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Abstract

The calixarenes are a diverse family of bowl-shaped molecules well known for their ability to form a variety of discrete and extended inclusion compounds. Both the tertiary butyl substituted and resorcinol-derived calixarenes have proven to be extremely versatile hosts, with the ability to form a variety of extended networks and include diverse guests. Typically, simple calixarenes such as 4-t-butylcalix[4]arene (4tBC4A) form 1:1 or 2:1 host:guest compounds, while c-methylcalix[4]resorcinarene (CMCR) will readily form hydrogen bonded structures with the resorcinarene assuming a closed cone conformation. Recently, we have observed that judicious selection of an appropriate guest and pH yield a much-extended chemistry for both 4tBC4A and CMCR. In our current study, we compare and contrast the structural motifs and physical properties observed in the polar clusters resulting from alkylamine inclusion in extended cavities formed with 4tBC4A. Similarly, we also examine the anionic frameworks that can be produced using various ions, bipyridines, and resorcinarenes.

New Polymeric Materials obtained from blending of Polypropylene and olefinic elastomers by using compatibilizers

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Abstract

The polypropylene can be improved by blending with other polymers. The aim of this study was to investigate the compatibilizing effect of functionalized PP as well as copolymers of ethylene-1-hexene and ethylene-1-octadecene on the compatibility of PP/PE- α -olefin blends. The effect of grafting of itaconic acid (IA) as polar monomer onto PP, ethylene-1-hexene copolymer (PE-C6) and ethylene-1-octadecene copolymer (PE-C18), via free radical reaction, on the processability, morphology and mechanical properties of PP/PE-C6 and PP/PE-C18 blends is presented in this work. Blends were characterized by tensile modulus, strength and elongation at break measurements. The blends containing grafted polymers show a higher toughness without any reduction of the strength and stiffness. The glass transition temperature of PP was increased slightly due to effect of PE-C6 domains on the segmental mobility of PP suggesting that an interpenetration between the noncrystalline portion of PP and the interface of PE-C6 exists.

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A photochemical method for the preparation of Zinc oxide thin films, and their potential use as gas sensor to CO

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Abstract

ZnO thin films have been successfully prepared by direct UV irradiation of amorphous films of B-diketonate complexes on Si(100) substrates. Deposited films were characterized by X-Ray Diffraction (XRD) and X-ray Photoelectron spectroscopy (XPS). The results showed that the stoichiometry of the resulting films is in agreement with composition of the precursor films. The optical properties of the films were transparent in the visible range above 400 nm and had sharp ultraviolet absorption edges at 380 nm aprox. The optical band gap energy was evaluated to be $E = 3.20-3.25$ eV. The surface characterization of these thin films was performed using Atomic Force Microscopy (AFM). This analysis revealed that zinc oxide films have a rougher surface, with rms values surface roughness varies between 14 and 20 nm. The experimental results of gas sensitivity of ZnO thin films, showed the highest CO gas sensitivity at 350-450 C.

Some experimental results with nanoscale assemblies and materials

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Abstract

Experimental results with molecular assemblies and materials in which at least one dimension is in the nanoscale will be described, and their properties discussed. These comprise:

a. Layer-by-layer electrostatically self-assembled enzyme multilayers with molecular (redox) wiring to electrodes and their structure-properties in particular electrocatalysis for biosensing, including molecular switches (molecular responsive transistors). b. Gold nanoparticle aggregation kinetics and optical properties c. Fabrication and manipulation of nanorods (Au, Ni, Au-Ni, etc.) d. Metallic conducting oxide nanotubes (LaNiO₃) e. Localized electropolymerization of poly(aniline) with a SECM

The techniques employed for the study of these systems include TEM and SEM electron microscopy, AFM, STM, FTIR and Raman spectroscopy, UV-Visible spectroscopy, electrochemical techniques, scanning electrochemical microscopy (SECM), quartz crystal microbalance, ellipsometry, etc.

Metallic Clusters Chemically Bound to Copper Surface

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Abstract

Several copper surfaces have been studied in order to chemically attach an organic spacer arm into the metal surface. The aim of this study is to prepare a well defined copper substate where a tri- or tetracobalt cluster can be placed and studied for its magnetical an resistivity properties. Though some authors believe that small thiols are siutable for SAM (Self Assembled Monolayers) we have checked the morphology of the adsorbate with different spacers (thiols). The lenght of the spacer arm has been varied in order to avoid destruction of the supporting layer by the smallest thiols. The resulting surface after thiol treatment has been studied by means of AFM. The effect of the presence and absence of oxygen during the adsorption of the thiol has also been studied, as well as the temperature and time evolution of the adsorbate. XPS was used to monitor the nature of the adsorbate observed by AFM.

New Metal Surfaces in Surface Enhanced Raman Spectroscopy for the Pollutants Detection

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Abstract

Contaminants polycyclic aromatic hydrocarbons (PAHs) are the major component of the soot formed in practically all combustion processes; their importance as pollutants stems from their documented biological activity. PAHs have been detected in the interstellar medium. Some results concerning the SERS spectra of PAHs have been published [1]; the scarce results mainly concern sol-gel embedded silver colloid and different coated silver systems for specific molecules. The main objective of this communication is to inform for the first time the SERS spectra of several PAHs at very low concentration levels by using a new metal surface. Present SERS spectra were obtained for pyrene, triphenylene, benzo(c)phenanthrene and chrysene. Each molecular system was deposited onto two different substrates: a silver colloid prepared by using hydroxylamine chloride as reducing agent and nitrate to favour the aggregation, and a self assembled 25,27-dicarboetoxy-26,28-dihidroxy-p-tert-butilcalix[4]arene silver colloid. Analytes were dissolved in acetone; final concentrations were lower than 10-12 M. Calix[4]arene was synthesized according well-known procedures. Spectrophotometer Bruker FT Raman model RFS 100/S was used for the spectral measurements; 1000 scans and 50 mW were the spectral conditions of scanning for the 1064 nm laser wavelength. A Renishaw spectrometer was used for the microRaman measurements by using the 785 nm excitation laser line. SERS spectra of several PAHs were obtained. The bands assignment of the solids was performed on the basis of previous data for PAHs and nitroPAHs [2] and references therein. Detection limits determined by using the 785 nm laser line goes to 10-12 M. The cavity diameter of the calixarene moiety is fundamental in the selective detection of the different PAHs.

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Bactericidal Properties of Chitosan Composite Films

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Abstract

The chitin (poly-b-D-glucosamide) from shrimp shells (*Pleuroncodes monodon*) by chemical methods is extracted. Later on, by means of basic treatment with NaOH the chitin was deacetylated and chitosan was obtained. The chitin and chitosan were characterized and several techniques such as: elemental analysis (characterization), FTIR, TGA (thermal properties), SEM (morphology), deacetylation degree and molecular weight were tested. Two chitosan were obtained, one of 100.325 g/mol and other 69.694 g/mol, with a degree of deacetylation 92 and 97 %, respectively. Subsequently, the chitosan is solubilized in weak organic acid at different concentrations and from that the chitosan film formation was tested. The biological activity against fungus such as *Candida albicans* and bacterias (gram (+) and gram (-)) were tested. The best activity against *Candida* was obtained and the best concentration was the lower molecular weight chitosan. The bacterial activity depends on the molecular weight. The higher molecular weight is more effective against gram (+) bacteria and for *Pseudomonas* is independent of the molecular weight.

Palladium and Germanium nanoparticles. HRTEM

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Abstract

Due to the interesting properties of these materials, it was proposed the Synthesis of Pd, Ge and Pd-Ge colloidal nanoparticles by means of CLD method. This method involves the resistive evaporation of metal and co-deposition at 77K with solvents like 2-propanol, acetone and THF. After a warm-up stage, colloidal dispersions of metal nanoparticles were obtained. Stable Pd colloids with average particle sizes between 2.2 and 2.8 nm were obtained, depending on the concentration and employed solvent. A study of the warm-up time variation allow us to control the particles size average in the 2-5 nm range. HRTEM studies in Pd colloids indicates three principal structure: cubooctahedron, tetrakaidecahedron and icosahedra. On the other hand, it was found that Ge colloid presents lower stabilities and the particle size depends strongly of the Ge concentration with average particle sizes between 3 and 30 nm.

Materials Science on Petaflop Computers

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Abstract

Predicting the properties and performance of materials is central to the success of major industries producing a vast range of consumer goods and to research programs at laboratories and universities around the world. For many years, scientists have longed to have computer simulations that predict the behavior of materials and track the evolution of their microstructures from the atomic to the engineering scales. Until recently, such simulations had been little more than an elusive goal. In recent years, the advent of ever more powerful, massively parallel computers, coupled with spectacular advances in the theoretical framework that describes materials, has enabled the development of new concepts and algorithms for the computational modeling of materials. As the field of computational materials science develops and matures, the notion is taking hold that modeling efforts should be an integral part of interdisciplinary materials research and just as it must include experimental validation. Lawrence Livermore National Laboratory will have 0.5 Petaflops (10^{15} flops) of computing power by early 2005. This represent more than the current TOP500 computers combined. What kind of scientific research can be done with such computer power? This talk will address this question through the work done at the Computational Materials Science Group of the Chemistry and Materials Science Directorate, LLNL. Applications from the electronic to the engineering scales, cover all relevant length and time scales.

Performance of new dispersion-precipitation strengthened copper-zirconium ceramic materials made by mechanical alloying

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Abstract

A new high temperature strength, high-conductivity copper based alloys were developed to achieve improved performance. The strengthening is provided by mechanical alloying during 12 and 30 h of milling under argon atmosphere with 1 vol % of ZrC or 1 vol % of ZrB₂ as fine dispersoids and by the interaction of others fine particles detected. The powder was hot consolidated by uniaxial hot pressing at 923 K and hot rolling with a 25% of reduction at 1073 K. After hot pressing, consolidated samples were microstructural characterized by microprobe EPMA, X-Ray Diffraction (XRD), and scanning (SEM) and transmission (TEM) electron microscopy (SEM-EDS). Hot consolidation process produced fully density MMCs materials with a satisfactory tensile strength as high as 650 MPa and electrical conductivity up to 48 % IACS. The effect of milling process on the microstructure and mechanical properties observed has been related to the pick up of iron, chromium, carbon and oxygen, with Fe-Cr oxycarbides and cuprospinel particles precipitated during hot consolidation. Transmission and scanning electron microscopy of consolidated alloys revealed that the strength of consolidated metal matrix composites Cu-Zirconium ceramics is consistent with estimates based on Orowan and Hall-Petch strengthening mechanisms.

Microstructure and Properties of PZT Ceramics With Grain Growth Control

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Abstract

Lead zirconate titanate ceramic powders have been surface modified by using phosphor ester 0.3% in volume. The phosphorous modification gave higher densities at lower temperatures associated with a reduction of the weight losses during the densification process. From the relationships between ceramic processing and microstructure, it was established that the phosphorous surface modification allows the effective grain growth control as well a higher homogeneity in the grain size distribution. Key words: Lead zirconate titanate (PZT), microstructure, sintering, grain growth control.

Hybrid Metal Oxide Framework Structures

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Abstract

Nanoporous inorganic materials, such as the aluminosilicate zeolites and the open-framework aluminum phosphates, find widespread applications in separation processes, ion-exchange, and catalysis. A large number of the other open-framework inorganics have been discovered in the last 20 years, often by using organic template molecules around which the inorganic frameworks are constructed. The rapid developments in the inorganic area have been paralleled by work on hybrid systems in which organic moieties are introduced into the framework itself, rather than merely occupying space in a pore system. This new generation of hybrid materials offers a wide range of chemical and physical properties that are only just beginning to be explored.

A major research theme in this field concerns *coordination polymers*, which we define as extended arrays composed of metal atoms or clusters bridged by polyfunctional organic molecules. Initial strategies focused on using rigid organic linkers to connect individual metal ions or clusters into extended networks, e.g. the work of Robson, Moore and Yaghi, who used connectors such as porphyrins ions to construct three-dimensional networks, often with the topologies of known structure types such as PtS and ThSi₂. More recent efforts, however, have clearly shown that flexible linkers can also be used to great effect.

A second class of materials contains infinite metal-oxygen-metal (M-O-M) arrays as a part of their structures. Early work in this area by Johnson and Jacobson showed how using diphosphonates to build connections between inorganic layers could create open, three-dimensional frameworks. It is now clear that hybrid frameworks can be made not only with layered metal oxide structures, but also with systems in which the metal-oxygen-metal (M-O-M) linkages are one- or three-dimensional. We collectively refer to this class of materials as *hybrid metal oxides*. The presentation will focus primarily on the structures and properties of this second class of hybrid materials.

Closed-shell cationic conducting polymers

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Abstract

A neutral conjugated polymer is not a good conductor of (DC) electricity. Only upon doping, either with an electron donor (n-doping) or an acceptor (p-doping) does the conductivity increase appreciably. If a closed shell polymer bearing formal charges could be prepared, the built in carriers would preclude the need for doping. Such a system should not only be highly conductive, but also much more robust than a traditional radical-ion polymer doped to a comparable degree (e.g. one charge per monomer). Polyaniline (PANI) seemingly behaves as a closed shell p-doped conducting polymer. From its un-doped state, the addition of a Brønsted-Lowry acid dopes PANI, however ESR investigations suggest a proton induced spin un-pairing that generates radical cations. Based on the remarkable stability of crystal violet, which reacts slowly in aqueous sodium hydroxide, and poly(thiophene) we aim to produce a conducting polymer bearing formal positive charges that remains ESR silent.

Study of Mononuclear and Binuclear Cu(II) Complexes derived from Redox Active Macrocycles and their Related Ligands

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Abstract

Robson type macrocyclic complexes are of interest as new materials and as models of biomolecules. The availability of a wide variety of planar ligands with different cavities offers the opportunity to study in detail magnetic phenomena, metal ion recognition, encapsulations, transport and separation effects, catalytic process, and new molecular devices^{1,2}. In this work we report the study of different copper (II) complexes with the macrocyclic and hemicyclic ligands, derived from condensation reaction of 2-hydroxy-5-methyl-1,3-benzenedicarbaldehyde with 1,2-diaminebenzene. Depending on the synthesis conditions it is possible to obtain three different complexes, a mononuclear copper(II) and dinuclear copper(II) hemicyclic complexes, and binuclear copper (II) macrocyclic complexes. The above mentioned compounds were characterized by different spectroscopic techniques, elemental analysis, magnetic susceptibility and electrochemical studies. Structural and physicochemical properties will be discussed.

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Tetranuclear Copper(II)Complexes:Structural Studies.

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Abstract

Since higher nuclearity copper(II) complexes are of current interest as model of copper metalloenzymes and inorganic materials. Special attention has been drawn to tetranuclear μ_4 -oxo bridged copper (II) complexes of general formula $[\text{Cu}_4\text{OCl}_6\text{L}_4]$ (L= Lewis-base ligand)

In this complexes the copper (II) atoms are configured in a tetrahedron around the μ_4 -bridging central oxygen. Each one of the four copper atoms is bridged by μ_2 -halides. In this work we describe the synthesis, and X-ray crystal structure of μ_4 -oxo-bridged copper (II) complexes with 2-methylimidazole and pyridine-N-oxide ligands.

Nanomaterials. Shape, size and properties

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Abstract

The properties of bulk materials essentially depend on the nature and on the geometrical arrangement of their individual atoms forming well defined crystalline or amorphous structures. However, the properties of nanostructured materials are also, and strongly, dependent on the size, shape and spatial correlation of their nanometric building blocks. The structure and mechanism of formation of nanostructured materials can be investigated by small-angle X-ray scattering (SAXS) and/or high resolution transmission electron microscopy (HRTEM). In this talk, a few experimental SAXS studies of the structure and process of formation of different types of nanocomposites will be reviewed, namely Bi liquid clusters and Ag nanocrystals embedded in a borate glass [1, 2], fractal zirconia-based sols and gels [3], and doped ZnO thin films [4]. Recent results of on going investigations of self-assembled nanoporous silica-based materials [5] and Pt-based catalysts [6] will also be presented. (*)

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(*) All reported experiments were performed using the LNLS synchrotron SAXS beamline (Campinas, Brazil).

Metallic Nanostructures from organometallic Polymers

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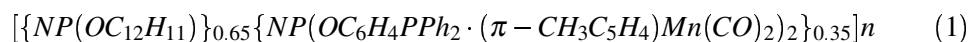
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Abstract

Among the methods used for to prepare metallic nanostructures those in solid state are the less available. This work describes the formation of metallic nanostructures from the organometallic polymer:



We have recently reported the synthesis and characterization of several organometallic polymers derived from polyphosphazenes [1,2] and here we report the formation of manganese containing nanostructures from the pyrolysis of the organometallic polymer (1). The polymer was thermolyzed in a conventional furnace in an air ambient. The resultant material was characterized by IR and Raman spectroscopy, TEM and SEM microscopy as well as by back scattered electron image. Elemental Analysis was obtained by EDAX. The pyrolyzed product exhibits metallic nanoclusters with size of about 74nm. Raman spectrum of the material indicated near-infrared photoluminescence. By analysing preliminary results with other organometallic polymers, a general solid state method for the preparation of metallic nanostructures is discussed.

Acknowledgements

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Preliminary Study of Calcium Salts Crystallization in Polymeric Gels and Films

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Abstract

It is well known that morphological changes in crystallization of calcium salts in nature is the result of the influence of biopolymers such as proteins and proteoglycans. These crystals subsequently grow until they become spatially restricted by the growing ends of adjacent crystals and by the proteins secreted into the palisade layer. Another hypothesis is that the structural organization is assisted by the organic matrix components or by the competitive crystal growth processes due to the presence of multiple nucleating sites. Chitosan, poly-b(1,4)-2-amino-2-deoxy-D-glucose, is the deacetylated product of chitin, poly(N-acetyl-D-glucosamine), a natural polymer found in the exoskeletons of crustaceans and insects and in the cell wall of fungi and microorganisms. In this work the influence of chitosan and modified chitosan by graft copolymerization with either acrylic acid or acrylamide on the crystallization morphology of calcium salts was investigated. The aim of this study was to approach the understanding of the changes in crystalline morphology of calcium salts induced by presence of the biopolymer. This in future could lead to the development of new materials. Both, high and low molecular weight chitosans were from Aldrich. They were purified before using for crystallization experiments or grafting reaction. Grafting reactions were carried out in solution at a predetermined time and temperature. Potassium persulfate (K₂S₂O₈) was used as initiator. In order to synthesize grafted chitosan with different degree of grafting, two different concentration of K₂S₂O₈ was used. The grafted polymers were characterized by FTIR spectroscopy. The crystallization was carried out by using the sitting-drop method, where a solution of CaCl₂ was put in contact with the biopolymer and in the presence of CO₂ produced by decomposition of NH₄HCO₃. The crystallization time was varied between 24 and 48 hours at 20 °C. Scanning electron microscopy (SEM) was employed to study the morphology of the obtained calcium salt crystals. A dramatic influence of the particular composition of grafted chitosan, used as structure-directing substrate, on the crystalline habit of calcium salts was found. The different active groups present in the grafted chains interact differently with the individual growing planes of the crystals. Potassium persulfate used as initiator in the grafting reactions with Polyacrylamide produced rosetts shaped calcium sulfate crystals together with calcium carbonate in some experiments using CH-gPAAM films. In the case of crystallization on CHI-g-PAA films small spheres or donuts-like shaped CaCO₃ particles were formed.

