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ABSTRACTS
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INTERNAL STRESS ANALYSIS FOR NANOSTRUCTURED Li-BATTERY ELECTRODES

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Due to the small Li-intercalation of carbon, which is used as the base material for the negative electrode in rechargeable Li-batteries, extensive research is being performed, for over two decades in order to find alternative anode materials. This research has suggested that some of the best candidates are Sn and Si, due to their high capacity. These materials, however, have not been used commercially because of their large volume expansion, which results in crumbling of the electrode after continuous electrochemical cycling. It is therefore of great importance to model the internal stress development inside these anodes. Since the miniaturization of the high-energy storage devices at hand is desired, gradient elasticity is employed to capture size effects as the scale of the microstructure is reduced to the nanoscale; comparison with solutions obtained from classical elasticity are made.

Spontaneous self-agglomeration of magnetic nanoparticles into nanowires

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A newly developed method for the formation of nanowires by self-aggregation of nanoparticles is presented in this paper. The first experiments have been performed using Co-rich nanoparticles dispersed on a holey carbon grid. The nanoparticles are inserted in a vacuum oven and are annealed at temperatures below 400C in the presence of a hydrocarbon vapour without the use of any externally applied electric or magnetic fields. High resolution electron microscopy (HREM) was extensively used to determine the shape, size distribution and crystallographic phase of the starting and produced materials. Interestingly, after an annealing circle of 72 hours, the nanoparticles seem to self-agglomerate into nanowires which have diameters in the 5-20nm range and lengths exceeding at cases 1 micron. The diameter of the produced wires is in the same range as the diameter of the initial nanoparticles, further supporting the notion that the nanowires have formed out of the nanoparticle agglomeration. Close inspection of nanowire HREM images shows that the structure of the nanowire body indeed resembles at cases linked nanoparticles. Phase identification has also been performed using the HREM images and a comparison between the starting material and the produced nanowires will be presented.The process presented here shows that nanoparticles can spontaneously self-align into nanowires in way never reported before. Therefore there is certainly scope for studying this method further to reveal more information about the catalytic action of transitional metals on hydrocarbons and the exact nanowire formation mechanism. Although it is currently a matter of speculation, this process might lead to the effortless growth of nanowires at particular places when building miniature circuits.

The Relationship Between Stability/Nanostructured Omega Phase/Mechanical Properties of Beta Titanium Alloys

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The mechanical behavior of various Ti-V alloys was studied at room temperature. The beta phase of these alloys, which has a BCC structure, contains a nanostructured omega phase. When a single phase beta Ti-V alloy was deformed, the primary deformation mechanism was found to be twinning. Upon twinning the omega phase, which is present in the parent crystal, reforms in the twin. However, when a beta phase with similar stability in the presence of alpha phase was deformed, the beta phase was found to deform by the formation of stress induced HCP martensite. When this martensite forms, the nanostructured omega phase was found to disappear, i.e. the omega phase was consumed during the stress induced transformation. The effect of this on the mechanical properties and the details of the investigation will be presented.
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Multi-scale Modeling of Titanium Dioxide: Controlling Shape with Surface Chemistry

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An important aspect in the use of titanium dioxide at the nanoscale for advanced photochemical applications is the controlled manipulation of the size, phase and morphology of the nanoparticles in solution. Solution pH is widely used to manipulate such properties at the nanoscale. We have used a multi-scale model designed to describe nanoparticles thermodynamics as a function of size, shape and chemical environment to investigate the effects of pH on the shape and phase stability of titanium dioxide nanoparticles. As input for the model, surface energies and surface tension of low index stoichiometric surfaces of anatase and rutile under hydrogen rich and hydrogen poor conditions have been calculated using density functional theory. Our results show how anatase phase is stabilized in acidic solution while the rutile is stabilized in basic solution, and that pH may also be used to control the particle shape and therefore the chemical functionality.

Computational Nano-morphology: Modeling Shape as well as Size

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As the demand for nanomaterials tailored to particular applications increases, so to the need for robust, monodispersed nanomaterials with reproducible and highly uniform properties will grow. It has been widely shown that many fundamental properties of nanomaterials have a strong dependence on particle size. Although great advances have been made in controlling the size of nanoparticles, variations of some properties still remain due to a dependence of the property not only on size, but also on the morphology. Individual particle properties such as quantum confinement, nanomagnetism, and catalytic properties have been found to be shape dependent, as have collective properties such as the self-assembly of metallic nanoparticles arrays. Therefore, nano-morphology must be carefully controlled to reliably synthesize large quantities of nanoparticles with uniform properties. We present results of a thermodynamic model designed to describe the shape of nanoparticle as a function of size and chemical environment; and show how the model may be used to explain how the shapes of nanoparticles differ from their macroscopic counterparts, and to predict the morphology of nanoparticles under desired conditions.

Synthesis and characterization of copper nanoparticles inserted in organic matrix

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Unsupported and supported copper nanoparticles are obtained by reduction of copper nitrate by the polyol process and characterized by X-ray diffraction, SEM, and TEM. The study we have undertaken on the preparation of copper nanoparticles showed that they can be obtained in a wide range of size depending on the concentration of the copper salt or ethylene glycol, the presence of a second metal, temperature and time of reduction, presence or not of a stabilizer or support, the metal loading in the case of supported materials. Addition of Ag and decreasing the copper content or increasing the EG/copper ratio decreased the metal particle size. Silica surface defects were suggested as catalytic sites which accelerated copper ions reduction in the presence of silica as surfactant or support. Strong metal- support interaction and reduction rate were the main factor determining the size and morphology of the supported metal particles formed. The thermal study of the copper nanoparticles evidenced the presence of an organic matrix and gave some structural information on the fresh samples.Hydrogen thermal treatment of the reduced phase showed also that the organic fragment, belonging to the precursor salt, still remained attached to the supported or unsupported copper particles as stabilizing matrix.The organic matrix retained on the reduced copper phase played a similar role as silica, that of stabilizing a agent of the metal nanoparticles

Nanocrystalline HF-CVD-grown Diamond and its Industrial Applications

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The correlation between the micro- and nanostructure of a material and its physical and chemical properties is the key issue in materials development. Considerable progress has been achieved recently by the development of new processing technologies (hot-filament-CVD-deposition) and new materials in a nanocrystalline state (nanodiamond) with superior mechanical strength and tribological properties. A novel fabrication method, based on CVD diamond deposition has recently been established at the University of Ulm. Reliable processing parameters have been developed in order to produce 30 - 40 micrometer thick samples of diamond with an average grain size of about 15 nm on 2 inch diameter silicon wafers. Further processes based on lithographic techniques known from silicon technology allow further microstructuring of CVD-diamond. This approach is unique world-wide. So far, the microstructuring of highly oriented columnar diamond has been hampered by the fact that the internal microstructure is being reproduced by plasma etching yielding rather rough surfaces. This problem now can be overcome by the production of nanoscale diamond. It can be expected that microparts (microtoothed wheels, atomically sharp cutting edges, functionalized diamond surfaces etc.) can be produced on a reliable basis in the near future. The fabrication of ultra sharp diamond cutting edges, resulting in radii of curvature below 10nm has already successfully been demonstrated. However, major stepping stones have to be overcome, such as, for example, the control of internal stresses limiting the film thickness, homogeneity of the films, doping procedures etc.

STUDY OF SELF-ASSEMBLED MONOLAYERS OF DNA AND DNA-CARBON NANOTUBE HYBRIDS AND THEIR APPLICATION TO DNA SENSORS

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Recent interest on the design and fabrication of new types of bionanosystems has increased the amount of studies regarding the functionalization of nanomaterials with biomolecules. These novel systems have the potential to be used in a variety of applications, including chemical and biological probes and sensors. This work presents the study of the supramolecular complex formed by the non-covalent functionalization of carbon nanotubes by DNA. The optimal conditions for the formation of these hybrids will be determined. In addition, gold substrates will be modified by self-assembled monolayers of mercaptohexanol, DNA and DNA-carbon nanotube hybrids, and the efficiency of the modification will be determined by microscopic, electrochemical, and spectroscopic techniques. Parameters such as concentration, immobilization time, and DNA length and sequence will be studied. These studies will enhance our understanding of the interaction between DNA and carbon nanotubes, which will lead us to develop more efficient bionanomaterials, in particular DNA sensors.