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Listening to bubbles on Gel

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Abstract

We input bubbles at the bottom of a vertical column made of Gel. Under Archimedes forces, the bubbles reach the top of the column, then explode. We listen to the sound of this exploding bubbles. It appears that the explosion is made of two distinct frequencies. The first one is high and linked to the expulsion of the air which fills the bubble. The second one, which is low, is linked to a surface wave.

The thorny issue is to explain why there's two so well defined frequencies for the explosion of a bubble. We show it is definitely not the fact of coalescing bubbles as proposed already.

We expect the same process to be involved in exploding bubbles on surface of lava, as the two frequencies can be heard. Thus understanding exploding bubbles on Gel is a way to probe the deep matter of earth, usually unreachable.

Teaching Old Materials New Tricks: Site-Specific Nanopatterning of Functional Nanostructures

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Abstract

Our recent research efforts at Northwestern University are geared towards designing intricate architecture of functional nanostructures, as well as using them as building blocks for device systems for sensing, diagnostics and therapeutics. Embedded in this scheme are several nanopatterning approaches, some are based on the original invention of Dip-Pen Nanolithography (DPN) developed at Northwestern.

The original DPN approach is modified to pattern, at the nanoscale, templates for inorganic and organic-inorganic complexes of arbitrary shape/size on arbitrary substrates, thus extending the efficacy and elegance of DPN. Subsequently, several direct methods (e.g. nano-fountain-pen) in conjunction with sol-based precursors have been developed for site- and shape-specific patterning of functional inorganics at nanoscale, thus circumventing the two-step template-based approach.

The talk will outline modified DPN and sol-based precursor Sinks as an enabling approach to pattern and characterize magnetic, electronic, chemical- and optical active nanostructures at the nanoscale. Success is already evident for magnetic oxides, inorganic mesoporous structures, ferroelectrics and optically-active nanostructures. The real need for characterizing structure/crystallography, 3-D morphology, local chemistry and conformation of such nanopatterns, as well as unambiguous measurement of their local properties, will be emphasized. The prospects for patterning at single-molecule resolution, especially for bioactive molecules, both by themselves and as templates for inorganics, will also be discussed.

It will be argued that functional nanostructures go beyond the shape, and present challenging yet exciting avenues for synthesis-structure-architecture -form-function-performance relationships, especially in hybrid organic-inorganic systems.

Luminescence Property of the Terbium 1,10 Phenanthroline Complex intercalated in natural Bentonite

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Abstract

In this work, we have studied the optical properties of the Terbium- 1,10 Phenanthroline Complex intercalated in a natural matrix, specifically Bentonite.

The complex and the intercalated compound were characterized by X-Ray Difraccction and elemental analysis. The optical measurements were carried out under UV-visible excitation.

The results demonstrated that the composite: Bentonite: Tb (Phen)₂ Cl₃ improved its luminescence compared with the complex. By UV-visible we could see that the absorption of the composite was increased compared with the complex and with Bentonite: TbCl₃. The absorption was below 300 nm in all cases.

The emission spectra of original complex and the composite consisted of two main lines:

(⁵D₄ - ⁷F₆) 489 nm

(⁵D₄ - ⁷F₅) 545 nm

The emission at 545 nm was the strongest. Moreover the emission of the composite were considerably greater than the complex.

These results indicate that the energy transfer takes place from the phenanthroline ligand to the Tb³⁺ ion.

Modification of calcium oxalate crystal morphology by specific macromolecules

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Abstract

Calcium oxalate is the main component of urinary calculi in humans, and the study of its crystallization is an important issue. Calcium oxalate presents two main degrees of hydration: the thermodynamically stable monohydrate (COM, whewellite) and the metastable dihydrate (COD, weddellite). Urinary calculi mainly consist of COM, while the urine of healthy people mainly contains COD crystals which do not aggregate into calculi. It has been demonstrated that some macromolecules contribute to the stabilization of COD. However, the mechanism by which these macromolecules stabilize COD crystals remains unsolved. Here we test the ability of individual or association of macromolecules with defined functional groups to change in vitro the morphology of calcium oxalate crystals viewed by SEM. In control conditions, COM crystals are formed. However, under the influence of particular macromolecules, noticeable modifications of the crystal morphology and hydration status was obtained. These modifications could be related with the nature and distribution of charged functional groups of the macromolecules. These results could provide some clues for designing molecules that could prevent the calculi formation.

Under Potential Deposition of Sulfides Compounds on Copper in Alkaline Solutions

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Abstract

Copper sulphide films find application application as condenser in satellite electronics, and ion sensors in analytical chemistry. Also this compounds was considered as a precursor reagent in the anodic electrochemical synthesis of films of the ternary semiconductor compound CuInS_2 . This compound can be formed by anodization of copper in $\text{NaOH} / \text{Na}_2\text{S}$ solutions and has been characterized at potentials more anodic than 1.0 V versus Standard Calomel Electrode (SCE). However the characterization of film formation at potentials cathodic with respect to 1.0 (SCE) has not been reported previously. This work presents a novel experimental methodology to characterize copper sulphide film formation at this low potential range.

The experiments were performed in a three-electrode electrochemical cell. The working electrode was a copper oxygen-free high conductivity copper (OFHC) doped with phosphorous. The surface exposed to solution was polished up to $0.5 \mu\text{m}$ with alumina powder. The counterelectrode was a platinum wire. The reference electrode was saturated calomel (SCE). The electrolyte was deoxygenated in a $0.001 \text{ M Na}_2\text{S} + 0.1 \text{ M NaOH}$ (Merck >98% purity) solution. Copper sulphide electrochemical formation was characterized by cyclic voltammetry and potential steps techniques. A potentiostat/galvanostat (EG&G Princeton Applied model 273A) was used as potential function generation and was connected to a data adquisition system. Copper sulphide films were characterized with X-ray photoelectron spectroscopy (XPS, Physical Electronics System model 1257), X-ray diffraction (DRX, Siemens D 5000) and scanning electron microscopy (SEM, JEOL model J8M-25-S2).

Experimental results suggested that the formation of sulphide specimen of copper that starts at $\sim 1.05 \text{ V (SCE)}$, a potential range lower than the previously reported. At this low potential range the net current is still cathodic and the film formation was evidenced from cyclic voltammetry peaks associated to the dissolution of the film. Growth of copper sulphide films at this low potential was also evidenced from XPS analysis which confirmed S-2 in the depth profiles of the copper electrode. DRX shows that the compound formed is gerite.

Influence of nanodispersoids on hot mechanical behaviour of dispersion-strengthened Cu alloys, prepared by reaction milling

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Abstract

The influence of nanodispersoids formed by reaction milling on the hot mechanical behaviour of Cu-2.5%vTiC-2.5%vAl₂O₃ and Cu-2.5%vTiC-2.5%vZrO₂ alloys was studied. The materials were prepared by reaction milling in an attritor mill, starting from elemental powders of the pertinent elements (Cu, Ti, Al, Zr and graphite), added in proper quantities as to form the nominal v% already mentioned. The hypothesis is that with the combination of two nanometric dispersoids in a copper matrix, which are resistant to different creep mechanisms, a greater hot strengthening will be obtained, in comparison with the case when the same volume fraction of only one type of dispersoid is considered. The mechanical behavior was evaluated by hot compression tests at 500 and 850 °C, at nominal strain rates of 10⁻³ and 10⁻⁴ s⁻¹. The strain-stress curves presented a typical hot-working shape: an initial maximum followed by a stationary plateau. An effective reinforcing effect was obtained at high temperatures. The temperature increase has a significant hot softening effect, while the rate of deformation has a low effect. The alloys that combine two types of dispersoids (Cu-2.5%vTiC-2.5%vAl₂O₃ and Cu-2.5%vTiC-2.5%vZrO₂), presented a greater resistance to softening and hot deformation than that of Cu-5%vAl₂O₃, Cu-5%vTiC and Cu-5%vZrO₂ alloys obtained in a previous research also using an attritor mill, thus validating the working hypothesis. This behaviour is explained in terms that in the alloys with two types of dispersoids, two strengthening mechanisms would be concurrently operative: incoherent particles (Al₂O₃ and ZrO₂) would limit dislocation detachment from particles and dislocation climbing, and TiC semi-coherent nanometric particles, observed by TEM, would limit grain boundary sliding through pinning. From analysis and observations in an Energy Filtered Transmission Electron Microscope (EFTEM), the presence of TiC elongated particles (20 to 30 nm thick), and of Al₂O₃ spherical particles (8 to 20 nm diameter) was observed. Intermetallic (Al,Ti) particles (20 to 100 nm size) were also detected, mainly in the alloy prepared in the high-energy mill. The formation and precipitation of these dispersoids would explain the observed improvements in the mechanical behavior of these alloys, even after a heat treatment at 900 °C.

Characterization of Some Macromolecules Involved in the Mineralization of Three Species of Scleractinian Corals

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Abstract

Scleractinian corals are the largest biomineralized structures in our planet. They constitute huge calcareous structures formed as exoskeletons by colonies of small invertebrates, the porifera (actinians).

As a step to the understanding of the mechanism of calcification of these structures, samples from three different species of scleractinian were studied, by looking to the occurrence and distribution of particular organic matrix components, the proteoglycans. The three species studied were *Favia stelligera* (Dana, 1846), *Lophelia pertusa* (Linnaeus, 1758), *Porites porites* (Pallas, 1766)

To analyze the general distribution of proteoglycans, Alcian Blue staining of proteoglycans was used, and for an specific characterization of these sulfated macromolecules, monoclonal antibodies against some proteoglycans present in other bioceramics, like chondroitin 4 sulfate, chondroitin 6 sulfate, dermatan sulfate and keratan sulfate were used.

These four macromolecules were present in the three species studied, but they differed in the distribution and spatial arrangement throughout the skeleton.

These results confirm the universality of the mechanism of biomineralization, where some ubiquitous macromolecules command the biomineralization process.

Effects of pH and other variables on catalytic currents and nanoarchitectures of redox enzymes biosensors. Models and Experiments

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Abstract

We electrostatically self-assembled electrodes to work as biosensors. We self-assembled layer-by-layer a redox polymer (PAH modified with an Os complex) with a redox enzyme (glucose oxidase) in multilayer nanostructures. The effect of polymer concentration, pH, and ionic strength on the nanoarchitecture of the multilayer electrode and on the generated electrical signal were studied by cyclic voltametry, quartz crystal microbalance and ellipsometric techniques.

We designed experiments to test the special kinetic cases in Pratt-Bartlett model of coupled diffusion/reaction processes, and to move from case to case by varying the experimental variables (thickness, concentrations, potentials, etc.) Layer-by-layer organised structures go from monolayer to thick layer that resembles a hydrogel where diffusion profiles are fully developed. Comparison of experimental results to digital simulation and case diagram predictions test the model.

This approach allows us to describe the concentration profiles across the enzyme film and the extension to multi-enzyme films and is used to contrast with the theoretical prediction with Pratt-Bartlett case diagrams.

We conclude about the catalytic capacity of the enzyme immobilized within different nanoarchitecturesadsfff

Growth and morphology of a Cu/Fe/Cu(100) system: preliminary results.

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Abstract

Both academic interests in novel nanomagnetic phenomena, as well as their technological importance for magnetoelectronics and high density magnetic storage devices make of the study of ultrathin ferromagnetic films particularly worthwhile. These extremely thin films, typically less than 10ML thick, exhibit significantly different magnetic properties in contrast to the bulk material. The epitaxial system Fe/Cu(100) has been studied extensively for the last decade owing to its ability to stabilize the fcc phase and also other entirely novel ferromagnetic phases of Fe at low temperatures. Besides their relevance for various other thin film issues, these experiments aim at a better understanding of the interrelation between structure and magnetism, which is of increasing importance for the design of special purpose magnetic thin films. The prototypical phase transitions of Fe are also of interest in others research are as including geophysics, metallurgy, and computational materials science.

Non-equilibrium metal on metal epitaxial growth and resulting are not readily probed with single techniques. Periodic structure revealed by diffraction, and composition from spectroscopy, are well complemented by real space imaging using STM. The structure of the initial deposition below 10ML, is not well understood due to the stabilization of Fe fcc and its resultant magnetic properties. The quality of the interface between the Cu substrate and Fe overlayer affects the magnetic properties of the very thin layers and sandwiched structures, but studies to date do not provide a complete or accurate picture of the microscopic growth structures and mechanism in this very low coverage regime.

On this work we present preliminary results of topographic studies with STM on ultrathin layer of Fe embedded in Cu, Cu/Fe/Cu(100). The Cu on the top surface was investigated, at room temperature, using different coverages ($\sim 7\text{ML}$). We have observed the apparition of a transition in the growth mode for 7ML.

This work was performed in the Laboratory for Surface Modification, in Rutgers University, with the partial support of the following grants: MECESUP FSM9901, FONDECYT, Fundación Andes and ICM.

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Polypropylene Reinforcement with Colombian Natural Fiber Bundles

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Abstract

This study reports the possibility of using natural fibers such as fique, banana and platane to reinforce modified polypropylene. The mechanical behavior of composites has been studied as a function of fiber type, fiber length, fiber content, fiber treatment and the content of maleated polypropylene (MAPP) used as a coupling agent. The experiment was carried out employing Taguchi method, looking forward to maximize flexural or impact resistance. Fiber treatments correspond to alkalization and steam explosion. The mechanical properties of treated fiber composites are higher than those for untreated fiber ones, due to the enhancement on fiber properties and fiber/matrix adhesion.

Fabrication Optimization of Dielectric Composite Materials with Taguchi method

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Abstract

Epoxy resins are widely used in different technical applications, including dielectrical composite materials, due to their high mechanical, dielectric, thermal and chemical properties. However, this behavior is strongly conditioned to curing conditions. In this study, the Taguchi method has been used to maximize the flexural behavior of dielectric epoxy resin reinforcement with glass fiber. The process parameters evaluated are: curing temperature, curing time, pressure and amine/epoxy group ratio. The study shows that the Taguchi method is suitable to solve the stated problem with minimum number of trials.

Physico- Mechanical Behavior and Morphology of Colombian Fibers After Different Treatments

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Abstract

In recent times, several researches have been carried out for analyzing the possibilities of vegetables fibers as potential reinforcement of thermoplastic and thermoset matrices. However, natural fibers usually are treated using physical and chemical processes in order to enhance the fiber/matrix adhesion. Generally, these treatments may cause changes on their mechanical, physical and thermal behavior, as well as alterations on morphology. In the present study, physical and behavior of untreated and treated Colombian natural fibers has been investigated. Fibers have been extracted from fique leaves and bunch of waste plants of banana cultivated in Colombia. Steam explosion and alkalization treatments have been evaluated. Mechanical properties of untreated and treated Colombian fibers have been evaluated. Alkalization treatment leads to significant increments on tensile properties whilst steam explosion treatments do not introduce important variations. Morphological analysis of untreated and treated fiber has been developed by optical (OM) and scanning electron (SEM) microcopies.

The Crystallography Laboratory Associated to the CIMAT

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Abstract

The main reasearch subject of the Crystallography Laboratory is the synthesis and crystal structure determination of inorganic complexes, as well as the study of the eventual correlation between structure and physico-chemical properties. In adition the Laboratory has developed a wide network of national and international (Argentina and France) collaborations with groups which produce organic and inorganic compounds. Presently the staff is composed by a senior scientist, two graduate and one under-graduate students as well as a chemical engineer. Regarding powder difraction the Laboratory runs a technical service for the chilean industry at the same time that provides teaching assistance and training support at a university level (Faculties of Physical and Mathematical Sciences, Chemical Sciences, etc).

Electrochemical study of copper nucleation on AISI316 stainless steel

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Abstract

The nucleation mechanism of copper deposited onto 316 stainless steel polished and anodized substrates from sulfate solutions were studied by electrochemical techniques (cyclic voltammetry and chronoamperometry). The electrolyte contained 0.04 M Cu^{2+} 0.1M H_2SO_4 in anaerobic conditions (N_2). Potential step were performed to characterize the deposition process during the early stages of nucleation. For both substrates, the current could be fitted to two different models that assumed instantaneous nucleation. The nucleation mechanism was confirmed by SEM analysis of electrode surfaces.

Thermal conductivity in granular materials.

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Abstract

We report two experimental studies of the thermal conductivity of granular materials.

When water is added to a granular packing, because of the formation of liquid bridges at the contacts between grains, the thermal conductivity increases. Below a critical amount of water, the number of bridges increases. Above, any additional water simply flows by gravity to the bottom of the container. Simple theoretical models account for both the critical amount of water and the measured thermal conductivity.

In addition, the response of a chain of beads to thermal cycles clearly shows why granular material are so good thermal insulators.

New Zeolite Topologies Based on Intergrowths of the FAU/EMT Systems

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Abstract

The impact of zeolites as catalysts for refining processes has been mainly associated to the regular distribution of channels and cavities which determine the distribution of product species on terms of geometry and size. In the search of new structures with new topologies the controlled synthesis of zeolites with stacking defects forming intergrowth structures looks very promising. In this work the controlled synthesis of intergrowths of zeolites FAU and EMT was carried out by the mixture of the organic templates 15 Crown-5 and 18-Crown-6 in different proportions. The materials were characterized by high resolution scanning electron microscopy (HRSEM), atomic force microscopy (AFM), nitrogen adsorption measurements, X-ray diffraction and m-xylene catalytic reaction at 773 K. The proportion of intergrowths was determined by the simulation of the X-ray diffraction pattern using DIFFaX computing program. HRSEM revealed the size and topology of the crystals. The average particle size for FAU is about 0.5 μm and for EMT around 4 μm . The intergrowth particles have an average particle size of 4 μm and are formed by hexagonal plates of EMT on which regions with the characteristic FAU morphology are observed. This morphology has been previously reported as characteristic of the intergrowth FAU/EMT. The photomicrographics shows the surface details for FAU, EMT and the intergrowth FAU/EMT. Detailed surface measurements using AFM on the intergrowth particles showed a minimum step height of 2.1 nm and multiples of this height were always found. Through the X-ray modeling the formation of clusters of intergrowth material was determined to represent blocks of FAU and blocks of EMT rather than random stacking arrangement of layers of FAU/EMT. Xylene isomerization reaction was used as a model reaction for elucidating the pore and cage size of the solid catalysts.

EXAFS, In-situ FTIR, and CO Oxidation Activity Studies of the State of the Active Surface and Particle Size Effect on Pt Supported Catalysts.