Rheology of CuO nanoparticle suspension prepared by ASNSS

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In this study, a low-pressure control method for an arc-submerged nanoparticle synthesis system (ASNSS) was proposed and developed for CuO nanoparticle fabrication. This study investigates into the rheology of CuO nanofluid having different mean particle sizes. Experimental results indicate that the pH value of the CuO nanofluid fabricated in this study is 6.5, which is far smaller than isoelectric point (i.e.p) of pH 10. The CuO nanofluid with larger mean particle sizes has a larger shear stress when the shear rate of different mean particle sizes are the same. Moreover, the smaller the mean particle size of the CuO nanofluid, the higher its viscosity is because of the larger the specific surface area, and the electrostatic force between particles would also be increased.

Multi-walled Carbon tubes combined with DNA: Synthesis and Characterization of covalent bonding

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We have developed a multi-step method to covalently link functionalized multi-wall carbon nanotubes (MWNT) to deoxyribonucleic acid (DNA) oligonucleotides. X-ray photoelectron spectroscopy (XPS) was used to characterize the initial chemical modification to form amine-terminated MWNTs, which were then covalently combined with DNA. The morphology recorded by atomic force microscopy (AFM) gave direct and explicit imagingimaging of the resulting DNA-MWNT adducts, showingshowing that chemical functionalization occurred at the ends and sidewalls of MWNTs. The adopted methodology is an important first step in realizing a DNA-guided self-assembly process for carbon nanotubes

Microstructure and mechanical properties of amorphous ? nanocrystalline mixed iron-tungsten alloy

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Iron-tungsten alloys with tungsten content ranging from 15 at. % to 50 at. % were prepared by electro-deposition on copper substrate. Transmission electron microscopy studies on the as-deposited sample show that the microstructure consists of a mixture of nanocrystalline phase and amorphous phase. The nanocrystalline phase shows a distorted body-centred-cubic structure with lattice parameter about 0.291 nm, larger than the 0.2866 nm of the equilibrium iron, while the amorphous phase shows the closest plane spacing of 0.2122 nm. It has been found that a 20 ?m thick deposited film enhances the hardness from 1GPa of the pure copper to 2.7GPa. TEM observations of in-situ straining and the relevant plastic deformation mechanism will be discussed.

Ceramic Film Formation via a Biomimetic Approach Based on Molecular Design and Organized Assembly

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A biomimetic approach is employed to deposit the ceramic films on organic, self-assembled monolayer (SAM) coated substrates. Specifically, a ZrO2 film is grown in situ in an aqueous solution at near room temperature (≈ 80?C). This process, directed by the nanoscale organic template, mimics the controlled nucleation and growth of the biominerals such as bones and tecth. It is shown that surface functionality of the SAM plays a crucial role by: i) providing surface nucleation sites for the ceramic materials, and ii) promoting electrostatic attraction between the SAM surface and the colloidal clusters or particles precipitated in the solution. The resultant zirconia films consist of sub-micron sized particles that are formed by an enhanced hydrolysis of zirconium sulfate precursor. The mechanisms of film formation are systematically studied by tailoring the film structure from solution chemistry and SAM functionalities. In particular, the cross-sectional TEM work is performed to quantitatively analyze the film structure as well as interfacial region of the biomimetic processed films. Further, the nanoindentation testing is used to characterize the mechanical properties of the films. This growth mechanism is sufficiently general that it may be applicable to other oxide systems. Therefore, the ultimate goal of this study is to develop a process that can yield dense, solid ceramic microstructure with desired properties.

Flow-limited Field-injection Electrostatic Spraying for Fabrication of Structured Nanoparticles, Nanofibers, and Thin Films

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Flow-limited field-injection electrostatic spraying (FFESS) is a process by which a material in liquid phase, when highly charged by field injection (i.e., field emission or field ionization), is ejected from the surface as charged nanodrops or nanojets, due to the resulting electrical tension forces. Since the precursor solutions may be prepared in desired chemical compositions and stoichiometries, nanoparticles, thin films, and nanofibers of a variety of materials can be produced using the FFESS process. The key parameters controlling FFESS are the field-injection current, and the flow rate and properties (such as dielectric constant, surface tension, and viscosity) of the precursor solution. By properly controlling these parameters, it has been possible to fabricate nanoscale materials with certain structures and morphologies tailored to specific applications. Because of its unique ability to control the force field inside a precursor solution before and after its nanodrops are ejected from the charged surface (due to the injected charge and solvent evaporation) the FFESS process may contribute to synthesis of uniquely structured nanoscale materials, potentially with novel properties.

ZnO nanostructured transparent thin films for gas sensing applications

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Zinc oxide transparent thin films (ZnO) with different thickness were prepared by pulsed laser deposition (PLD) technique using ZnO sintered ceramic target and a typical homemade PLD deposition chamber, using XeCl Excimer Laser 308 nm wavelength, in oxygen atmosphere onto silicon and Corning glass substrates, in different growth conditions. Structural investigations carried out by Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD) shown a strong influence of deposition technique parameters on the film surface topography and material optical, electrical properties. Film roughness (RMS), grain shape and dimensions were found to correlate with the deposition parameters and to reflect strongly on the optical and electrical film properties. On these films highly oriented nanostructures were identified and a clear evidence for the nucleation of nanorods with preferential orientation were identified. XRD measurements proved that the films grown by PLD technique have a polycrystalline structure following the characteristic zincite XRD spectra. This work indicates that the film characteristics are strongly influenced by the deposition technique conditions applied, thus providing a tool for the enhancement of the film sensing capabilities.

OPTIMIZATION STUDIES OF SOFT AND HARD MAGNETIC MATERIALS WITH NANOMETRIC STRUCTURE

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The influence of replacing different elements on the magnetic properties of well known soft and hard magnetic systems was studied. FeSiB and NdFeB based alloys with structures in the nanometric scale have been thoroughly investigated because of their high performance as soft and hard magnets respectively. For the case of soft magnetic materials, we herein present results obtained when Co, Al and Ge, or a combination of them, were added to the FINEMET (FeSiBNbCu) system. In particular, limited additions of Ge improved soft magnetic responses by reducing coercivity and increasing permeability and saturation magnetization. At the same time, the presence of Ge seemed to increase crystallization temperature of borides by stabilizing the Fe3Si nanocrystalline phase. High Ge contents (□13 %) caused an increase in the amorphous phase Curie Temperature of about 50□C without lowering saturation. As regards the hard magnetic systems, NdFeB alloys with low Nd content are an interesting alternative because of their low cost and better corrosion resistance. Magnetic and structural properties of these low Nd content alloys (4.5%) were studied and compared with those of NdFeB alloy prepared by partially replacing Nd with Mishmetal (MM), a rare earth alloy which is three times more economical.

Mechanically milled Al-Pb nanocomposites consolidated by HERF technique

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By axissymmetrical powder compaction High Energy Rate Forming (HERF) method pore-free bulk samples were produced for different application purposes in case of the very different immiscible Al-Pb metal pair.By mechanical milling of atomised Al and Pb powders Al-Pb nano composites were made partly by a SPEX 9000 and with a Fritsch Pulverisette 4 mill. Due to the fact that milling was carried out in air atmosphere, the originally existing PbO surface layer at the atomised Pb powder, ruptured and was also distributed in the composite. By XRD. SEM and TEM (BF, DF, SAED) the presence of the nano Pb and PbO particles could be seen. Using high energy milling parameters the PbO crystallites became so small that they nearly can not be shown by XRD technique. XRD and process diffraction method of SAED are both useful to the evaluation of the result of the milling process and compaction

Microstructure and Photoluminiscence Properties of Mg-Doped ZnO Powders

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ZnO is a direct bandgap semiconductor (Eg=3.36eV) which is been extensively studied due to its unique optical and electronic properties and thus for its potential use in many demanding technological applications, such as blue and ultraviolet light emitter and detector. Substitution on the cation site modifies the bandgap of ZnO, increasing in the case of Mg but maintaining the wurtzite structure. Mechanical milling has proved to be an effective and simple technique to produce nanocrystalline powders and the possibility of obtain large quantities of materials. In this work we present a structural and optical characterization of Mg-doped ZnO powders obtained by mechanical milling. The starting materials were commercially ZnO and MgO powders. The samples were prepared by mechanical milling in a Restch PMMM 400 rotating ball mill. The milled powders were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), positron annihilation spectroscopy (PALS) and photoluminescence spectroscopy (PL). The mixing of both oxides is followed by means of XRD and SEM. As milling proceeds a clearly reduction of grain size and homogenization are observed.The evolution of annihilation parameters and PL spectra with milling time were analyzed and related with the kind of mechanical induced defect involved.