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Abstract

The effect of the precursor used, different pretreatments and the particle size effect on the activity of Pt-supported catalysts have been studied by in-situ IR and controlled atmosphere EXAFS spectroscopies, and kinetic studies during CO oxidation. Catalysts containing 1.5% Pt/Al₂O₃ were prepared by incipient wetness from H₂PtCl₆ and Pt(NH₃)₄(NO₃)₂ precursors. At low reactant concentration (0.3 vol.% CO, 16 vol.% O₂) the Cl-free catalyst was at least 10 times more active than the Cl-containing catalyst during complete oxidation. Addition of HCl to the Cl-free catalyst rendered its activity identical to the catalyst prepared from Cl-containing precursors. The presence of Cl also affects the activity of 2% Pt/SiO₂ catalysts, but to a lower extent. IR results show that chlorine significantly reduces the amount of CO adsorbed on metallic Pt sites. The catalyst activities correlate well with the amount of reduced surface sites, and a model is proposed to explain the mechanism of chloride poisoning, which is shown to occur mainly by site blocking. EXAFS studies show that calcination of Pt catalysts leads to Pt(IV) with 6 nearest neighbors, 6 Pt-O in the Cl-free catalyst and 2.5 Pt-Cl and 3.5 Pt-O in the Cl-containing catalyst. No Pt-Pt distances are observed in the calcined catalysts. Reduction at 300°C in H₂ results in the complete reduction to small metallic Pt particles with no presence of Pt-Cl distances. After further oxidation in oxygen at 300°C, the Pt-Pt coordination distance of 2.7 Å with coordination numbers of 3.6 (Cl-free) and 0.9 (Cl-containing) indicates that the small metallic Pt particles are not fully oxidized. In the Cl-free catalyst there are Pt-O distances at 2.05 Å; while in the Cl-catalyst there are both Pt-O and Pt Cl distances. The activity of catalysts with different crystallite sizes was measured after two different pretreatments. Half of the samples were calcined at 200°C in air for 3h, whereas the other half was reduced in 50% H₂-He mixture for 3h at 200°C before reaction. The results indicate that the calcined catalysts show no measurable activity below 100°C whereas the reduced catalysts exhibit activity at low temperature. As the temperature increases the TOF of both reduced and calcined samples tend to be similar for each dispersion. It was also observed that for both pretreatments, calcination and reduction, the catalysts with lower dispersion exhibit a slightly higher activity than the catalysts with the highest dispersion. When the specific reaction rates were analyzed in an Arrhenius plot the apparent activation energy decreases as the dispersion of the Pt/SiO₂ catalysts decreases, clearly demonstrating that the small crystallites have sites that are less active than the large crystallites. EXAFS results show that only metallic Pt surfaces are present after reduction at 300°C and that when these surfaces are re-oxidized the highly dispersed catalysts are easier to oxidize than the larger crystallites. The results of an in-situ IR experiment with a sample that was not reduced but only calcined at 400°C show

no CO adsorption at room temperature. As the sample is continuously heated in the reaction mixture, at 100°C a small and broad band at 2105 cm⁻¹ appears. However as the temperature increases a band at 2077 cm⁻¹, corresponding to linearly adsorbed CO, starts developing while the band at 2105 cm⁻¹ decreases. Ignition starts at about 160°C but it is not abrupt as in the case of the reduced sample, with adsorbed CO not detected above 180°C. The interpretation of these IR results is that the surface starts fully oxidized and only a small amount of CO is adsorbed on such oxidized surface. As the temperature increases 1% CO in the reactant stream is sufficient to start reducing the surface presumably through an Eley-Rideal mechanism. Further exposure to CO at higher temperatures reduces even further the surface until the temperature is high enough so the LH mechanism starts operating, as it is the case on the reduced surface.

Stress distribution and basic mechanisms of fracture in natural bioceramic materials

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Abstract

We have built a machine to apply localized forces on a small sample of bioceramic material like nacre, in order to study the induced strain/stress fields in a plane geometry configuration. We shall be able to study bending and fracture phenomena by performing three- and four-point mechanical tests on thin or thick samples of any biological rigid material. In order to obtain the displacement field we use Electronic Speckle Photography (ESP). Within this method, a laser beam, focused on the surface of the sample, changes when the latter is subject to deformation. By evaluating the correlation of the speckle patterns prior and after deformation in successive subregions of the entire image, we obtain the displacement in each subregion. The strain field is estimated via differentiation.

Hydrothermal- Stable Mesoporous Aluminosilicates Obtained from Zeolite Seeds

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Abstract

Aluminosilicates of zeolite type are important catalysts for cracking processes in the petrochemical industry. However, their small pore size limits the molecular size of the compounds to be treated. Thereafter, mesoporous aluminosilicates (pore size $> 20 \text{ \AA}$) are currently investigated in order to transform major molecules. Since the discovery of MCM-41, numerous mesoporous materials have been obtained, among which HMS, MSU-X, KIT-1 and SBA-15 are important representatives. However, the low hydrothermal stability of the solids decrease notably their practical applications. This work presents the synthesis and characterization of mesoporous aluminosilicates obtained from zeolite Y and ZSM-5 seeds under hydrothermal conditions and basic pH. The samples were characterized by means of adsorption of N_2 , XRD, ^{27}Al MAS NMR, SEM and TEM. The presence of acid sites was confirmed by means of FTIR spectroscopy using the pyridine adsorption method. The mesoporous aluminosilicates presents high surface areas (around $500 \text{ m}^2/\text{g}$) with pore volumes between 1.0 and $1.3 \text{ cm}^3/\text{g}$. Since their surface area remained higher than $350 \text{ m}^2/\text{g}$, the materials synthesized from zeolite seeds showed very good hydrothermal stability under the strong conditions (24 h at $150 \text{ }^\circ\text{C}$). These results shown that the presence of protozeolitic units provide additional stability to the aluminosilicate network.

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Crystal and Molecular Structure of the 3,3'-Dioctyltetrathiophene

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Abstract

The title compound crystallizes in the Triclinic System, space group P-1, where the asymmetric unit consists of two molecules of 3,3'-dioctyltetrathiophene, rather similar. In the crystalline space the structure is stabilized by vander Waals forces that link the molecular chains in a zig zag way.

A quantitative model of eggshell growth

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Abstract

Eggshells present remarkable properties, both from mechanical and structural point of view. It may thus be of practical importance to understand and model eggshell formation. The basic model we consider has two stages. In the first stage, calcium and carbonate ions are deposited on each mamilla (the nucleation structures of the eggshell) in the form of columns of expanding thickness which eventually meet, and the interaction among the different growth sites is neglected. The second stage is initiated as the columns meet, and the shell grows as a whole due to two effects: diffusion and surface curvature. These two effects are captured by the Kardar–Parisi–Zhang (KPZ) equation, which gives a local description of growth. Good agreement is obtained with observed pore structure as well as with observed surface roughness.

Growth and Characterization of Thin Films of Tungsten Carbide (WC) on Steel Substrates

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Abstract

The Tungsten Carbide, is a material of great use in the industry, mainly in the area of coatings. In this work one has focused to grow tungsten carbide by the pulsed Plasma technique and thus to create an ample protocol that indicates optimal conditions of growth and a complete characterization of the required procedure to obtain WC, with a very good level of adhesion. The done characterization, by the technique of XRD, to the first produced films has demonstrated the formation of WC in cubical phase, which demonstrates that the technique of pulsed arc is favorable for the production of this coating. The improvement of the tungsten target, an ample control of the temperature of the same one in the unloading process and to make gas mixtures to be used like work gas, is efforts that are made aiming to improve the films in which to superficial adhesion.

Fabrication and Characterization of CaTiO₃ Ceramics and Coatings

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Abstract

Raman spectroscopy was performed to characterize CaTiO₃ ceramics in the temperature range from 80 K to 870 K. The samples were prepared under different pressure and temperature conditions, and the temperature is seen to be the most important factor. Calcium titanate coatings on titanium were obtained by the hydrothermal-electrochemical method and these were examined by Raman at room-temperature. The films showed CaTiO₃ spectra in polycrystalline form. Scanning electron microscopy (SEM) was used to observe the surface morphology and also cross sections revealing the growth of films up to 300 nm in thickness. The energy dispersive spectrometry (EDS) analysis showed carbon, calcium, titanium, oxygen and magnesium on the titanium surface, which can be useful in biocompatible applications.

Electrochemical Studies and Modelling of Anodic Dissolution of Chalcopyrite in H₂SO₄ solution at 70 °C

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Abstract

Study the Enrolled Mechanism to Vanadium Pentoxide and Molybdenum Disulphide Nanotubes

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Abstract

Template-directed synthesis represents a promising route to formation 1D nanostructures. In this kind of approach the template (long primary amines) act like a structural direct agent, also the mainly function is to generate nano structure in situ [1].

Vanadium pentoxide xerogel have rich intercalation chemistry [2], also the formation of vanadium pentoxide nanotubes (VO_x-NTs) is possible by hydrothermal treatment of lamellar V₂O₅-long-chain primary amine (e.g. hexadecyl- or octadecylamine) intercalated [1]. Other material promising is the molybdenum disulphide [3, 4] to obtain nanotubes through the same approach.

In this work we will describe the synthesis and characterization of molybdenum disulphide nanotubes by electron microscopy techniques (SEM, TEM), XRD, FT-IR, Raman, but focusing in the description the mechanism to formation of this kind of nanostructures, using our experience in the intercalation of MoS₂ [2]. We discuss the differences in the formation of VO_x-NTs and MoS₂-NTs both obtained by hydrothermal treatment of lamellar products.

VO_x-NTs with dimensions of about 60 nm diameter and lengths in the range 1-3 μm were obtained; the molybdenum disulphide nanotubes have lengths in the range 2-12.5 μm and diameters in the range 400-60 nm (outer), 100-25 nm (inner).

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Sulfidation of Modified Fe-9Cr-1Mo Alloy in Reducing Environments with Hydrocarbons at High Temperature

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Abstract

Sulfidation resistance of modified 9Cr-1Mo ferritic steel (ASTM A-335 Gr.P91), has been evaluated at three different temperatures, 550, 650 and 750°C, in a CO - CO₂ - CH₄ - H₂ gas mixture and additions of 0.1 and 1.0% Vol.H₂S, with exposition times between 1 and 300 hours. Tests were carried out in function of weight gain with the exposition time. The P91 steel was sulfidized according to a complex kinetics with an initial lineal rate law, followed by a parabolic rate law, for a concentration of 0.1% Vol.H₂S. However, for the same gas mixture and concentration of 1.0% Vol.H₂S, the kinetics behavior was inverse, initially parabolic and after lineal. The scales formed on the steel surface, consist basically of three layers: an internal layer which is adjacent to metallic substrate, with low content of iron and chromium oxides; an intermediate layer composed by iron and chromium oxides in different proportion, and finally an external layer composed mainly by iron and chromium sulfides, and some times, by silicon oxides. It was observed an acceleration of the sulfidation kinetics when the content of H₂S was 1.0% and the detachment of the external layer in the surface, with evidence of weight loss of the base metal. This detachment has been explained by formation and accelerated growth of a layer, due to its size, it generates internal stresses that produce the detachment of the external layer of FeS, with a strong influence of the concentration of H₂S in the gas mixture; in some cases, also, by the presence of pores in the external-intermediate layer interface. At low concentrations of H₂S, the layers formed are continuous, homogeneous and adherent, contrary to high concentrations of H₂S that are friable, porous and little adherents. It was found that the size of the layers is function of temperature and concentration of H₂S.

Key words: Sulfidation, High Temperature Corrosion, Modified 9Cr-1Mo steel ASTM A-335 Gr. P91, Kinetics, Ferritic Steels.

Synthesis and Properties of NiSn Colloids Using Different Metal Ratios by CLD

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Abstract

The NiSn colloids were synthesized by the Chemical Liquid Deposition method in which the Ni and Sn atoms, were co-deposited at 77K with acetone, 2-propanol and 2-methoxyethanol vapors to obtain colloidal dispersion. The molar relation is 1:1, 2:1, 3:1, 1:2 and 1:3, the evaporation of solvents produces fine divided solids. The characterization of colloids and active solids is using TEM, FT-IR, UV-Vis, TGA and Electron Diffraction. The greater stability is represented in the NiSn colloids prepared with 2-methoxyethanol (>30 days). The UV-Vis measurements showed absorption bands at 204 and 270 nm. A 3-day study in which samples were taken every hour showed that the absorption bands decrease probably due to clustering. Studies in TEM reveals an average size distribution between 6 to 14 nm depending on the solvent. The FT-IR spectra show the presence of the solvent incorporated in the active solids. The thermal stability of these bimetal powders was studied by TGA up to 550°C.

New Metal Surfaces in Surface Enhanced Raman Spectroscopy for the Pollutants Detection

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Abstract

Contaminants polycyclic aromatic hydrocarbons (PAHs) are the major component of the soot formed in practically all combustion processes; their importance as pollutants stems from their documented biological activity. PAHs have been detected in the interstellar medium. Some results concerning the SERS spectra of PAHs have been published [1]; the scarce results mainly concern sol-gel embedded silver colloid and different coated silver systems for specific molecules. The main objective of this communication is to inform for the first time the SERS spectra of several PAHs at very low concentration levels by using a new metal surface. Present SERS spectra were obtained for pyrene, triphenylene, benzo(c)phenanthrene and chrysene. Each molecular system was deposited onto two different substrates: a silver colloid prepared by using hydroxylamine chloride as reducing agent and nitrate to favour the aggregation, and a self assembled 25,27-dicarboetoxy-26,28-dihidroxy-p-tert-butylcalix[4]arene silver colloid. Analytes were dissolved in acetone; final concentrations were lower than 10⁻¹² M. Calix[4]arene was synthesized according well-known procedures. Spectrophotometer Bruker FT Raman model RFS 100/S was used for the spectral measurements; 1000 scans and 50 mW were the spectral conditions of scanning for the 1064 nm laser wavelength. A Renishaw spectrometer was used for the microRaman measurements by using the 785 nm excitation laser line. SERS spectra of several PAHs were obtained. The bands assignment of the solids was performed on the basis of previous data for PAHs and nitroPAHs [2] and references therein. Detection limits determined by using the 785 nm laser line goes to 10⁻¹² M. The cavity diameter of the calixarene moiety is fundamental in the selective detection of the different PAHs.

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New zeolites with structure of defects: Synthesis and Characterization

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Abstract

The synthesis of intergrowths of the zeolite systems MFI and MEL was carried out. Detailed characterization of the materials obtained was performed by combined use of different structural analysis techniques such as x-ray diffraction, high resolution scanning microscopy (HRSEM) and high resolution transmission microscopy (HRTEM), electron diffraction and atomic force microscopy (AFM). The images obtained by HRSEM showed that solids consisted of spherical granules (MFI), ovulate granules (MEL) and intermediate morphology (intergrowth MFI/MEL) having a size between 4-6 micras. The particles of these zeolites were assembled by many individual blocks which differed in dimensions from about 25 nm to 140 nm as well as in shape from very frequently almost rectangular (for MFI, MEL and MFI/MEL) to sometimes roundish or irregular habits (mainly for MFI/MEL). A detailed study of the surface topography was performed by AFM, the fine surface structure of zeolites particles was terrace-like with steps between adjacent terraces typically in the range of 20 nm to 60 nm; the minimum step measured was approximately 4 nm. HRTEM images of the intergrowths system show the presence of stacking faults, twins and pore coalescence. Streaking in the electron diffraction pattern evidenced the stacking disorder present in these system.

Performance of New Dispersion-Precipitation Strengthened Copper Zirconium Ceramic Materials Made by Mechanical Alloying

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Abstract

A new high temperature strength, high-conductivity copper based alloys were developed to achieve improved performance. The strengthening is provided by mechanical alloying during 12 and 30 h of milling under argon atmosphere with 1vol % of ZrC or 1vol % of ZrB₂ as fine dispersoids and by the interaction of others fine particles detected. The powder was hot consolidated by uniaxial hot pressing at 923 K and hot rolling with a 25% of reduction at 1073 K. After hot pressing, consolidated samples were microstructural characterized by microprobe EPMA, X-Ray Diffraction (X-RD), and scanning (SEM) and transmission (TEM) electron microscopy (SEM-EDS). Hot consolidation process produced fully density MMCs materials with a satisfactory tensile strength as high as 650 MPa and electrical conductivity up to 48 % IACS. The effect of milling process on the microstructure and mechanical properties observed has been related to the pick up of iron, chromium, carbon and oxygen, with Fe-Cr oxycarbides and cuprospinel particles precipitated during hot consolidation. Transmission and scanning electron microscopy of consolidated alloys revealed that the strength of consolidated metal matrix composites Cu-Zirconium ceramics is consistent with estimates based on Orowan and Hall-Petch strengthening mechanisms.

Micromagnetic simulation of Nanomagnets

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Abstract

Using micromagnetic simulations we perform a detailed study of square, circular, triangle and Relax triangle nanomagnets. Iron, permalloy, cobalt and nickel are used as material of the nanomagnets. The sizes of nanomagnets are almost the same and their magnetic behavior is studied for three different thickness (10, 20 and 40 nm). A rich of magnetic states is found and the dependence of hysteresis loops on the nanoelement shape is presented.

Synthesis and Characterization of Metal Oxides Foams

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Abstract

In the search of new materials, the functional material have appeared, there are especially interest the material super-structured with high porosity, high surface area, and conductors and catalytic characteristic. The functional activity of these materials this intimately related to the thickness of the material. If the layers thickness are thinner, its properties semiconductors and catalytic are modified considerably. Among the methods to obtain nanoestructuras are the processes: sol-gel [1], and the templeted use in routes non-hydrolytic [2]. An interesting type of materials are the foams. That are material ultra-light with a high macro- porosity that are generated for the intercalation of a surfactante and the production of bubbles of oxygen in situ [3,4].

In the work, we describe the synthesis of metal oxides foams (TiO₂, CrO₃, MoO₃, V₂O₅). The hexadecylamine are the templeted and H₂O₂ is source of oxygen. The products are characterized by Elemental Analysis, X-Ray Diffraction, DSC, DTG y FT-IR. We study the intercalation of amine in oxide and we obtain sponge-like nanoporous materials with lamellar mesostructure.

The optical properties of foams are determined using Difusse Reflectance UV- VIS spectroscopy (DRS). The products show displacements of the pattern of absorption with respect to the initial oxide which depend of the nature of the same oxide. Those changes in function of the huesped-host effects are discussed.

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Compoasting Process of Cast ZAMAK Particulate Composites

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Abstract

In this work is described the synthesis of two base Zamac particulate composites that were processed by compoasting in an experimental equipment that was built during the research. The obtained materials were reinforced in one case with calcined fine coke particles with low sulfur content which comes from processes of drying and sifting of hydrocarbon remainders, and in a second case, with fines particles of SiC-Bheta obtained from the pyrolysis of rice husk. For this last case, the synthesis of the SiC was carried out in a gas furnace and the process was optimized by an experimental design that includes variables like the temperature, pyrolysis times, catalyst type and atmosphere of the process.