In situ high resolution transmission electron microscopy of nano-sized metal clusters: challenges and opportunities

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This presentation concentrates on challenges and opportunities to control the microstructure in nano-structured metal systems via a relatively new approach, i.e. using a so-called nanocluster source. An important aspect is that the cluster size distribution is monodisperse and that the kinetic energy of the clusters during deposition can be varied. Interestingly the clusters are grown in extreme non-equilibrium conditions, which allow obtaining metastable structures of metals and alloys. The combination of factors such as temperature, kinetics, impurities, and surface energy effects could lead to unusual nanoparticle shapes and size distributions. We will show the excitements of the nanocluster deposition by starting with the basic building block of Fe, Nb, Mo and Co, i.e. the structure and properties of a single cluster studied with high-resolution transmission electron microscopy, followed by an in-situ TEM study of the coalescence and diffusion of clusters (sizes ranging between 3 nm and 10 nm) leading to the growth of nano-structured metal films. Growth front aspects of Cu nano-cluster films deposited with low energy onto silicon substrates at room temperature have been investigated with atomic force microscopy (AFM). Various in-situ observations appeared to be in contrast with theoretical descriptions of coalescence assuming initially a point contact as a pathway to coalescence. As far as the properties are concerned the magnetic properties of Co films are investigated with MFM and electron holography suggesting a super-spin glass state.

Formation of Palladium nanoparticles from molecular cluster precursors

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Formations of nanoparticles of noble metals have been studied during the last decades because they belong to a new category of materials, which is different from both conventional bulk material and from atoms. These nanometer-sized metal particles attracted much attention of researchers from different scientific and technological view points, because of their unique physicochemical properties and their importance as catalysts. Ideally, the metal nanoparticles would be perfectly monodispersed, but special properties are to be expected even if the ideal is not perfectly realized. The use of molecular cluster precursors has been studied in order to obtain small and uniform nanoparticles.[1] Highly ordered pyrolytic graphite (HOPG) surfaces were modified by the adsorption of Pd molecular precursors from solution. Different palladium-containing molecular precursors will be studied, a mononuclear one, binuclear one and a trinuclear one, to compare their affinities, sizes and distributions at substrate surfaces. To obtain Pd nanoparticles, these neutral molecular precursors will be reduced under hydrogen atmosphere. Thermogravimetric analysis (TGA) will be carried out to establish the behavior of these precursors at various temperatures. Understanding the thermal stability of these compounds is very important in order to establish the appropriate conditions to form metallic Pd. The modified surface will be characterized by X-ray photoelectron spectroscopy (XPS), Auger Electron Spectroscopy (AES) and atomic force microscopy (AFM). In addition the reductive process will be monitored by XPS and AES. Pd particles will be analyzed by Transmission Electron Spectroscopy (TEM) and the techniques mentioned above. Preliminary Results present remarkable differences between the mononuclear and trinuclear compounds in terms of dispersion, particle size and homogeneity. The preference of the trinuclear one was to deposit at HOPG defects, in contrast to that of the mononuclear one, which agglomerated evenly over the surfaces. Moreover for the trinuclear, not only Pd nanoparticles, but also Pd nanowires were obtained.References: 1. Toshima, N.; Yonesawa, T. New J. Chem. 1998, 1179.

EFFECT OF SEVERE PLASTIC DEFORMATION ON ATOMIC STRUCTURE OF METALS AT STUDY OF FIELD ION MICROSCOPY METHOD

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It has been revealed that in Iridium influenced be SPD a UFG structure is formed (the grain size of 20-30 nm), but in the bodies of grains there are practically no defects of structure, however, after irradiation a subgrain structure, (subgrain size of 3-5 nm) is formed, and in the bodies of subgrains there are defects. The subgrain structure was also revealed in UFG Nickel and Copper after SPD (subgrain size of 3-15 nm), but in the latter case the observed boundary region is broader and subgrain are highly disoriented.

Optical and electronic properties of the aluminophosphate glasses doped with 3d- transition metal ions

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We present a wet non-conventional method for preparing alumino-phosphate glasses doped with iron, manganese and chromium ions. The advantage of this method consists in a higher optical homogeneity of the glass, a shorter duration of melting and annealing processes and the removal of the usual mechanical homogenization of the melt. The method provides chemical reactions of the metaphosphates in the earliest stages of the preparation, before the melting stage. The obtained aluminophosphate glasses belong to the oxide systems: Li2O-BaO-Al2O3-La2O3-P2O5 . The influence of the vitreous matrix composition and the effect of the doping ions on the optical properties of the glasses have been investigated in relation to micro-structural and local electronic phenomena. Structural information were provided by IR absorption spectra in the range 2000-500 cm-1. The optical phonon modes in pure P2O5 glass were compared with those of presently prepared glass samples for that the following features can be mentioned: P=O stretch, P-O-P antisymmetric stretch, P-O-P symmetric stretch, PO32- symmetric, PO32- antisymmetric and AlO45- antisymmetric. The distortions of the PO43- tetrahedral could be due to the Al-O-P bonds that play the role of network former besides P-O-P bridges. The optical behavior (transmission and refractive index) of Li2O-BaO-Al2O3-La2O3-P2O5 glasses doped with 1% mol.FeO (1), 1% mol.FeO-1% mol.MnO2 (2) and 1% mol.FeO-1% mol.CrO3 (3) has been studied by UV-VIS spectrometry and the Fe valence state and local coordination were also analysed via 57Fe Mossbauer spectroscopy. Both Fe3+ and Fe2+ species in octahedral and tetrahedral configurations were evidenced, their relative amount depending on the doping elements. The redox equilibrium in glasses (2) and (3) is discussed based on the Mossbauer data and taking into account the oxidation and reduction potentials of the doping ions.

Investigation of electro-mechanical properties of 1-3 nano-composites made of ZnO nano-crystalls

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Within framework of nanomechanics we investigate the static and dynamic problems of 1-3 nanocomposites, which a based on ZnO nano-crystals. The composites with chaotic and regular distribution of nano-crystals are considered. The effective elastic, piezoelectric and dielectric constants are obtained. Some models of nanopiezocomposites of 1-3 connectivity are created using the effective modules method. These models have heightened piezosensibility and low acoustic impedance in comparison with pure piezoceramic. Static, modal and harmonic analyses of 1-3 nanopiezocomposite transducers are realized by using finite element method and computer packages.

On the multilayered ZnO thin films growth modeling

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For the layer by layer growing multilayered epitaxial ZnO thin films on c-plane sapphire grown by multi-step pulsed laser deposition, the mathematical model is proposed which possess to optimize the stress filed in the upper layer of film. The finite element simulation is applied for definition of thermal and piroelectrical stresses in multilayered films. The electrical and optical properties of such films are studied in [1, 2]. Now we investigate the elastic and piezoelectric behavior of ZnO films. The proposed model is based on the constitutive equations of pre-stressed piezoelectric bodies under small strains which take into account different physical properties of films layers. The bending of multilayered films for nanosensor application is considered.References 1. Kaidashev E. M., Lorenz M., Wenckstern H., Benndorf G., Rahm A., Semmelhack H.-C., Han K.-H., Hochmuth H., Bundesmann C., Riede V., Grundmann M., High electron mobility of epitaxial ZnO thin films on c-plane sapphire grown by multi-step pulsed laser deposition // Applied Physics Letters. 2003. 82. p. 3901-3903.2 Lorenz M., Kaidashev E. M., Wenckstern H., Riede V., Bundesmann C. Spemann D., Benndorf G., Hochmuth H., Rahm A., Semmelhack H.-C., Grundmann M. Optical and electrical properties of epitaxial (Mg, Cd)xZn1-xO, ZnO, and ZnO:(Ga, Al) thin films on c-plane sapphire grown by pulsed laser deposition // Solid State Electronics. 2003. 47. p. 2205-2208

Construction of three-dimensional nanostructures employing two-photon nano-stereolithography

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We report two-photon polymerization of a polymer composite using a femtosecond laser at 1028 nm. The polymer composite is a viscous liquid consisting of an acrylate-based polymer, a free-radical photo-initiator and a photo-sensitizer. The material is transparent to infrared laser radiation and allows for deep penetration. By scanning the tightly focused laser beam, we can use two-photon absorption to polymerize and selectively solidify the material.Multi-photon photo-polymerization of organic composites permits the construction of complex-shaped three-dimensional structures of sub-micron resolution. Due to their versatile optical and chemical properties and the ability to mix them with active molecules, these materials are particularly useful for a variety of applications in the nanotechnology field such as photonic devices, actuators and micro-fluidic devices.

Theoretical study of Hydrogen Storage in Nanotubes and Nanoscrolls

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A combination of ab-initio and Molecular Dynamics methods is used for investigating the nature of atomic and molecular hydrogen interaction in carbon Nanotubes and Nanoscrolls. The curvature of the tube walls together with the direction of the hydrogen approach is considered and evaluated. In addition the improvement of the storage capacity is tested under various conditions of doping, pressure and temperature.