The characterization of both composites was made using mechanical tests and microscopic observation. About the tensile strength, improvements with respect to the base material after adding the reinforcement material are obtained for both cases. On the other hand, the hardness results show that the carbonaceous particles diminish the hardness of the composite whereas the SiC particles increase it.

Synthesis of Organo-Inorganic Hybrid Films and their Potentialities as Functional Materials

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Abstract

The hybrid films in which silica is combined at molecular or nanodominion scale with organic polymers present great interest in the field of biocompatible materials, nanolithography, etc. Using the sol-gel method, a network-forming precursor sol and organic compounds can be combined under soft conditions to develop this kind of materials. Recently we have developed hybrid polymeric films from chitosan (CHI), poly(monmethyl itaconate) (PMMI) and silica (SiO₂) based on the formation of an interpolymeric complex between CHI and PMMI. The siloxane sol is generated by controlled hydrolysis of tetraethoxysilane using acid catalyst and low relative quantity of water. The products can be obtained in the form of self-supported transparent films and also as coating of glass and graphite surfaces due to the great adherence of these hybrid materials.

In this system it is possible to control the concentration of amino and carboxylic groups in the film and therefore change the ionic properties varying the composition of the organic components. Due to the adherent properties of these films, they constitute an attractive material to be used as transparent coatings for ion exchange reactions. They were cast on the surface of a graphite electrode of the all-solid state type and the sensor properties of the hybrid films as ion selective membranes were studied. The sensing capacity of the nanocomposite was examined for different anions, where best results were obtained for NO₃⁻ ions by using a film of composition 0,6:1:0,3 (CHI:SiO₂:PMMI). The response time of the electrode was 20 seconds and it could be used without divergence for a period of two weeks. Also, the hybrid films, with adjustable protonation degree by means of a simple pH variation, can be used as matrix for the incorporation of functional inorganic particles such as semiconductors or magnetic particles. The in situ formation of CdS nanoparticles was studied. The absorption and emission spectra of the CdS demonstrate quantum size confinement effect. As the CHI concentration increases in the films the UV threshold of the samples is blue-shifted relative to bulk CdS at 520 nm and at the same time a maximum associated to the excitonic transition is observed. This indicates a narrow distribution of the particle size. The combination of the adherent properties of these films and the optic transparency jointly with a further functionalization with inorganic particles may lead to the development of new functional materials.

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Nucleation and selective growth of polymorphs of calcium carbonate in organic-inorganic hybrid films

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Abstract

The biological systems use organic molecules (fundamentally proteins and polysaccharides) to control the nucleation and growth of minerals in an organic matrix. In this way such hybrid materials are formed as bones, teeth, and shells of mollusks by means of the biomineralization process. The biomacromolecules that participate in the production of these composites can be classified into water-soluble proteins and water-insoluble macromolecules such as chitin and collagen that work as solid matrixes. The study of the influence of structured organic surfaces and soluble organic macromolecules in the orientation and growth of inorganic crystals is a fundamental aspect in biomimetic mineralization processes that has attracted a great attention.

A fundamental factor for the heterogeneous nucleation of mineral crystals in organic substrates is to increase the charge density on the surface of the matrix. In this work, our approach has been to study the crystallization of calcium carbonate (CaCO_3) in organ-inorganic ternary hybrid films constituted by poly(monomethyl itaconate) (PMMI), silica (SiO_2) and chitosan (CHI) or gelatin (GE). The ternary hybrid films possess a high mechanical stability and they do not disintegrate in water, contrarily to what happens when any of a binary combination of these precursors is used. By varying the composition of the films, it is possible to change the concentration of the functional groups present in the organic macromolecules and to study their influence in the morphology and the stabilization of a particular polymorph of the CaCO_3 crystals that are formed in the surface. The crystals and particles with different morphology that crystallize in the hybrid CHI/ SiO_2 /PMMI films only consist of calcite. However, significant changes in the morphology and orientation of the formed crystals were observed in the films with a higher content of PMMI. In the ternary films that incorporate gelatin (G/ SiO_2 /PMMI) the formation of vaterite and calcite was identified. The stabilization of vaterite, that is the less stable polymorph, is controlled by increasing the concentration of gelatin in the films.

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Synthesis, characterization, and antimicrobial behavior of water-soluble polymers and its polymer-metal complexes

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Abstract

The modern world have the necessity of control possible health and contamination problems, this make necessary a bigger regulation in sanitary control, although is require to adequate processing of waste solutions, specially when this contaminants are found in low concentrations to be recovery. In this sense, the water soluble polymers (WSPs) have more value in technology world and have been employed in a great variety of processes like water purification, oil separation, minerals processing, etc. The retention of metal ions for this macromolecules depends of several factors where exist intrinsic and extrinsic variables. The presence of atoms with free electrons like O, S, N y P in these polymers allow the interaction with different metal ions.[1] Polymer-cation interactions are present in two ways a) complexes formation b) electrostatic interaction. One of the most important applications of WSP are in biomedical area as biocides, i.e., chemical composites that allow inhibit or stop the bacterial growing. This activity can be improved with PMC and cationic polymers because the partial negative charge on bacterial surface.[2]

This study involves the homopolymerization of 4-acryloylmorpholine and copolymerizations of 4-acryloylmorpholine with acrylamide, 2-acrylamido glycolic acid, and 2-acrylamido-2-methyl-1-propane sulfonic acid. The polymerization was carried out by radical way in aqueous solution with a constant molar ratio. Ammonium peroxydisulfate (1-5 mol%) was used as initiator. Commercial poly(ethyleneimine) was studied to compare the metal ion retention. The polymer-metal interaction was studied by Polymer-based Liquid phase Retention (LPR) technique. The metal ions studied were: Ag⁺, Cd²⁺, Co²⁺, Cu²⁺, Ni²⁺, Pb²⁺, Zn²⁺, Al³⁺ and Cr³⁺ at pH 3, 5 and 7 changing the filtration factor, Z. The biocide activity was studied for these polymers and for the commercial cationic poly(acrylamide-co-diallyldimethyl ammonium chloride). The bacteria studied by the NCCL method with concentration from 1032 μg/mL, incubating at 36°C for 24h in trypticase broth. were: Escherichia coli (ATTC) and Staphylococcus aureus 6538P,

The results of this study show that all polymers were soluble in water. The behavior as polychelator shows a retention over 80%, for example, with poly(4-acryloylmorpholine-co-acrylamide) for the metal ions like Cr³⁺ at pH 3, Cd²⁺, Co²⁺, Ni²⁺, Zn²⁺ at pH 5 and 7, where the polymer-metal interactions occur by complex formation. Similar results were obtained with poly(ethyleneimine), where at these pH the amino groups are deprotonated favoring the complex formation, even at Z=10. The biocide behavior of these WSP indicate that these polymers shown a low bacteriostatic activity at 1032 mg/mL, against Staphylococcus aureus 6538P and Escherichia coli (ATTC).

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3D composition profiles of Ge:Si (001) domes

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Abstract

The growth of 3-dimensional structures offers the ability to implement in solid-state objects with electronic properties that emulate those of an atom. The Stranski-Krastanow growth mode provides a path for the synthesis of coherent, defect free islands with a band gap that is narrower than the surrounding matrix. Ge on Si has been regarded as a prototypical system allowing the understanding the growth of Quantum Dots. Understanding the electronic properties of such systems requires the assessment of structural properties such as size, composition, and strain. Several independent studies with electron microscopy and x-ray techniques have targeted the issue of Si diffusion into Ge islands grown on Si(100), which is a significant factor in determining the shape and size distribution of an island ensemble. All support the existence of a distinct SiGe vertical composition variation, with most of the Si concentrated at the base of the island. Different growth conditions produce distinct lateral profiles. Hence, the assessment of lateral composition profiles is important to both identify the dominant growth mechanisms and model the confining potential of quantum dots. We report Grazing Incidence Angle X-ray Scattering (GIAXS) measurements on an ensemble of Ge domes with a uniform size distribution. We determined the (average) three-dimensional composition of the domes from an analysis of the anomalous scattering reciprocal space intensity maps near the Ge K absorption edge by first segmenting the domes into a stack of layers and then mapping the lateral concentration of Ge in each layer. Finally, we performed additional selective-etching experiments and qualitatively confirmed our proposed structural model. This work was funded by FAPESP (contract 98/14757-4) and HP Brazil.

Production and Performance of an Aluminosilicate Pozzolan From Colombia

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Abstract

Metakaolinite is a manufactured pozzolan produced by thermal processing of Kaolinitic clay to specified temperature. The main objective of this study was to investigate the potential use of metakaolin produced from different sources of Colombian kaolin as a supplementary mineral admixture in cementitious composites. In this work, five representative kaolins were studied. The effect of heating temperature (400 - 1200°C) and the process of dehydroxylation of kaolinite in order to produce metakaolin was characterized by different Instrumental techniques such as X-ray Diffraction (XRD), Differential thermal / Thermogravimetric analysis (DTA/TGA), Fourier Transform Infrared Spectroscopy (FTIR), and Scanning / Transmission electron microscopy (SEM/TEM). These techniques were used for the characterization of raw materials too. The pozzolanic activity of thermally treated samples as a function of heat treatment parameters was investigated by chemical and mechanical tests. Mortars specimens with five levels of Metakaolin replacement of 0, 10, 20, 35 and 50% were prepared in accordance with ASTM procedures. Mortar properties, such as compressive strength, water absorption capillary and chloride penetration resistance, were investigated. It is concluded that the pozzolanic activity of metakaolin is strongly related with the heat treatment, chemical and mineralogical composition of the raw material. So, thermal treatment at 600-800°C increases the activity pozzolanic. The presence of MK in cement mortar causes refinement in pore structure, decrease the threshold diameter and increase the percentage of small pores. Resistance to chloride migration increased with the increasing metakaolin content. Reductions in diffusion coefficients compared to control specimens were of the order of 46% and 80% for mortar with 10% and 20% respectively.

In general, this study shows that it is possible to produce a high effective supplementary cementing material which can be used for architectural and special cementitious materials. These results obtained are important for a next optimization of a process of the metakaolin large scale production in our country.

Keywords: Pozzolans, Fired kaolin clay, Metakaolin, Thermal Process, Durability properties, Blended mortar.

Shock wave propagation in chains of elastic beads.

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Abstract

We explore experimentally the propagation of shock waves in tapered chains of elastic beads. Contrary to a chain of identical beads, in which an impulse can propagate as a solitary wave, the beads diameter progressively decreases in a tapered chain. Symmetry is thereby broken, and the impulse cannot ever propagate as a solitary wave. In accordance to a theoretical model (S.Sen et al, *Physica* 299, 2001), this symmetry break may implies that the initial impulse finally splits into a multitude of negligible impacts, which leads to strong attenuation of the amplitude of shock waves propagating through such a system.

Study of GaInAs/InAlAs by means of Photoluminescence of Quantum Wells

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Abstract

The presence of fluctuations in the thickness or ruggedness in the interfaces of the Quantum Wells (QW) originates modifications in the emission spectrums of the excitonic recombination, due to the presence of located states for the energy of the exciton in the well. So, the ruggedness of the well can be considered as a parameter that introduces a certain degree of inhomogeneous or disorder in the Hamiltonian of the ideal well. In this work the results of the evaluation of the photoluminescence answer are presented for GaInAs/InAlAs Multiquantum Wells (MQW) as a function of the temperature. It is found that the variation of the medium width of the photoluminescence pick evidences the existence of excellent quality quantum wells where the ruggedness can be considered worthless compared to the method of characterization.

Magnetic structure determination in REBaCuMO₅ perovskites (M = Fe, Co; RE = Y, La, Pr, Nd, Er, Tm, Lu)

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Abstract

While the HTc superconductor YBCO presents a square pyramid as the coordination polyhedron around the Cu²⁺ ion, REBaCuMO₅ perovskites exhibit two apex-sharing CuO₅ and MO₅ square pyramids. The magnetic structures in these systems have been determined by Rietveld refinements using neutron powder diffraction data. These data were collected at BT1 high resolution diffractometer, NIST (Gaithersburg, MD) and the OSIRIS instrument, ISIS (Didcot, UK). Joint refinements using synchrotron radiation data obtained at XRD1, LNLS (Campinas, SP, Brazil) were also performed. Both series, the Co and the Fe ones, exhibit important differences in the magnetic structures, mostly due to original different crystal structures. The magnetic order within each series is dependent on the size of the lanthanide. This influence plays a key role for the existence of a wide variety of magnetic ordering, ranging from simple to helical antiferromagnetism, with commensurate or incommensurate superstructures. For example in LuBaCuFeO_{5+d}, the crystal structure is tetragonal P4mm ($a = 3.774(1) \text{ \AA}$, $c = 7.474(2) \text{ \AA}$) and the magnetic structure ($aM = 2a$ and $cM = 2c$) shows a magnetic propagation vector $k = (1/2, 1/2, 1/2)$. A low temperature ($T < 170 \text{ K}$) commensurate magnetic superstructure is detected with $cM_{\text{comm.}} = 8c$. This structure evolves to a distribution of commensurate and even incommensurate superstructures. A transition to a simple antiferromagnetic structure occurs at $T = 303(3) \text{ K}$. Analogous results for other members of both series will be shown.

Study of the effect of polypropylene molecular weight on the preparation of nanocomposites with different clays

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Abstract

In the present work we investigate the effect of polypropylene molecular weight prepared from Conventional and Metallocenic, in the exfoliations of two natural clays, Montmorillonite (MMT) and Hectorite (HRT). The products were characterized by X-Ray Diffraction (DRX) and Scanning Microscopy Electronic (SEM).

Study of a superelastic Cu-base alloy intended for applications in earthquake engineering.

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Abstract

Superelastic alloys exhibit pseudoelastic deformations and energy damping when submitted to strain-stress cycling. Superelasticity is related to the reversible strain-induced diffusionless transformation of austenite into martensite. Cu-Al-Be alloys have been recently developed as to exhibit superelastic behaviour at room temperature. The present study is part of a research effort to consider these alloys for energy dissipation devices in civil structures. The material should dissipate, at environmental temperature, substantial seismic energy, through repeated stable cycles at large strains, with little degradation in properties and low sensitivity to frequency in the 0.1-5 Hz range. To ensure that behavior, a great effort has still to be done in order to produce alloys and devices for engineering applications, beyond a laboratory environment. Some early results of the mechanical characterization of a Cu-11.8wt.%Al-0.5wt.%Be alloy, under the form of polycrystalline wires about 3 mm diameter, are presented and discussed: monotonic and cyclic tensile curves; temperature evolution with time along mechanical tests, related to adiabatic heating; and fractographic analysis.

Combustion of dichloromethane over titania supported Pd and Ni catalysts

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Abstract

The emission of chlorinated compounds to the atmosphere contributes to ozone depletion, smog formation and global warming. Besides, Cl-VOCs, such as methylene chloride, have suspected toxicity and carcinogenic properties. Incineration is the most widely applied technique for destruction of Cl-VOCs. However, it is a relatively fuel-intensive technique and may lead to a large amount of more complex chlorinated products of incomplete combustion. The catalytic oxidative destruction of Cl-VOCs significantly lowers the process operating temperature, requires little or no supplementary fuel to sustain combustion and can operate with dilute effluent streams (0.1-1% Cl-VOCs). Single or binary metal oxides modified by sulfate ions are strong solid acids that have arisen increasing interest in recent years because of their high thermostability, strong acidity and unique catalytic activities in many environmentally benign reactions. In this contribution the behaviour of Pd and Ni as catalytically active components supported on xerogel sulfated titania carriers are compared for the oxidative destruction of methylene chloride in the presence of water vapor. Two methods were used to introduce Pd and Ni, namely cogellation and impregnation. In the first method the metal precursor was introduced into the initial solution while in the impregnated samples the metal was spread over the carrier surface. The physicochemical properties of catalysts were investigated by XRD, XRF, N₂ sorption, TGA, DTA, SEM and FTIR. Catalytic tests were carried out using 0.1 g of catalyst sample in a Pyrex tubular reactor at atmospheric pressure. The total gas flow was 20 ml/min consisting of 1945 ppm of CH₂Cl₂, 4.8% O₂, 1 % H₂O and He as balance. The range of temperature examined was 100°C to 500°C. The effluent gases were monitored using a FTIR gas analyzer. The temperatures at which 50% conversion is achieved, T₅₀, were 260, 265, 269 °C over Ni/TiO₂(S), Pd/TiO₂(S), and over the sulfated titania support, TiO₂(S), respectively. The T₅₀ values of the cogelled catalysts were 330 and 360 °C over Pd-TiO₂(S) and Ni-TiO₂(S), respectively. In contrast, the homogeneous reaction was observed at temperatures higher than 400°C and a minimum temperature of 500°C was required to obtain 30% conversion. The main oxidation products from the decomposition of methylene chloride over Ni/TiO₂(S) and TiO₂(S) were carbon monoxide (65%) and hydrogen chloride (80%) while carbon dioxide was favored over Pd/TiO₂(S). On the other hand, carbon dioxide selectivity was higher than 90% over Pd/TiO₂(S). The production of higher chlorinated byproducts was not observed over the investigated catalysts. The highly active performance of sulfated titania supported samples in dichloromethane conversion could be accounted for by the generation of strong acid sites, which were preferentially Brønsted sites.

Magnetic Properties of Low Dimensional Physics

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Abstract

The magnetic properties of low dimensional systems has become a very active subject of truly interdisciplinary character, spanning such diverse areas as complex electronic structure calculations; the chemistry and metallurgy of transition metal and rare-earth compounds; the technology of thin films and overlayers; the chemistry and materials science of small particles; and the very recent production of metal transition nanowires. Here we present some results of two particular systems: i) non-collinear magnetism in small Mn clusters and ii) the magnetic properties of Fe nanowires.

We acknowledge partial support of CONACyT under Grant 42428.

New Structures of lanthanids with croconate pentagonal ligand

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Abstract

Lanthanides with their rich stereo chemistry and abundant nature are currently underutilized in crystal engineering development. Here, we report the crystal structures of lanthanide complexes with croconic acid which structures have been characterized by single crystal X-ray diffraction. Complexes consists of a polymeric form of $[\text{LnCC}_2(\text{H}_2\text{O})_5]_n \cdot (\text{H}_2\text{O})_n$, The last being crystallization water molecule. In these complexes, the ligand is coordinated in a monodentated mode by one of the oxygen atoms and there are four ligands and ten coordinated water molecules per lanthanide atom pair. The repeating unit is a dimeric form of this and because of the pentagonal nature of the ligand, there is a rising opportunity for the crystal design of unprecedented shape coordination network.

Water soluble polymers with ability to bind metal ions.