A NEW REPRESENTATION FOR THE PROPERTIES OF ANISOTROPIC ELASTIC FIBER REINCORCED COMPOSITE MATERILAS

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The number of anisotropic materials is increasing by the addition of man-made anisotropic single crystals and technology developed anisotropic materials. For a deep understanding of the physical properties of these anisotropic materials use of tensors is inevitable. The decomposition of tensors has many engineering applications in anisotropic elastic materials which are, both qualitatively and quantitatively, different from isotropic materials. In analyzing the mechanical properties of anisotropic linear elastic composite medium a tensor of fourth rank is required to make up a linear constitutive relation between two symmetric second-rank tensors, each of which represents some directly detectable and measurable effect in the medium. The stress- strain relations for elastic anisotropic composite material have not been very well established as compared to those of the isotropic material in the classical theory of elasticity. In the mechanics of continuous media, i.e. in elasticity studies, a procedure for decomposing Cartesian tensors in anisotropic continua into orthonormal parts is developed. This procedure based on constructing orthonormal tensor basis using the form-invariant expressions which can easily be extended to any tensor of rank n. We present a new innovational general form and more explicit physical property of the symmetric fourth rank elastic tensors. A new orthonormal decompositions of symmetric elastic tensor is given for different symmetries like isotropic, monoclinic, transversely isotropic, and orthotropic media. Besides, each decomposed term represents a physical meaning and more featured and transparent physical property. Introducing a new method to measure the stiffness in the elastic fiber reinforced composite materials using the norm concept on the nanosacle, it can be investigated the effect of orientaion, number of plies, material properties of matrix and fibers, and degree of anisotropy on the stiffness of the structure. The results are to be compared with those available in the literature through group III-V semiconductor compounds, reinocored composite materials, and biomaterial examples.

NANO-COMPOSITE BASED MATERIALS FOR ORGANIC BASED PHOTOVOLTAICS

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Organic based solar cells offer the potential for moderate efficiency at very low cost over large areas and could be the next generation for PV power. The potential to process them entirely by atmospheric based roll to roll processing is potentially a new paradigm for electronic device manufacturing. However, to get to this goal will require a significant amount of materials science. Key is that the length scale for the elements of the cell must all be on the nanoscale due to the lifetimes of both excitons and carriers in the organic materials. Building a complex composite structure at this length scale with a high level of control of all of the electronic properties, interfacial properties and mechanical properties has not been accomplished for any other structure to date. None-the-less initial cell efficiencies are approaching 5% for polymer fullerene bulk heterojunction cells. We will report on the development of a cell based on a low cost substrate with a controlled oxide nano-carpet (TiO2 or ZnO) as an electron conductor and an electroactive polymer as the hole conductor. This cell which can be made with atmospheric processing below 200 C has demonstrated initial efficiencies above 0.5%. We will also discuss the potential for cells employing the same oxides as capped nanoparticles in a phase separated bulk heterojunction cell. The application of such nanostructured oxides reduces synthesis complexity, increases morphological control and leads to a new class of 3D structured opto-electronic devices.

Synthetic reinforcement materials for the polymer-inorganic nanocomposites

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The main purpose of the present study is to develop the new kind of the reinforcement material for the polymer-inorganic nanocomposites with the improved properties. The majority of the research works in the field of the polymer-inorganic nanocomposites are focused on the materials on the basis of the natural layered silicates (namely montmorillonite). Natural montmorillonite clays are inhomogeneous by the chemical compositions and particles size. This fact does not allow the researches to obtain the nanocomposites with the predicted properties. To solve this problem the method of the synthesis of the layered silicates and nanotubed materials under hydrothermal conditions was developed. The materials obtained are characterized by the definite chemical composition and particles sizes and can be considered as perspective reinforcement materials for the polymer-inorganic nanocomposires.