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Abstract

The resins, insoluble polymers, are materials much more stable than many chelating polymers with high metal uptake ability¹⁻². They have higher selectivity and larger adsorbing capacities than other adsorbents and they are also easily eluted and regenerated. The desirable properties of chelating resins are fourfold: a high capacity for the metal(s) of interest, high selectivity, fast kinetics and rapid equilibrium with metal-containing solutions and high mechanical strength and toughness of the exchanger particles. In this work, we report the synthesis of the resins poly(4-styrenesulfonate of sodium) [P4ES], poly(4-styrenesulfonate of sodium-co-4-vinylpyridine) [P4ES-co-4VPy], and poly(4-styrenesulfonate of sodium-co-acrylic acid) [P4ES-co-AA] and the metal ion retention properties by using the batch equilibrium procedures. The synthesis of the resins was carried out by radical polymerization, using ammonium persulfate (AP) as initiator and N,N-methylene-bis-acrylamide (MBA) as crosslinking reagent. The resins were filtered and washed with abundant water, and dried up to constant weight. Yield 99%. Afterwards, the resins were sized by screening and the fraction with mesh size in the range of 180-250 μm was chosen. The batch metal uptake experiments were performed at pH 1-5 depending on the metal ion under non-competitive conditions. The metal ion were selected according to their environmental impact and are the following: Cd(II), Cr(III), Zn(II), Al(III), Pb(II), and Hg(II). All experiments were performed in flasks mounted on a shaker at 20°C for 1h, the samples were filtered, washed with water and dried. The resin:metal ion ratio (in mol) was 20:1. The solution obtained from the washed resin was collected in a 50 ml flask. The metal ion in the solution was determined by atomic absorption spectrometry. The all resins have a particle size > 1000 μm but it does not depend on the crosslinking ratio. The resins also shows a high thermal stability up to 200°C with a weight loss lower than 20%. The resins shows good metal ion retention for the all cations, but the highest retention was observed for Cr(III) and Al(III) ions in all pH range. The results demonstrated a dependency on the pH for the Cd(II), Zn(II), Pb(II) and Hg(II). The resins have high retention at pH= 5, which is higher than that 90%. It was also studied the maximum load capacity at optimum pH, metal ion retention properties under competitive conditions, the regeneration capacity by using different eluents, and cycles of retention-elution.

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Characterization of Some Macromolecules Involved in the mineralization of Red Claw Lobster (*Cherax quadricarinatus*)

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Abstract

Gastroliths are calcium storage structures present in Crustaceans. During the premolt period, the extensive resorption of the cuticle is followed by the liberation of calcium, most of which is stored in the gastroliths formed at the anterior part of the stomach. Gastroliths are a good example of biomineralization, they are composed mainly of calcium carbonate and in addition, they contain a small amount of organic materials, including proteins associated with chitin and carbohydrates, which are probably important in calcification. As a step in the understanding of the mechanism of calcification, we undertook the characterization of the organic matrix of the gastroliths, searching for the presence of some sulphated macromolecules. For structural characterization, partial decalcified gastroliths were observed by scanning electron microscopy (SEM). The presence of proteoglycans was studied by using monoclonal antibodies against some proteoglycans present in other bioceramics. To study the role of organic macromolecules in mineralization, in vitro mineralization assays in the presence of macromolecules from the gastroliths were performed and remineralization assays using decalcified gastroliths as substrates were done. To characterize the mineral component of these concretions X-ray diffraction (XRD) and photoelectron spectroscopy (XPS) were used. We observed that specialized mineralization macromolecules are present in the gastrolith. In vitro mineralization assays showed crystal modifications when decalcified gastroliths were used as substrate. Using organic matrix, obtained from decalcification of gastroliths, as additive, crystal modification was also observed. Keratan sulfate was detected as the only proteoglycan present in the organic matrix. By using XRD and XPS the presence of amorphous calcium carbonate as a mineral phase in the gastroliths was observed.

Influence of the Polymethylsiloxane Sulfonic Acid Derivated on the Nucleation and Growth of Calcium Carbonate Crystals

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Abstract

The main synthetic routes leading to functionalized polymethylsiloxane is the hydrosilylation of unsaturated functional compounds with polysiloxanes containing SiH active groups. Sulfonic polymethylsiloxane compound was obtained through reaction of functionalized polymethylsiloxane with sulfuric acid. For the mineralization experiments of the functionalized polymethylsiloxane were done by using the Sitting-Drop method. The crystallization experiments were done using a chamber consisting of plastic Petri dish having a central hole in its bottom glued to a plastic cylindrical vessel. Inside the chamber, microbridges were filled with CaCl₂ solution in TRIS buffer in the range of pH 9-12. The central hole allows the diffusion of CO₂ vapor from the (NH₄)HCO₃ into the buffered CaCl₂ solution on the polymorphism of CaCO₃. Crystals morphology varied for growth in the absence and in the presence of sulfonic polymethylsiloxane compound. The sulfonate content of the functionalized polymethylsiloxane subsequently interact with the newly formed overgrown crystals, resulting from to 5 μm to 40 μm long piles of modified calcite crystals. The resulting morphology of the synthetic crystals is an expression of different growth rates in variuos crystallographic directions and strongly depend of the functionalized polymethylsiloxane concentration and pH unit, modulated by the adsorbed additives present in solution and/or on filter.

Synthesis of Hydrogels by Inverse Suspension Copolymerization of Acrylic Acid and Acrylamide for a Fertilizer Controlled Release

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Abstract

Inverse suspension polymerization was studied as a method for synthesis of geometrically homogeneous hydrogels. This work was intended to gain a better understanding of the polymerization process's stability, the final product's swelling, and urea release performance. A comparison was performed on release properties of hydrogels obtained by this method with materials synthesized by other polymerization techniques.

Acrylic acid and acrylamide were polymerized in presence of N,N-metilenbisacrylamide in aqueous solution and dispersed in toluene, M-Grade paraffin oil or VAROL[®] isoparaffinic oil as continuous phase. A series of experiments were carried out in two stages. Firstly, preliminary evaluation to investigate the influence of suspension and operation parameters on bead size and morphology and suspension stability. A number of parameters were investigated during this stage such as type of continuous phase, disperse/continuous phase rate, impeller type, dispersing agents and stirring rate. The material obtained was evaluated for physical appearance, color and bead size; and the suspension polymerization process was evaluated by particle size distribution and agglomeration rate of the suspended particles.

Some samples were characterized by Scanning Electron Microscopy (SEM) images in an effort to describe bead morphology and particle agglomeration process during the polymerization.

The second experimental stage evaluated the influence of monomer ratio, thermal initiator and crosslinker initial concentration on hydrogels swelling and Urea release rate, based on fixed values for parameters evaluated on the first experimental stage. Particles obtained were classified by sieve analysis; water absorption capacity, water/Urea absorption rate and Urea release rate are measured for a desired particle size fraction. Analytical methods employed in hydrogels characterization include UV spectrophotometry for Urea release evaluation, gravimetric method for swelling properties, Differential Scanning Calorimetry (DSC) for thermal properties and bound water studies, SEM for particle morphology and FTIR for identification of functional groups.

The hydrogels obtained exhibited water absorption capacities of 300 to 500 times the dry weight with equilibrium swelling times of 60 to 70 minutes. Particle from 400 to 500 microm in diameter were selected for final experiments with present spherical forms as observed by SEM images. A high urea release rate is observed for the mayor of samples with the 90 percent of Urea released during the first 60 to 70 minutes. This release rate is higher than the rate for hydrogels synthesized by solution or bulk polymerization with the same monomers and monomer initial concentrations.

Cyclopalladated Complexes and their catalytic activity in polymerization reaction of ethylene

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Abstract

Mononuclear cyclopalladated complexes of type I $\text{PdCl}(\text{Ph}_2\text{N}-\text{N}=\text{CR}1-\text{C}-\text{R}2=\text{N}-\text{NPh}_2)$, where $\text{R}1=\text{R}2=\text{H}$, $\text{R}1=\text{R}2=\text{CH}_3$, and $\text{R}1=\text{H}$, $\text{R}2=\text{CH}_3$ and type II $\text{PdCl}(\text{RRS}-\text{S}=\text{CH}-\text{C}-\text{CH}_3=\text{N}-\text{NPh}_2)$ where $\text{R}=\text{CH}_3$, $-\text{CH}_2\text{CH}_2-$ were synthesized by the reaction of palladium chloride and hydrazones¹. Additionally, the catalytic activity in the reaction of polymerization of ethylene was studied, giving high activity (> 100) in the relation co-catalyst (Al)/catalyst (Pd) =4000, there value are considered higher for non-metallocene catalysts. The molecular weights, are near 100.000 and present of polydispersity near 2 characteristic of these type of initiators. The melting point for the crystalline form, correspond to a linear polyethylene.

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Production and characterization of thin films of c-BN obtained by pulsed vacuum arc discharge.

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Abstract

Using pulsed vacuum arc system thin films of c-BN were produced by a PAPVD (Plasma Assisted Physical Vapor Deposition). The equipment for the discharge is formed by a reactor composed by a vacuum chamber with two opposite electrodes and a RLC circuit to produce the arc discharge. We was used a target of h-BN placed on the cathode and substrates of silicon placed on the anode. In order to improve the adherence of the c-BN film, it was grown an interlayer of TiN. The chamber was filled with N₂ to produce the TiN coating, with a pressure of 1,7 mbar. and a voltage of 300 V. In the case of c-BN the filled gas was also nitrogen at a pressure of 4.4×10^{-1} mbar and a voltage of 240 V. By means of XRD , it was determined the existence of TiN finding different crystalline orientation in FCC phase. FTIR was employed to determine sp³/sp² bonding ratio in the c-BN film. It was realizing I-V curves in order to study the electrical properties of the bilayer, observing a semiconductor behavior and this result was compared with the silicon substrate without coating.

Study of structure transformation of chalcopyrite during its dissolution in acidic solutions

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Abstract

Chemical and electrochemical studies of chalcopyrite have suggested that the dissolution process of this mineral involves a number of stages, leading to the formation of non-stoichiometric intermediates at the surface of the solid level.

This mechanism is likely to show up several structural changes, which may lead to the formation of a solid, with a lack in metallic content.

Variations in the chalcopyrite oxidation rate are attributed to the existence of this layer, which makes difficult the transport of soluble species, to be consumed as well as products to be released to solution bulk.

There is no a unique opinion in the structural and chemical characteristics of this layer. The main point to be rationalized and solved is that the surface layer constitutes clusters or heterogeneous reaction zones or it might just be as a part of a complete phase being formed throughout the oxidation.

The present work aims is to study the formation and characterization of a solid type cubic chalcopyrite, which might be produced during the dissolution of the chalcopyrite at a pH and a temperature conditions, which makes possible the utilization of thermophilics micro organisms.

The structural characterization of the intermediate specie formed in the chalcopyrite dissolution process was identified by X-ray diffraction (XRD) analysis.

And then the structural parameters were obtained, employing the method put forward by Rietveld. The methodology has not been usually used in mineral systems characterization , since for these purposes crystalline materials are needed.

KEYWORDS : Chalcopyrite,X-ray diffracction,Rietveld method,

Titania-Silica-Zirconia Mesoporous Oxides Obtained by Sol-Gel Method

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Abstract

Pure titania, silica and zirconia have been extensively studied as catalyst or catalyst support for heterogeneous catalytic reactions. For example, titania is a well-known catalyst for photocatalytic reactions. Recently TiO₂ and ZrO₂ mixed oxides have received much attention as catalysts for its high surface area and acid-base property. The preparation of binary or multicomponent solid oxides can be carried out at low temperature by the sol-gel method, being the control of the hydrolysis and condensation rates of the various molecular precursors used of paramount importance. The difference in reactivity can be minimized by controlled prehydrolysis of the less reactive precursor or by chemical modification of the precursors.

In this work mesoporous titania-silica-zirconia with highly dispersed titania and zirconia have been prepared by an alcoxide sol gel process. An acid hydrolysant was added to a solution of tetraethylorthosilicate and ethanol. In order to control the relative hydrolysis rates of zirconia and titania precursors, the tetraisopropoxytitanium (IV) was modified by methoxyethanol and n-propoxide zirconium by acetylacetonate and then they were added to the silica sol. A Polyethylenimine (PEI) solution as pore forming agent was incorporated to the titania-silica-zirconia precursor sol, producing a hybrid polymer. The resulting titania-silica-zirconia / PEI hybrid materials were dried at 70°C/24h. Further calcination of this hybrid resulted in the formation of a continuous, purely inorganic network. The influence of preparation parameters (Zr and Ti- relative contents, the drying method and calcination temperature) on the structural and textural properties of the oxides was studied by means of N₂-physisorption, X-ray diffraction, thermal analysis and vibrational spectroscopy (FTIR). The resulting networks have different structures and surface areas ranging from 100-650m²g⁻¹. It was found that an increase in silica content increase the surface area and pore diameter. The materials obtained remain amorphous after calcination at 550°C/2h

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Nucleation Kinetics Of Potassium Jarosite In The System Fe₂(SO₄)₃-H₂SO₄-KOH At 70°C

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Abstract

The kinetics of K-jarosite precipitation in the system Fe₂(SO₄)₃-H₂SO₄-KOH at 70°C was studied. It was found that the rate of Fe⁺³ precipitation can be described according to the following equation:

$$r = -\frac{d[\text{Fe}^{3+}]}{dt} = k' \cdot (\Omega - 1)^n = k' \cdot \left(\frac{IAP}{K_{PS}^o} - 1 \right)^n$$

where Ω is the saturation ratio and corresponds to the ratio between the ionic activity product (IAP) and the solubility product constant (K_{PS}^o), k' and n are derived empirically from fitting rate (r) versus saturation state data (Ω). The kinetics of K-jarosite nucleation was characterized from measurements of the induction time in [Fe⁺³] - time curves obtained at different initial acid concentrations. The induction time was observed to increase with the supersaturation decrease. When the saturation index (SI = log Ω) was over 24,0 nucleation was homogeneous, but when SI < 24,0 nucleation was heterogeneous. Employing the classical nucleation theory, the interfacial tension between potassium jarosite and supersaturated solutions was estimated to be about 160.3 mJ/m².

Acknowledgements:

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Properties of Propylene/ α -Olefin Copolymers Synthesized with a Metallocene Catalyst

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Abstract

A study is made of the main properties of propylene/ α -olefin copolymers (1-hexene, 1-octene and 1-octadecene as comonomers) synthesized with a metallocene catalyst. An effect of comonomer incorporation on the polymer's thermal properties and crystallinity is seen. Changes in some viscoelastic relaxation and mechanical properties such as Young's modulus and yield point are also seen. It is found that not only the incorporation of the comonomer is important, but also its size, noticeable especially in the glass transition temperature.

Study of Mononuclear and Binuclear Cu(II) Complexes derived from Redox Active Macrocycles and their Related Ligands

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Abstract

Robson type macrocyclic complexes are of interest as new materials and as models of biomolecules. The availability of a wide variety of planar ligands with different cavities offers the opportunity to study in detail magnetic phenomena, metal ion recognition, encapsulations, transport and separation effects, catalytic process, and new molecular devices^{1,2}.

In this work we report the study of different copper (II) complexes with the macrocyclic and hemicyclic ligands, derived from condensation reaction of 2-hydroxy-5-methyl-1,3-benzenedicarbaldehyde with 1,2-diaminebenzene. Depending on the synthesis conditions it is possible to obtain three different complexes, a mononuclear copper(II) and dinuclear copper(II) hemicyclic complexes, and binuclear copper (II) macrocyclic complexes.

The above mentioned compounds were characterized by different spectroscopic techniques, elemental analysis, magnetic susceptibility and electrochemical studies. Structural and physicochemical properties will be discussed.

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Study of the influence of ferrous and ferric ions on the growth of copper electrodeposits from CuSO₄-H₂SO₄ solutions

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Abstract

Calcite Crystallization in a double Diffusion Reacting Conditions

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Abstract

The Crystallization of calcite is being studied in a quasi bidimensional double diffusion cell which consist in three chamber separated by cellulose membranes. The purpose of these study is to investigate, by in situ microscopic observations, the nucleation and growth of calcite under varying supersaturation conditions depending on the time and position of the Ca^{2+} and CO_3^{2-} along the cell. The diffusion media correspond to a gel (Agarose type 1) confined within a very thin chamber 100 micrometer height. The local supersaturation is the main experimental variable, which controlling the nucleation and crystal growth features as well as the morphologies developed after nucleation taked place.

Effect of dispersed Al₂O₃ on the phase transitions and ionic conductivity of KH₂PO₄

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Abstract

Differential scanning calorimetry (DSC) and impedance spectroscopy (IS) were used to study the composite solid electrolytes (1-x)KH₂PO₄-xAl₂O₃ in the concentration range x=0.0-0.5. The composites were prepared by mechanical mixing of the components followed by heating at temperatures below the KH₂PO₄ (KDP) melting point at 259 oC. We grew single crystals of pure KDP. The DSC curves of the KDP single crystals show three endothermic peaks at 185, 223 and 256 oC, respectively, on the first heating run. For the polycrystalline KDP, the first peak sometimes appear at 183 oC and it tends to disappear, the second one shifts down to 195 oC and the third one appears at 261 oC. For the composites, only two endothermic peaks are observed on heating runs, at about 210 and 250 oC, respectively. The conductivity data for single crystal and polycrystalline KDP samples show an Arrhenius behaviour with temperature but the values for the crystal samples remains about one order of magnitude higher than those for the powdered ones in the whole temperature range. Moreover, the Arrhenius conductivity plots for the single crystal samples shows a change of slope to higher values at about 190 oC. The dc conductivity data for the composite samples show similar behavior to that observed in KDP single crystals. The conductivity data vs. alumina concentration showed two conductivity maxima at about x=0.1 and x=0.3 at different temperatures. The results are discussed in terms of the approximation effect of Al₂O₃ dispersed particles on the proton behavior of KDP.

Heterogenization of metallocene on supports based on inorganic oxides, obtained via Sol-gel technique and their use as catalysts in the ethylene polymerization.

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Abstract

The present work shows results obtained for the heterogenization of metallocene with different supports obtained via Sol-Gel technique. Supports utilized were SiO₂, MgO and TiO₂, those that presented high superficial area, and in general they turned out to be mesoporosos. Et(Ind)₂ZrCl₂ was used as metallocene. Activities turned out to be lower in the supported systems than in the homogeneous systems, but higher than conventional support using commercial silica. On the other hand, the interaction between the metallocene complex and the modified support was studied for different concentrations of MAO by diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS). This technique allows information about the variation of isolated hydroxyl groups on the surface support.

Key words: metallocene, supports, ethylene, catalysis, polymerization

Heterostructures Based On Epitaxial Oxide Thin Films

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Abstract

For many possible electronic applications as well as fundamental studies, it is essential to fabricate epitaxial layered structures of insulators, semiconductors or normal metals as well as magnetic layers together with high temperature superconductors (HTS). However, HTS materials have complex lattice structures and this makes difficult to grow multilayers with sharp interfaces, preserving epitaxiality through the whole structure. In this work we describe transport measurements and microstructural analysis of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}/\text{PrBa}_2\text{Cu}_3\text{O}_{7-\delta}/\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO/PBCO/YBCO), $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}/\text{Bi}_2\text{Sr}_2\text{YCu}_2\text{O}_{8+\delta}/\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO/BSYCO/BSCCO) and $\text{La}_x\text{Ca}_{1-x}\text{MnO}_3/\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (FM/HTS) heterostructures deposited on (001) SrTiO_3 substrates by using an in situ DC sputtering technique at high oxygen pressures. Conductance measurements on this type of multilayers showed a clear quasiparticle tunneling indicating a gap structure around 25 mV in the case of YBCO compounds, 30 $\dot{\text{U}}$ 35 mV and a zero bias anomaly in the case of BSCCO materials. We will discuss also the Josephson behavior of heterostructures based on BSCCO compounds as well as the interplay between superconductivity and magnetism in superconductor/ferromagnetic heterostructures and superlattices.

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Catalysts for New Materials based on Polyolefins

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Abstract

The discoveries of organometallic polymerization catalysts and stereoselective polymerization initiated a chain of innovations promoting the rapid growth of the polyolefin industry. The development and progress of the last decade in single-site metallocene catalyst technology finally indicates that the advancing polyolefin industry has moved, in anticipation, towards even more modern technologies meeting the ultimate goal of employing clean processes that provide environmentally green products. These catalysts have reached now their full industrial maturity and offer themselves as a new class of commercially viable and environmentally clean alternatives for producing a wide range of varieties of polyolefin homo- and copolymers. Emphasis is being placed upon new approaches, basic correlations between catalyst and polymer architectures, and new opportunities for producing polymeric materials with new property profiles, especially due to the development of new catalytic technologies and processes. One of the biggest challenges for modern organometallic chemistry is its application in new technologies and new materials. For this purpose, in many cases already known types of complexes have been synthesized, modified, and applied to new catalytic processes or applications. During the last 10 years, in our research laboratory we have been studying not only metallocene catalyst, but have also started working on the activity of non-metallocene catalysts for the homo and copolymerization of ethylene, α -olefins and polar monomers. Results showing a series of Organometallic Complexes that present Catalytic Activity and also New Materials like: Membranes, Nanocomposite, Elastomer etc. that have been prepared through the polymers obtained via Metallocene Catalyst will be discuss. We can correlate: Catalyst Structure-Polymer Structure-Polymer Properties

Raman study of phase transitions in KNbO₃

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Abstract

The influence of grain size on the phase transitions of the ferroelectric crystal KNbO₃ was studied by Raman spectroscopy and it was found that large particles ($\sim 500 \mu\text{m}$) show sharper transitions than small ones ($\sim 50 \mu\text{m}$), i.e. the character of the first order transition becomes weaker when the size is reduced. The transition temperatures also depend on the size of the particle, and all particles show hysteresis. Further, evidence has been obtained that in small particles monodomains of the monoclinic and orthorhombic phases can coexist above the transition temperature.

Coarse-grained models for nano- and mesoscale soft matter systems

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Abstract

We will discuss a novel coarse-grained rigid blob approach developed specifically to study nano and mesoscale soft matter systems. The approach is based on a partitioning of the components of the system into "blobs" that move as rigid particles. The blobs interact with each other through potential energy functions that reflect the full three-dimensional shape of the blobs. We have developed very efficient algorithms that allow simulations of the morphology and dynamics of many thousands of blobs for long periods of time. We will discuss simulations of phase separation and morphology changes for diblock polymers in solution.

Nucleation and selective growth of polymorphs of calcium carbonate in organic-inorganic hybrid films

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Abstract

The biological systems use organic molecules (fundamentally proteins and polysaccharides) to control the nucleation and growth of minerals in an organic matrix. In this way such hybrid materials are formed as bones, teeth, and shells of mollusks by means of the biomineralization process. The biomacromolecules that participate in the production of these composites can be classified into water-soluble proteins and water-insoluble macromolecules such as chitin and collagen that work as solid matrixes. The study of the influence of structured organic surfaces and soluble organic macromolecules in the orientation and growth of inorganic crystals is a fundamental aspect in biomimetic mineralization processes that has attracted a great attention. A fundamental factor for the heterogeneous nucleation of mineral crystals in organic substrates is to increase the charge density on the surface of the matrix. In this work, our approach has been to study the crystallization of calcium carbonate (CaCO_3) in organ-inorganic ternary hybrid films constituted by poly(monomethyl itaconate) (PMMI), silica (SiO_2) and chitosan (CHI) or gelatin (GE). The ternary hybrid films possess a high mechanical stability and they do not disintegrate in water, contrarily to what happens when any of a binary combination of these precursors is used. By varying the composition of the films, it is possible to change the concentration of the functional groups present in the organic macromolecules and to study their influence in the morphology and the stabilization of a particular polymorph of the CaCO_3 crystals that are formed in the surface. The crystals and particles with different morphology that crystallize in the hybrid CHI/ SiO_2 /PMMI films only consist of calcite. However, significant changes in the morphology and orientation of the formed crystals were observed in the films with a higher content of PMMI. In the ternary films that incorporate gelatin (G/ SiO_2 /PMMI) the formation of vaterite and calcite was identified. The stabilization of vaterite, that is the less stable polymorph, is controlled by increasing the concentration of gelatin in the films.

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The characterization of porous materials with ^{129}Xe NMR spectroscopy

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Abstract

Over the last twenty years, ^{129}Xe NMR spectroscopy has developed to a point where it can be considered to be a useful and versatile tool for learning about the presence of void space, including pore size, structure, and the interconnectivity and distribution of pores of various sizes. As well, recently the introduction of optically enhanced (hyperpolarized) Xe has added a new dimension of sensitivity, thus expanding capabilities tremendously. This talk will start with an overview on ^{129}Xe as an NMR nucleus, and how chemical shifts and chemical shift tensors relate to the shape and size of small voids in crystalline materials where structural data, experimental chemical shift tensors and modeling calculations are available. Then, for larger pores, eg mesoporous silicas and controlled pore glasses, how exchange-averaged chemical shifts allow the determination of pore sizes up to 50nm. Since Xe NMR spectroscopy is inherently limited by the level of thermal polarization (number of spins, the strength of the magnetic field), and the spin-lattice relaxation time, the increase in sensitivity by factors of up to 105 by using optical pumping to produce a hyperpolarized version of xenon has increased prospects tremendously. The general principles and apparatus required to generate hyperpolarized Xe in a continuous flow system will be described. Many spectra can be obtained with single-scan sensitivity even with very low concentrations of Xe gas (1%), allowing time- and temperature dependent studies to be carried out with relative ease. Besides information on pore size, one can determine heats of adsorption and specific surface areas, one can study competitive sorption with Xe gas as tracer, and one can follow material transformations in-situ in the NMR spectrometer. One can also obtain three-dimensional chemical-shift resolved images in a reasonable length of time. Applications to crystalline metal-organic polymers and host-guest networks, and non-crystalline aerogels and solid-lipid nanoparticles will be described.

Polymeric Materials To Remove Metal Ions

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Abstract

Polymers containing metals have emerged as a new generation of material with tremendous potential in fields like superconducting materials, ultra-high strength materials, liquid crystals, catalysts, and biocompatible polymers [1]. The structures of some polymer-metal ion complexes have been reported in the literature [2-3]. Insoluble polymeric supports are widely investigated and applied for metal recovery from dilute solutions [4-5]. There are different natural and synthetic products that show ion-exchange properties. The organic resins are by far the most important ion exchangers. The main advantages are high chemical and mechanical stability, high ion-exchange capacity and ion-exchange rate. Another advantage is the possibility of selecting the fixed ligand groups and the degree of cross-linking. The separation methods based on membrane process are among the most promising techniques for enrichment of various species from solutions [6-8]. Thus, a number of soluble and hydrophilic polymers have been prepared through addition polymerization and by functionalizing various polymers, and found to be suitable for the separation and enrichment of metal ions in conjunction with membrane filtration. Membrane filtration allows easily the separation of metal ions bound to soluble polymers from non-bound metals. This method is known as the liquid-phase polymer-based retention (LPR) technique. Applications of water-soluble polymers to the homogeneous enrichment or selective separation of various metal ions from dilute solutions have been reported. Water-soluble polymer materials are commercially available or can be synthesized by different routes. The polymers, prior to being used in the LPR technique, are fractionated by the same method using different membranes of known molecular weight exclusion limit. Thus purified, they are then lyophilized and characterized. For LPR experiments, the highest molecular weight fractions are normally used in combination with a low molecular weight exclusion limit membranes to ensure no macromolecule exits the ultrafiltration cell. Metal ions with high interaction rates with the polymer are retained by the polymer, which is not able to pass through the ultrafiltration membrane, while other ions are eluted through the membrane.

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Precipitation Behaviour Of 8090 Alloy Developed Upon Retrogression And Reaging Treatments

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Abstract

As the reduction of density is one of the primordial requirements for innovative aerospace materials, great efforts have been dedicated in the last decades to the study of Al-Li base alloys. The addition of alloying elements such as Cu, Mg and Zr, promote the formation of stable and metastable phases and is intended to improve the mechanical behavior of these alloys. The main metastable phases observed are: T1 (Al₂CuLi), Al₃Li and Al₃Zr. During a prolonged reaging, one can also observe the precipitation of stable S (Al₂CuMg) phase. In the present investigation, we have studied the microstructure stability of the strengthening precipitates in an Al-Li base alloy subjected to a two-stage heat treatment of retrogression and reaging.

The material used for the study was the 8090 T3 Al-Li alloy supplied by Pechiney Recherche in the form of a 3.3 mm thick plate. Homogenization annealing of the alloy was carried out at 550C for 1 hour followed by quenching in water. Reaging treatment was performed at two different temperatures of 150C and 200C during different time intervals, ranging from 10 to 5000 minutes.

The results obtained have indicated an overall polycrystalline arrangement developed upon heat treatment of retrogression and reaging. This corresponds to incoherent high angle grain boundaries together with low energy sub-grain boundaries composed of dislocations arrays. It is also noticed that the background is not continuous because of the strain field contrast of the nanoscale homogeneous Al₃Li precipitates. In view of the non-planar (at the atomic scale) topology of the foil sample with respect to the incident electron beam, some bend contours were helpful in establishing appropriate diffraction conditions to resolve this fine precipitates even at the low magnification. The retrogression treatment produces partial dissolution of the precipitates, and therefore spherical particles of Al₃Zr phase could still observed. Reaging at 150C during 1000 minutes results in a homogeneous precipitation of very fine particles corresponding to Al₃Zr phase as well as spherical particles of about 20 nm in size which correspond to Al₃Li phase. In fact, after a prolonged reaging time (1000 minutes), the precipitation of Al₃Li phase also occurs around existing Al₃Zr nanoparticles resulting in a formation of very fine donut shaped nano-composite precipitates of about 50 nm in size. The presence of other phases, such as T1, is observed in the alloy reaged during 100 and 1000 minutes, indicating conditions of peak age and over aged respectively. The S phase is observed only when the alloy is reaged during 5000 minutes. For this condition one may noticed the coarsening of other precipitates such as Al₃Li and Al₃Zr and the presence of inclusions interacting with dislocations. The deformation texture introduced in the alloy due to its fabrication process (rolling) still persists after the retrogression treatment. TEM observations also indicate the presence of

persistent inclusions, which are independent of the heat treatment cycle induced in the sample. Indeed, EDS analysis has shown such inclusions to be iron containing, which is considered typical in Al alloys.

A New Obtention method of Nickel Nanoparticles.

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Abstract

The physical properties of materials as they progress from the bulk to nanoscale regime (1 - 100 nm) continue to be of immense interest and increasing importance for future technological applications. Metal nanoparticles display properties generally found to be scientifically different from the bulk material which they can be derived. The potentialities in areas of nanoscience a technology of nanoparticles are mainly due to the quantum size effect. Preparation of nanoparticles generally involves the reduction of metal ions in solutions or in high temperature gaseous environments¹. In our case, we develop a new simple method to synthesize nickel nanoparticles. The synthesis carried out mixing bis(1,5 cyclooctadiene)-nickel(0) in THF and thiourea in methanol. Transmission electron microscopy (TEM), electron diffraction and UV spectroscopy were used for the characterization of nickel nanoparticles. TEM images showed uniformity of particles size (10-15 nm). By the analyses of electron diffraction pattern were confirmed metal natures of the resultant particles. UV absorption spectrum showed a maximum absorption at about 250 nm, which corresponds neither to the solvent nor 1.5 cyclooctadiene².

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Obtention of SnO₂-Based Varistor of High Performance

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Abstract

Varistor (variable resistor) is a electronic ceramic that change its resistance with voltage. This device is a resistor with nonlinear current (I) - voltage (V) characteristic. Varistor ceramics have become technologically important because of their highly nonlinear electrical characteristics enabling them to be used as reversible solid - state switches with large-energy-handling capabilities. The processing of varistors is no different from that of any other multicomponent ceramic. The result product is a polycrystalline ceramic with a unique grain-boundary property that contributes to the well-know nonlinear I-V characteristic of the device. Commercial varistors used in protection systems are based on SiC (silicon carbide) or on ZnO (zinc oxide). However, in recent years, a new class of high-density nonohmic polycrystalline ceramics based on SnO₂ (tin oxide) was discovered. All of the SnO₂-based varistor systems reported to date are destined for high-voltage applications due to their high breackdown voltage. In this CIAM project, the current densities versus applied electric field behaviour of high dense SnO₂ ceramic were studied. Transition metal oxides were used as densifying agent. Other goal of this work is show that it is possible to combine the features of SnO₂ and TiO₂-based ceramics in an oxide matrix of (Sn,Ti)O₂ to obtain ceramics with nonohmic properties similar to those of pure components. SnO₂ doped with other oxides were prepared by coprecipitation and polymeric precursor (Pechini method). The influence of several dopants on the microstructure development, on the secondary phases formation and on the electrical behaviour of SnO₂-based varistor was studied.

Magnetic properties of toroidal graphite and their implication in magnetic carbon

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Abstract

Using a pi-orbital nearest neighbour tight-binding Hamiltonian in conjunction with the London approximation, we have studied the magnetic response of different toroidal carbon nano-arrangements. It is found that torii generated by coalescing C60 fullerenes, exhibit intrinsic large paramagnetic moments, independent of the size of the torus. In addition, toroidal Haeckelites also possess paramagnetic behavior. Both, Haeckelites and the coalesced C60 structures exhibit negative Gaussian curvature due to the presence of heptagonal and octagonal carbon rings respectively. Contrarily, pure hexagonal carbon tori created by connecting the ends of single walled carbon nanotubes, exhibit a clear paramagnetism, which is only dependent on the size and diameter of the structure. Our results indicate that it may be possible to find ferromagnetism in pure graphitic sp² arrangements possessing negative curvature.

Study of Mononuclear and Binuclear Cu(II) Complexes derived from Redox Active Macrocycles and their Related Ligands

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Abstract

Robson type macrocyclic complexes are of interest as new materials and as models of biomolecules. The availability of a wide variety of planar ligands with different cavities offers the opportunity to study in detail magnetic phenomena, metal ion recognition, encapsulations, transport and separation effects, catalytic process, and new molecular devices^{1,2}. In this work we report the study of different copper (II) complexes with the macrocyclic and hemicyclic ligands, derived from condensation reaction of 2-hydroxy-5-methyl-1,3-benzenedicarbaldehyde with 1,2-diaminebenzene. Depending on the synthesis conditions it is possible to obtain three different complexes, a mononuclear copper(II) and dinuclear copper(II) hemicyclic complexes, and binuclear copper (II) macrocyclic complexes. The above mentioned compounds were characterized by different spectroscopic techniques, elemental analysis, magnetic susceptibility and electrochemical studies. Structural and physicochemical properties will be discussed.

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A new method to obtain the degradation of semiconductor materials using an extra high impedance DC current source

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Abstract

In this paper we present the Voltage- Current V-I characteristics of semiconductor materials obtained with an extra High Impedance current source. This source, called ETHICS, is able to deliver a constant current in an extremely large range of the load resistances. At the present moment we have applied constant DC currents of both polarities in the range of 0.1 mA to loads varying between 1 Ohm to 10 Mega-Ohm. With the source ETHICS we have obtained the V-I characteristics of semiconductor devices such as varistors and paintings used in electrical insulators. In the case of varistors, it was possible to notice small differences in the V-I characteristics by changing the varistor's temperature. Additionally we compared new and aged units and it was clearly established differences in their behaviour. In the case of semiconductor paintings it was possible to differentiate the V-I characteristics of similar test objects with small differences in its composition. In the near future we will construct a new ETHICS model which will produce currents in the range of several mA. The current source ETHICS has advantages when it is compared with a voltage source. In the later, the current given by the source is affected by the load. The source ETHICS could be used in aging material testing and we investigate its application in battery charging.

Modeling Plastic Deformation Effects on Magnetic Hysteresis Loops in Steels

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Abstract

Plastic deformation affects the hysteretic magnetic properties of steels because the plastic deformation changes the dislocation density, which affects domain wall movement and pinning, and also because it places the specimen under residual strain. In earlier papers, a model was proposed for computing hysteresis loops based on the effect of grain size d and dislocation density Gd . In that paper, hysteresis loops were compared that all had the same maximum flux density B_{max} . The result was that coercivity H_c exhibited a linear relationship with inverse grain size ($1/d$) and $Gd^{1/2}$. The same was true of hysteresis loss WH . If one compared hysteresis loops all with the same maximum magnetic intensity H_{max} , the linear dependences were only approximately found. Because the relationships are simpler, core loss experimenters compare loops that all have the same B_{max} .

In this paper, we present the results of modifying the above model to study the effect of plastic tensile deformation on hysteresis loops with the same B_{max} . In this case, linear relationships are found between H_c and residual plastic strain, and between WH and residual plastic strain. With increasing residual tensile strain, H_c increases; whereas with increasing elastic tensile strain, H_c decreases. Also, with increasing residual tensile strain, the slope of the hysteresis loop decreases; whereas, with increasing elastic tensile strain, the slope increases. Compressive plastic deformation effects will also be discussed.

Building Complex Nanostructures by Using Molecular Films

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Abstract

Self-assembled monolayers (SAMs) of alkanethiols and silanes on metal and semiconductor surfaces have been widely used as elemental blocks for building different types of nanostructures. These molecules exhibit a functional group with a marked affinity for the substrate surface and a hydrocarbon chain with a length that can be varied by increasing the number of $-CH_2-$ units. SAMs are formed by the self-assembly of molecules (usually silanes for oxidized surfaces or alkanethiols for clean metal surfaces) by simple adsorption from the vapor or liquid phases. At the saturation coverage SAMs consist of ordered arrays of standing-up molecules strongly adsorbed on the substrate by S- (alkanethiolates) or Si-O- (silanes) bonds. The terminal group can be hydrophobic ($-CH_3$) or hydrophilic ($-OH$, $-NH_2$, $-COOH$). Thus, different ions and molecules can be trapped on/into the SAMs by electrostatics, hydrogen bonding or hydrophobic interactions. Therefore, SAMs-covered materials offer new possibilities in the field of sensors/biosensors development and drug delivery strategies. Deposition onto $-CH_3$ terminated SAMs on metallic or semiconductor templates allows direct pattern transfer from the template to the deposited material (polymers, metals, ceramics). SAMs are stable under different deposition conditions and different deposition techniques (polymer casting, thermal physical vapor deposition, electrodeposition, reactive sputtering). Pattern transfer from the template to the deposited materials is allowed with at least 50 nm lateral and 6 nm vertical resolutions. After deposition, easy detachment of the deposited film takes place due to the excellent anti-adherent properties of the $-CH_3$ terminated SAMs. Patterned metallic surfaces can be modified again by alkanethiolate SAMs to be used as a further mold for template replication. The patterned metallic surfaces are excellent templates to produce nanopatterned metal-semiconductor hybrid surfaces by controlled chemical reactions.

Production And Characterization Of Titanium Nitride - Titanium Aluminium Nitride (TiN/TiAlN) And Titanium - Titanium Aluminium Nitride (Ti/TiAlN) Bilayers By Means Of The Arc Pulsed PAPVD Technique

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Abstract

It was grown TiN/TiAlN and Ti/TiAlN bilayers on 304 stainless steel substrates, by using the pulsed arc PAPVD technique in a non commercial chamber. The bilayers were characterized by Scanning Probe Microscopy (SPM) in Atomic Force Microscopy (AFM) mode, where it was determined the grain size and the square medium roughness of the coatings; moreover, the X ray diffraction (XRD) technique was employed in order to identified the TiAlN crystalline phase in both bilayers. These coatings were exposed to temperature controled increase, from room temperature to 1000 C, with steps of 100 C to observe the phase transitions and the structural changes in each one of the bilayers grown.

Titanium Aluminium Nitride (TiAlN) has been shown to enhance the performance of cutting tools in dry, high speed machining of cast iron and die steels when compared with TiN coatings [1]. The inclusion of vanadium and others elements in the coatings of TiAlN is also found to stabilize the layers and promote diffusion-resistance and wear-resistance [2], for this reason that it was placed interlayers of Ti and TiN between the substrate and the TiAlN coating.

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Metal Clusters and Carbon Nanotubes: Towards Building Functional Materials

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Abstract

The presentation will focus on the following three related topics, namely, spectroscopy of ligated metal clusters in the gas phase, fabrication and applications of metal clusters in solutions and, fabrication and gas adsorption properties of single-walled carbon nanotubes.

InfraRed MultiPhoton Depletion (IR-MPD) spectroscopy is a powerful method to study cluster structures and chemistry in the gas phase. The presentation will feature recent work at the Free Electron Laser Facility in the Netherlands on Rh, Au, and Si clusters ligated with either CO or NH₃.

Laser vaporization and irradiation of powders suspended in solutions can be efficiently used to prepare copious amount of metal clusters in solutions. Following a proof-of-principle demonstration with Au/Ag, the talk will focus on the preparation and characterization of magnetic nano-clusters and their utilization in biology.

Single-walled carbon nanotubes (SWNT) can be prepared by laser vaporization of carbon targets or by chemical vapor depositions. We have improved the efficiency of these methods either through a combination of laser irradiation schemes and sample preparations or catalyst particles (cluster) designs and delivery. The most relevant results will be presented and discussed. If time permits, the adsorption properties of SWNT with respect to rare gases and molecular hydrogen will be discussed.

Developing Nano-structured Materials by Controlling Phase Transformations and Synthesis Processes

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Abstract

One of the major goals of Materials Science is to design alloys with pre-specified, desirable, technological properties. To reach this goal it is necessary to have a thorough understanding of the fundamental mechanism underline materials behavior. Of central importance is the understanding the effects on materials properties as response of changes in composition and how combination of processing parameters, such as temperature, time, applied deformation affect the microstructure. In addition to the equilibrium phase to the information available in phase diagrams, non-equilibrium dynamic processes and meta-stable phases are known to be crucial in determining materials properties. Diffusion-controlled nucleation and growth processes affect long-term phases and microstructural stability. A comprehensive understanding of the basic, underlying phenomena is indispensable in controlling these factors.

Given the above mentioned perspective, this contribution will address a variety of phase transformations taking place in the solid state, as a mechanism for tailoring materials structure at the nano and micro scales. For the purpose of a phenomenological treatment, it is common to consider two major categories of diffusional phase transformations: transformations controlled by interphase diffusion and those controlled by lattice diffusion. The former correspond to a classical heterogeneous and segregation phenomena at stationary grain boundaries and also to discontinuous precipitation, coarsening and dissolution processes in polycrystalline alloys. The latter is related to a number of homogeneous transformations such as meta-stable precipitation, spinodal decomposition and ordering reactions. After presenting the fundamentals underline the above mentioned phenomena, a number of examples will be presented as occurring in metallic and ceramic systems of a technological importance. It will be shown, by means of well-documented examples that the application of analytical electron microscopy (AEM) and high-resolution electron microscopy (HREM) allows one to obtain, respectively, nano-scale compositional data together with structural information down to the atomic level. The synthesis, processing and characterization procedures apply to these materials will, thereby, be presented based on worked examples aiming at illustrating the control of phase transformations at the nano-scale level together with the physical and mechanical properties of structural materials and devices.

Ferroelectricity in Achiral Liquid Crystal Systems

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Abstract

The ferroelectric and antiferroelectric properties are among the most spectacular manifestations of cooperative phenomena in condensed materials. These effects are observed in a wide diversity of materials such as solids, composite ceramics, polymers, and liquid crystals. The most explored systems studied corresponds to perovskites as inorganic and chiral liquid crystal as organic materials. This work shows that ferroelectricity can also be detected in systems consisting of liquid crystalline monomer \dot{U} polymer mixtures possessing no chiral centers at all, thus being the first known reported materials of this nature. The mixtures manifested high pyroelectric activity with a spontaneous polarization close to the theoretical limit.

Chiral liquid crystalline systems are very interesting since the ferro- or antiferroelectric properties may be controlled structurally. The usually applied routine approach for the preparation of such materials is essentially based on the use of chiral liquid crystalline substances possessing a tilted smectic phase. In this case the spontaneous polarization arises as a secondary order parameter[1-2].

In 1996 we have spearhead the discovery of the first achiral, macroscopically polar liquid crystalline system consisting of achiral side chain polymer and its monomer[3]. The mixtures show antiferroelectrics polarization hysteresis curves in the smectic C phase and, reveal high pyroelectric responses thus being of potential interest for applications such as IR or piezo detectors[3]. Almost at the same time, novel schemes were developed successfully introducing antiferroelectric or ferroelectric properties in liquid crystalline material systems without chiral centres. The bend shaped molecules exhibit a different smectic-like ordering having in-plane spontaneous polarization[4].

In this report we shows our first results on new achiral ferroelectric polymer - homologous monomer mixtures. Now the composites consist of the side chain polymer PM6R12 and different monomers, like M4R5, M4R6 and M4R8, mixed in a 2:1 molar ratio. The aim of this work was to study the relationship or the influence in the pyroelectric response for the PM6R12-M4R5, PM6R12-M4R6 and PM6R12-M4R8 composite. The molecular length variation of the monomer with respect to the side chain polymer gives the possibility for the monomer to allocate in a different fashion between the mesogenic side chains in the polymer. The new composites show pronounced ferroelectric switching, a phenomena that need to be reviewed. We will inform the piezoelectric coefficient d_{31} , pyroelectric coefficient and spontaneous polarization P_s for the mentioned composites.

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Granular matter transport: hydrodynamics and beyond

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Abstract

Granular materials, composed of many individual particles are present in many common-day and industrial phenomena. One of the many problems that are still unsolved in full detail is the transport of granular materials. When two grains collide, there is some kinetic energy that is lost (in friction, plastic deformation or other mechanisms); thus to sustain a macroscopic motion energy must be supplied continuously. The usual methods are trough external forces and vibrating walls. Depending on the energy injection rate the system can behave as a solid, a fluid or a mixture of both. The fluid phase is relatively known, but there are some important differences with molecular fluids, like clustering, shear instabilities and anomalous energy transfer. In the solid phase there is also some understanding and the key problems deal with force transmission. But the mixed phases, where solid and fluid phases coexist lacks for a description.

In this seminar, some of the features of the fluid phase will be detailed with emphasis on the energy transport mechanisms. Some peculiarities of the mixed phase will be enunciated.

Influence of Shell Matrix Macromolecules on Biomineralization of Freshwater Bivalve Mussel (*Diplodon chilensis*)

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Abstract

Biomineralization refers to the processes by which living organisms form minerals. Biogenic minerals (biominerals) distinguish from their inorganically produced counterparts in their unusual external morphologies, crystallographic orientations and the way they are formed. The process of biomineralization has received much attention from materials scientists, because the biominerals produced are inorganic-organic hybrid composites formed by self-assembled bottom up processes under mild conditions, showing interesting properties, controlled hierarchical structures and remodeling or repair mechanisms that are still remaining to be developed into a practical engineering process. Through the analysis of many biominerals from seawater organisms, a myriad number of macromolecules have been described to be involved in the control of biomineralization. However, little is known on the mechanisms controlling freshwater organisms mineralization.

The present study reports the partial isolation and function of shell macromolecules obtained from the freshwater bivalve (*Diplodon chilensis*). Soluble and insoluble fractions and insoluble films from decalcified shells were used to modify the in vitro crystallization of calcium carbonate. Fractions and/or films were added to buffered calcium chloride solution under a CO₂ and analyzed by scanning electron microscope (SEM).

The different fractions and their combination produced noticeable changes in the calcium carbonate crystal morphology. These changes remain to be correlated with the structure of the macromolecules.

Solid -State Coordination Chemistry: Hydrothermal Synthesis of Oxovanadium Phosphates (Phosphonates) with Copper Coordination Compounds.

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Abstract

Many recent papers have highlighted the great flexibility of polyoxovanadates to adopt a wide range of different cluster, chain and network frameworks. The rich and subtle chemistry found in the hydrothermal synthesis of polyoxovanadates illustrates the ability of vanadium to adopt different coordination environments (octahedral, square pyramidal, trigonal bipyramidal and/or tetrahedral). These structures can be greatly enriched and diversified by adding phosphate or phosphonate groups, together with copper coordination compounds. By combining substructures it is possible to generate a composite which possesses a combination of their individual properties, such as catalytic, optical or magnetic.

In this work some new oxovanadium and oxovanadium / phosphate (or phosphonate) frameworks, modified by the presence of copper complexes, will be presented together with their magnetic properties. All the analyzed compounds present diamagnetic vanadium (V) ions, so the paramagnetic centers which generate the measured magnetic properties correspond to the copper (II) ions present in the structures.

Acknowledgements

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Directed Assembly of Nanomaterials for Miniaturized Sensors

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Abstract

The abundant knowledge about synthesis of nanomaterials has paved the way for the controlled construction of miniaturized sensors and sensor arrays. However, self-assembly methods lack precise position control, the ability to pattern multiple species and overall reproducibility, among other considerations. In view of these challenges, directed assembly of nanobuilding blocks by various site-specific patterning approaches is desired. We have resorted to dip-pen nanolithography (DPN) to pattern diverse nanomaterials (semiconducting metal oxides) as building blocks which assemble into final functional form. The site-specific and multiple-ink patterning capabilities of DPN are put to use in fabrication of miniaturized chemical sensor arrays with sol-based inks which yield gas sensitive semiconducting metal oxides. The miniaturized sensors constructed in this manner show ultra-fast response and rapid recovery, and can be further integrated to form sensor array that have excellent gas recognition capabilities. We have extended this approach to "electronic nano-nose", whereby multiple sensor elements are integrated in an array for multiplexed gas sensing.

Template Synthesis of LaNiO₃ Nanotubes by a Precursor Method

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Abstract

Nickel and lanthanum perovskite, LaNiO₃ (LNO), have attracted attention for its low resistivity and its structure. The later is similar to perovskite-type ferromagnetic materials like Pb(Zr,Ti)O₃ and (Ba,Sr)TiO₃, so it is expected that these materials could be grown over LNO. Thus, the creation of nanostructures of LNO may be interesting not only because of their own possible applications but also because more complicated materials can be created from them.

In our work, LNO nanotubes have been chemically synthesized employing a precursor method. The pores of an alumina membrane are filled by capillarity with a solution of (NH₄)LaNi(NO₂)₆ which gives LaNiO₃ by thermal decomposition.

The precursor was characterized by FTIR spectroscopy in KBr, UV spectroscopy in solution and thermogravimetry; powder x-ray diffraction was used to characterize LNO. The LNO nanotubes were observed by SEM/EDAX, TEM, HR-TEM and DF-TEM. These methods reveal that they are hollow, with internal partitions. Their diameter is highly monodisperse around 300 nm. The wall is exceptionally thin, being only a few nanometers thick.

On Growth and Form of Graphitic Structures

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Abstract

Graphite has proved to be very flexible forming not only fullerenes and nanotubes, but other more complicated arrangements such as onion-like structures, cones, coalesced fullerenes inside single walled nanotubes (peapods) coalesced tubes, etc. First of all, this work shows several possibilities of new graphitic nanostructures with amazing properties waiting to be discovered. The other part of the present account is devoted to growth mechanisms and self assembly of new graphitic architectures. Understanding the growth and form of graphite will allow us to understand other layered materials and make a substantial contribution in future nanotechnological applications.

Fabrication of Vapor and Gas Sensors Using Films of Aligned CN_x Nanotubes

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Abstract

We have succeeded in sensing rapidly (0.1 - 0.5 sec response), relatively low concentrations of toxic gases (e.g. > 1% for ammonia), and organic vapors (e.g. acetone, ethanol, gasoline, pyridine, chloroform, etc.) using electric devices integrating films and compressed pellets of aligned CN_x nanotubes. We demonstrate, for the first time, that CN_x nanotubes could be more efficient for monitoring toxic and hazardous species, when compared to pure carbon nanotubes. This is due to the fact that CN_x nanotubes exhibit nitrogen rich islands on their surface, which are highly reactive. Using first principles calculations we confirmed that pyridine-type regions on the tube surface bind strongly (chemisorption) to ammonia, acetone and OH groups, thus altering their density of states (DOS) and minimizing the electron conduction causing a decrease in the states around the Fermi energy (E_f). The fabricated sensors are sensitive to physisorption and chemisorption when exposed to different gaseous species. Our results demonstrate that CN_x nanotubes could be used as fast responsive sensors due to the nitrogenated sites on the tube surface, thus opening novel avenues in the sensor industry especially in the fabrication of reusable alcoholmeters.

Advances and Challenges of Nanotube Science and Technology

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Abstract

Experimental and theoretical research on nanomaterials continues to accelerate and, as a consequence, novel structures with remarkable chemical reactivity, as well as mechanical and transport properties are being predicted and developed. In particular, the synthesis of novel nanostructures (e.g. nanotubes, inorganic fullerenes) using layered materials such as graphite, BN, BC₂N, WS₂, MoS₂, VS₂, NiCl₂, CN_x, etc. may revolutionize technology in less than 10 years.

However, at this point and from the experimental viewpoint, it is important to carefully control stoichiometries of elements, homogeneity of the nanomaterials and to develop novel self-assembly processes to grow or interconnect such fascinating structures. In this context, it will be shown that that “substitution reactions” involving carbon nanotubes or metal oxide nanorods in the presence of B₂O₃ or H₂S yield stable B_xC_yN_z nanotubes and MS₂ (M = W, Mo, Re, Ta, Nb) nanotubes and nanoparticles respectively. These results provide vital information for achieving growth control in the production of inorganic nanotubes and homogenous heteroatomic structures.

The importance of doping in carbon nanotubes will be emphasized, since it is possible to alter significantly the electronic, mechanical and chemical properties of the tubes. This opens up new avenues in the production of nanomaterials with desired properties and stoichiometries. Therefore, the controlled production of nanotubes made of layered BC₂N and CN_x will be presented. In this context, the electronic and field emission properties, as well as the density of states (DOS) of CN_x and CB_x nanotubes using scanning tunneling spectroscopy (STS) will be discussed. It is also demonstrated that the presence of low concentrations of N and B inside carbon nanotubes are responsible for introducing donor and acceptor states near the Fermi Level. Novel applications of these doped materials will also be discussed in areas of chemistry (as chemical sensors), biology (as protein immobilizers) and electronics (metallic and semiconducting nanowires).

Regarding single-walled carbon nanotubes (SWNTs), we will demonstrate, that irradiation exposure at elevated temperatures, can be used as an effective tool to covalently coalesce and weld SWNTs in order to create larger tubules and molecular junctions of various geometries. We have fabricated “Y”, “X” and “T-like” junctions, that are stable. Tight binding molecular dynamics calculations demonstrate that vacancies, formed under the electron beam, trigger the formation of molecular junctions involving seven or eight membered carbon rings. We envisage that our results will pave the way towards controlled fabrication of novel 3-dimensional nanotube based molecular circuits, nanotube fabrics and network architectures.

III-V Quaternary Semiconductor Materials Based on Ga, In, As and Sb

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Abstract

The III-V semiconductor ternary and quaternary compounds are, at the present days, one of the most popular materials for technological applications in electronic devices. These materials are especially important for heterostructure devices; the best semiconductor lasers and high electron mobility transistors all use heterostructures based on ternary and quaternary compounds. Due to the ability of these alloys to optimize their parameters for different device applications and, at the same time, matching their lattice constants to a desired substrate, they are very attractive materials for the development of new devices. In this work we present epitaxial layers based on Ga, In, As, Sb quaternary alloy, over GaSb, Te doped and undoped single crystals, their fabrication technique and characteristics such as surface morphology, crystallinity, chemical composition and stoichiometry.

This work was supported by Colciencias and Universidad del Quindío.

Optical and structural characterization of MoO₃ thin films prepared by thermal evaporation using a CO₂ Laser.

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Abstract

MoO₃ thin films were growth by evaporation using a CO₂ laser working at continuum wave. Substrate temperature and pressure of oxygen were varied to determine their influence over the optical and crystallographic properties of samples. Thin films were growth on to glass substrates using powder of MoO₃ (99.9 sublimates due to the incidence of a 9 watts power beam over its surface. Samples were prepared raising the substrate temperature from room temperature to 350 oC. A base pressure of 2×10^{-5} Torr was established in chamber, and some samples were deposited under an oxygen atmosphere with partial pressures ranging from 10^{-5} to 10^{-3} Torr. Samples were characterized with optical transmittance measurements at the visible range using a PERKIN ELMER Lambda 2 spectrophotometer. X-ray diffraction patterns were obtained with a Phillips diffractometer, with the K- α line of copper, and a 40 mA current at 40KV . The experimental transmittance spectra were simulated by using a theoretical model for the transmittance of a thin film deposited on to a transparent substrate [1]. From the simulation process the optical properties as absorption coefficient, refractive index and samples thicknesses were determined. Samples prepared at substrate temperatures below 250 oC were amorphous, from 250 oC to 350 oC samples exhibited a polycrystalline structure [2]. At long wavelengths (880 nm) it is present a strong absorption band likely due to oxygen vacancies in the sample [2]. Refractive index is increased as the substrate temperature is elevated. From the calculated absorption coefficients it was possible to determine the material energy gap, it is observed a strong dependence of this parameter with substrate temperature being shifted from 2.83 eV on samples prepared at 300 oC to 3.16 eV on samples prepared at room temperature [2].

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Synthesis and crystal structures of three new copper perchlorate complexes

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Abstract

The structure and reactivity of the copper complexes are very sensible to the nature of the ligands. In this poster we present the synthesis and crystal structures of three new copper complexes : (1) Di-(bis - (2-pyridylmethyl-benzilamina) (bis - μ - chloro) di-copper (II), (2) Di- [(6-methyl-2-pyridylmethyl)- (2-pyridylethyl)benzilamine] (bis - μ - metoxo) di-copper (II) and (3) Di-4-carbomethoxy catecolate cuprate II of 4-methyl-2,6- bis - [2-(2-pyridyl)ethyl]iminomethyl]phenol di-copper (II).

All three complexes are dimeric and present perchlorate as counterion. The third complex shows in addition one extra counterion in the form of a bis- catecolate of copper (II).

Hydrogenation of palm oil to obtain fatty alcohols using heterogenous catalysis

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Abstract

The methyl esters hydrogenation reactions from palm oil were studied using heterogeneous catalysts like Cu-Ni, Cu-Sn and Ni-Sn supported in titanium, tin and zinc oxides, prepared by impregnation method and activated with hydrogen at 400°C, the reactions were carried out to 50 bar of hydrogen and 200°C, with magnetic agitation in a Batch reactor during 6 hours. Palmitate, oleate, estearate and methyl linoleate esters from palm oil weren't transformed to alcohols, but double bond partial hydrogenation reactions of polyunsaturated esters being obtained selectively methyl oleate and positional isomerization reactions in methyl oleate.

New hybrid organic/inorganic copper oxovanadium phosphates

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Abstract

Recently, many researchers have used a hybrid approach in which an organic ligand is combined with an inorganic one. Such organic/inorganic hybrid materials combine the characteristic features of both the organic and inorganic substructures in design of solid state phases with novel physical properties.

In this work we report the hydrothermal synthesis and characterization of new hybrid organic/inorganic copper oxovanadium phosphates $\text{Cu}_4\text{bipy}_4\text{V}_4\text{O}_{11}(\text{PO}_4)_2 \cdot x\text{H}_2\text{O}$ ($x = 5$) and $\text{Cu}_2\text{bipy}_2\text{V}_2\text{P}_2\text{O}_{12}$ (bipy-2,2'-bipyridine) which crystallize in the triclinic symmetry. The two structures present different oxovanadium phosphate anionic units which result from the vertex-sharing of PO_4 and VO_4 tetrahedra and are coordinated to copper diimine cationic groups to form a 1D framework.

Acknowledgements

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Investigations on the Ion Transport Mechanism in Conducting Polymer Gels

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Abstract

The change in the electrical properties of polymer membranes based on poly (vinyl alcohol) (PVOH) and potassium hydroxide (KOH) have been investigated as a function of the environment relative humidity (RH%) and temperature. The membranes were characterized by electrical conductivity (using impedance spectroscopy) and thermal measurements (using differential scanning calorimetry DSC) and thermogravimetric analysis). It has been found that the temperature dependence of the ionic conductivity (keeping constant the relative humidity) follows an Arrhenius-type behavior associated with the ion transport mechanism in water swollen polymer films. A treatment of the experimental data is proposed to explain the conductivity trend as a function of Rh% based on the Onsager equation valid for electrolytic solutions. The equation has been applied to the relevant parameters of the polymer membranes and it describes change in its conductivity as a function of its water content satisfactorily.

Keywords: Solid polymer electrolytes, poly (vinyl alcohol), electrical conductivity.

Nanomagnetism

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Abstract

In this talk fundamental concepts in magnetism like hysteresis, blocking temperature and magnetization reversion are introduced in relation with recent experimental results and possible technical applications. Some new results in magnetic nanostructures and granular systems will be presented. Finally, dynamical aspects of the reversion problem will be addressed.

Inhomogeneidad de Esfuerzos en Películas de ZnSe Determinada por la Técnica de Fotorreflectancia

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Abstract

Se presenta el análisis de esfuerzos por medio de la técnica de fotorreflectancia (FR) de películas de ZnSe crecidas sobre sustratos de GaAs. El objetivo es realizar un estudio de los esfuerzos presentes y de la homogeneidad de estos en la película. El de ZnSe se creció por la técnica de epitaxia de haces moleculares (molecular beam epitaxy, MBE). Para las mediciones de FR se emplearon láseres de diferentes longitudes de onda como: el HeNe 6328, 5430 Å, HeCd 4416 y 3250 Å. El valor de la banda prohibida se obtuvo por medio del ajuste de la curva mediante la expresión de la tercera derivada de Aspnes. La línea de FR muestra dos contribuciones a la señal en 2.673 y 2.695 eV. El primer valor corresponde a la contribución a la curva de una región cercana a la interfaz ZnSe/GaAs y significa que el ZnSe se encuentra tensando debido a la deformación térmica. El segundo valor corresponde a la señal donde la influencia de las tensiones es menor y esto ocurre para regiones cercanas a la superficie del ZnSe. El valor de la deformación hidrostática que experimenta la película de ZnSe, es de -5.9×10^{-3}

Copolymerization of propylene and alpha-olefines by using metallocene catalyst

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Abstract

In the search of new catalysts for polymerization of alpha-olefines, metallocenes have arisen in the last decades like an alternative for the obtaining of polymers with tacticity (1), molecular weight and distribution of molecular weight control. Ligands bonded to the transition metal, as well as the type and length of the bridge among rings, can change metallocene geometry, and consequently the stereoselectivity of the catalyst, existing a relationship between the symmetry of the catalyst and the structure of the produced polymer (2).

Supporting of metallocene catalyst (deposition of the catalyst on an insoluble support) allows to obtain products (3,4) with much more stereoregularity and with higher molecular weight than in homogeneous systems; supported metallocenes provides kinetic control of the reaction and morphologic control of the polymer particle.

On the other hand, synthesis of propylene copolymers with alpha-olefines allows the obtaining of new polymeric materials (5,6), from thermoplastic until elastomeric products.

In this work it has been obtained propylene copolymers with alpha-olefines from 6 to 18 atoms of carbon, using catalytic metallocenes based on zirconium, with methylaluminoxane (MAO) as cocatalyst. This work will be continued with supported catalyst. Isoselective and syndioselective zirconocenes has been used, in a slurry polymerization system. Polymerization products of homogeneous systems, have been analyzed by means of GPC, ¹³C-RMN and DSC. It has been observed that the comonomer reactivity decreases when increasing the long of chain, and that the molecular weight of the copolymer decreases when comonomer incorporation increases. Melting temperature diminishes when comonomer incorporation increases, in a lineal relationship.

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Different DFT Approximations for the Calculation of Crystalline Packing Effects on Magnetic Exchange Interactions

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Abstract

The interpretation of some physical and chemical phenomena in solid state, requires the utilization of theoretical models. It is known that the magnitude of the value of the magnetic exchange between two metal centers is strongly dependent on the metal-bridge-metal angle and the distortion of the plane generated by these atoms. At a molecular level these are the relevant parameters, however, once the crystalline packing is considered, new interactions appear. These interactions have not been extensively studied and show however an important influence on the magnitude of the value of the magnetic exchange.

In the present work we will show the results of the calculations performed on a copper (II) binuclear macrocyclic complex. The macrocyclic ligand corresponds to the product of the <2+2> condensation of 2-hydroxi-4-methyl-1,3-benzenedicarbaldehyde and 1,3-diamine-2-propanol. All the calculations were performed using the crystalline geometrical parameters. The variable in this study was the number of the axial ligands existing in the crystalline arrangement. Several DFT calculations using different functionals (local and non-local) and basis sets (analytical and effective core potentials) were performed on each of the structures.

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Restrictions to Ferro and Antiferroelectric Behavior in Highly Polarized non Chiral Polymeric Materials

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Abstract

The conversion of thermal energy to electrical energy using pyroelectric materials has been known since ancient times [1]. Up to 1960 all piezo and pyroelectric devices made, use either a single-crystal structure such as quartz and lithium tantalite, or a polycrystalline ceramics such as lead titanate zirconate perovskites in which the dipole moments of individual crystalline units could be oriented by an applied electric field. The discovered strong piezoelectric [2] and pyroelectric effects [3] induced in the polymer poly(vinylidene fluoride) or PVDF by application of an electric field open a wider possibilities of applications. The great potential of a completely flexible rugged piezoelectric and pyroelectric material which can be inexpensively transformed to large area thin sheets was immediately realized in a wide variety of prototype devices [4]. It was until 1974 when chiral liquid crystals begin to dominates this field of research [5]. As it was demonstrated by Soto et al. in 1996 [6], it is possible the existence of systems without optical activity by themselves that posses comparable or even better characteristic when compared with other quiral related materials. The described system consist of a mixture of a polymer and 33% of its respective monomer, assuming an anticlinic structure of the mesogen units that are perpendicular to the main chain in a herring bone structure. The first remarkable observation made on the systems was a very low saturation voltage of around 10 V/ μm , that can be only understood if a cooperative process as ferro- or antiferroelectric is present in the samples. These preliminary observations initiated a further detailed study of the system electrical behaviour using the pyroelectric effect, where the observed electrical properties can be easily related with the polarization of the material. Applying this technique with the restriction already discussed to the samples, we succeed to find a maximum macroscopic polarization three times higher compared with our standard in a PM6R12-M6R12 sample. Later on, measurement of bias field dependence of the pyroelectric coefficient in the smectic C2 phase temperature range shows a typical hysteresis curve for a ferroelectric material. In an ongoing program we are interested in the design of reliable and stable pyroelectric materials suitable for device applications. To enhance our knowledge of the system, and temperature range applicability, measurements at low temperature of the order of 100 K has been carried out. The pyroelectric studies on a series of polymeric mixtures where the spacer will be fixed with 6 methylenic groups (PM6Rn) and the aliphatic chain with 12 carbon atoms (PMnR12) will be discussed. The analysis will be done based on the hysteresis loops of the pyroelectric coefficient at a constant temperature and their respective pyroelectric curves.

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Study about anticorrosive protection mechanisms of organic coatings using electrochemical impedance spectroscopy

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Abstract

The models of the electrochemical behaviour of three different pigments, Zinc chromate, Micaceo iron oxide and metallic zinc, used in coatings formulation, are deduced from diagrams of Electrochemical Impedance Spectroscopy (EIS), and other techniques of surface analysis as X-ray photoelectron spectroscopy (XPS), and the Scanning Electron Microscopy (SEM). The coatings were applied on carbon steel coupons with superficial preparation SSPC-SP5 and evaluated in a controlled atmosphere of saline spray cabinet according to the standard American Society for Testing and Materials (ASTM) B117. The spectrum of EIS were obtained using a Schlumberger instrument, SOLARTRON SI1280B. The described models show the functionality of these pigments in the coating, these models allow to understand the characteristics in order to improve the anticorrosive properties of them. The results allow the implementation of the EIS for the evaluation of the organic coatings performance in simulated environment, once the mechanism protection are known. Three different equivalent circuits were proposed for each evaluated coatings. The analyses of X-ray photoelectron spectroscopy (XPS) confirm the reduction from the Cr⁶⁺ to Cr³⁺, through the exposure time and as it arrive to the steel interface. Similarly the oxidation of Fe²⁺ at Fe³⁺, from the contact with dichromate ions is demonstrated

Electronic Quantum Step Confinement in Ag/Al(100)

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Abstract

Physical properties of thin metal layers and metal-metal interfaces are of importance in several applications in nanotechnology. It is in particular interest to study the evolution of the electronic properties of these systems as a function on thickness of the metal layer, which is the main electronic confining direction in a metallic quantum step. Using inverse photoemission spectroscopy (IPS) we have studied the empty electronic states of ultra thin Ag layers on Al(100). The IPS spectra obtained at normal incidence for several thickness of Ag deposited at temperature less than $\tilde{U}100\text{zC}$ show specials resonances, which cannot be attributed to silver or aluminum density of state. Nevertheless, we observe an intensity dependence in the IPS spectra as function of the Ag thickness. By help of numerical calculations we show the potential effect of this system on the electron wave function. We distinguish two possible resonances that are quantum step resonance(QSR) and surface state resonance(SSR).

Optical properties of coatings based on liquid crystals dispersed in polymer blends

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Abstract

Films that can be thermally switched from opaque (translucent) to transparent states, called thermally-reversible light scattering films (TRLS), have potential uses in privacy windows, displays, thermal sensors, active elements in thermal memory all-optical devices and other optical applications. Materials developed for these purposes consist of two phases that exhibit a mismatch of refractive indices at a characteristic temperature, where one of the phases undergoes a disorder-order transition (i.e. a crystallization or an isotropic-nematic transition). A usual composition for TRLS films consists of domains of a relatively low-molar-mass compound (i.e. a fatty acid or a liquid crystal), dispersed in a polymer matrix. This compound exhibits a relatively high solubility in the polymer matrix that depends on temperature. This leads to a low activation energy for the variation of optical transmission with temperature which is one of the main drawbacks for practical applications. Besides, changes in morphologies in the course of successive cooling/heating cycles lead to corresponding variations of optical properties.

In this presentation it will be shown that the mentioned drawbacks may be eliminated by adding a small amount of a thermoplastic polymer to a solution of a liquid crystal in thermoset precursors. The thermoplastic polymer must have a refractive index matching the one of the fully cured thermoset, and should exhibit a high compatibility with the liquid crystal and a low compatibility with the thermoset precursors. This would lead to phase separation of thermoplastic/liquid crystal solutions at low conversions in the polymerization reaction. This process has the following potential advantages: a) a dispersion of droplets of adequate size for the scattering of visible light may be achieved with smaller liquid crystal concentrations than those used in commercial products (growth and coalescence processes are favored when phase separation occurs at low conversions), b) this primary morphology should be stable at room temperature or in the course of successive cooling/heating cycles due to the high viscosity of droplets containing the thermoplastic polymer, c) the residual concentration of liquid crystal in the thermoset may be decreased leading to an increase of its glass transition temperature. Although we will focus on generating an efficient TRLS film, these ideas can be as well applied to the development of new families of polymer dispersed liquid crystal films (PDLC).

Properties of Porous Membrane from Polypropylene Copolymers Prepared by the TIPS Process

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Abstract

In the present work, a study related to the effect of the comonomer type (1-Hexene and 1-Octadecene) and content in the iPP on the membrane morphology and its properties will be presented. We have found that for copolymer membranes from iPP with 1-Hexene the permeability increase when the incorporation of the comonomer increase. For the copolymer membranes from iPP with 1-Octadecene the behavior is opposite.

New Polymeric Materials obtained from blending of Polypropylene and Olefinic Elastomers by using Compatibilizers

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Abstract

Mechanical properties of polypropylene can be improved by blending with other polymers. The aim of this study was to investigate the compatibilizing effect of functionalized PP as well as copolymers of ethylene-1-hexene and ethylene-1-octadecene on the compatibility of PP/PE- α -olefin blends. The effect of grafting of itaconic acid (IA) as polar monomer onto PP, ethylene-1-hexene copolymer (PE-C6) and ethylene-1-octadecene copolymer (PE-C18), via free radical reaction, on the processability, morphology and mechanical properties of PP/PE-C6 and PP/ PE-C18 blends is presented in this work. Blends were characterized by tensile modulus, strength and elongation at break measurements. The blends containing grafted polymers show a higher toughness without any reduction of the strength and stiffness. The glass transition temperature of PP was increased slightly due to effect of PE-C6 domains on the segmental mobility of PP suggesting that an interpenetration between the noncrystalline portion of PP and the interface of PE-C6 exists.

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Production and Characterization of Ferromagnetic Alloyed-Nanowires inside Carbon Nanotubes

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Abstract

We describe the production of aligned multi-walled carbon nanotubes filled with Fe-Co alloys. The method involves the aerosol thermolysis of toluene-ferrocene-cobaltocene solutions at temperatures ranging from 650 to 800°C in an inert atmosphere. The materials have been carefully characterized using state-of-the-art high-resolution transmission electron microscopy (HRTEM), energy electron loss spectroscopy (EELS), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), electron diffraction, HREELS-STM elemental mapping, X-ray powder diffraction and SQUID magnetometry. The results indicate that different stoichiometries of Fe_xCo_y alloys could be produced at different temperatures. We noted that the formation of FeCo alloys only occurs at relatively low pyrolytic temperatures (e.g. 650 - 750 °C). Above this temperature, segregation of Co and Fe domains start to occur. The alloy nanowires (5-30 nm OD; 1 micron long) are monocrystalline and always exhibit the FeCo (110) parallel to the carbon nanotube axis. The Fe_xCo_y nanomaterial has shown unusual ferromagnetism and large coercive fields at room temperature (e.g. 1500 Oe). We envisage that these aligned ferromagnetic nanowires could be used in the fabrication of high-density magnetic storage devices.

Glass Myths

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Abstract

In this talk I review and discuss, in light of experimental evidence and theories, two well-known histories about glass: the possible (slow) flow of medieval stained glass, and coloured sacred images that miraculously appear on some contemporary windows. Reportedly some stained glass windows from 12th century cathedrals are thicker at the bottom than at the top, suggesting that glass is a liquid which flows (albeit slowly) downward under the force of gravity (see video show). When I first heard about sagging medieval windows, I thought it was just a Brazilian myth. But then I heard the same tale from colleagues in Chile, and found echoes of it the Encyclopaedia Britannica and even in engineering textbooks. Although window glass isn't supposed to flow at room temperature, old glass has many impurities that might help it ooze. So I looked up the chemical compositions of some 300 medieval glasses and calculated (extrapolated) typical viscosities at room temperature. With the help of P.K. Gupta we then determined the time scale necessary for window glass to flow. Since July 2002, an image on a old window has been mobilising thousands of people in Ferraz de Vasconcelos, on the outskirts of São Paulo city, Brazil (see video show). It is a face that is reminiscent of the Virgin Mary, the mother of Jesus. After countless television reports, similar effigies started to be noticed in homes from several other cities in Brazil. There has been also a report of a similar image in Clearwater, FL, USA. To attend a request from the Vatican to check up a possible miracle, we demonstrated that these images are the result of natural phenomena. Finally, I will show a video and demonstrate and discuss a third "surprise" glass myth.

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