Bio-composite nanostructured materials for selective electronic noses

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Encapsulation of biomaterials in the pores of inorganic materials produced by sol-gel chemistry results in the formation of three-dimensional nanostructured matrices consisting of solid colloidal particles and a mesoporous network filled with the dopant bio-molecules. Non-transparent, metal oxide (MoO_3) sol-gel matrices were used for the first time to encapsulate enzyme (urease) molecules. Thin films of these hybrid materials were used as urea biosensing elements having the advantage of reduced response time and high sensitivity to the target analyte. Furthermore, electrospinning has been used as a promising technique for encapsulating biomolecules in nanostructured, non-woven organic membranes. Successful encapsulation of enzymes in electrospun nanofiber membranes of synthetic and natural polymers has been demonstrated in our groups research, as well as usage of these bio-composites as on-line bio-detection tools.This paper focuses on characterizing the structural characteristics of the bio-doped gels and bio-composite membranes, by means of transmission electron microscopy techniques, showing evidence of the enzyme encapsulation and the metal oxide- or polymer-biomolecule interactions. The use of gas sensitive matrices (sol-gel or polymer) in these studies offers the advantage of resistive type biosensing through the detection of the gaseous products of the biochemical reaction between urea and urease (e.g. ammonia detection). Formation of metal oxide nanowires by combining polymer solutions with metal oxides sol-gels and electrospinning the resulting mikxture is also discussed.

Functional Nanoparticles in Thin Films as Sensing Media

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The combination of unique properties offered by materials on the nanoscale with the increased role of surface chemistry in nanostructured solids makes core-shell nanoparticles extremely attractive for application to "smart" thin-film coatings. Sensing properties of nanoparticle-based thin films were studied in several systems containing organic-coated semiconductor and metallic particles. In semiconductors, the interaction of organic shell and/or thin-film "matrix" with the environment results in changes in the nanoparticle's surface states, altering the optical properties of the thin film. Measuring the electrical properties of thin films composed of metallic cores with hydrocarbon shells offers another mechanism to monitor the local environment through the swelling of the hydrocarbons in the presence of external compounds. The sensing mechanism was also studied using reactive nanoparticles. Increasing temperatures were found to loosen the protective shells, leading to oxidation of the metallic cores. These mechanisms and their potential application to novel sensors will be discussed.

Synthesis of nanostructured WC/Co powders by Chemical Process

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WC/Co hard alloys are widely used for wear resistance machine parts or tools material. Reduction of the tungsten carbides size generally gives a marked increase in hardness, wear resistance and transverse rupture strength of WC/Co alloy. In order to produce nanostructured WC powder, new chemical approach were made from gas phase and liquid phase. Nanoscale size WC/Co composite powder of less than 150nm particle size can be synthesized by mechanochemical process using water soluble metallic salt precursors as starting materials. This method allow the production of components homogeneous mixing state and offer homogeneous ultra fine sintered body microstructures. CVC process was adapted for forming the nanosized clusters by homogeneous condensation from decomposed metal-organic precursor in the gas phase. And it has been reported to be appropriate for synthesizing high purity and non-agglomerated ultra-fine particles with superior functional properties.

Functional magnetic nanostructures based on self-assembled arrays and polymer nanocomposites

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Magnetic nanostructures hold tremendous potential as basic building blocks in spin-electronic devices and high-density data storage. Since these structures are often formed as clusters through various synthetic methods, it is important to understand the collective dynamic properties in such materials. Magnetic nanoparticles embedded in polymer matrices are useful in applications like EMI shielding due to their unique properties such as light-weight, mechanical strength, non-corrosiveness, frequency agility. We have synthesized a variety of interacting magnetic nanoparticle clusters (Fe, Fe3O4, Fe2O3, Mn-Zn and Ni-Zn ferrites) in the form of blended polymer composites and self-assembled arrays deposited by Langmuir-Blodgett method. The resulting composites are processed as spin-coated thin films, multilayers and in bulk forms. We have optimized the processing conditions to achieve high quality, uniform dispersion and tunable magnetic response. Static and dynamic magnetization studies have been done to monitor the systematic changes in superparamagnetic and ferromagnetic properties. In particular, a unique RF susceptibility technique developed by us has been used to precisely probe the magnetic anisotropy in these systems. Our studies reveal insights into the collective behavior of strongly and weakly interacting clusters of magnetic nanoparticles and their promise in applications ranging from EMI shielding to refrigeration based on the magneto-caloric effect (MCE).Work supported by the US National Science Foundation through Grants ECS-0140047 and CTS-0408933

Synthesis and encapsulation with polymer of nanophased YSZ particles in supercritical carbon dioxide

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Material synthesis in supercritical carbon dioxide is of growing interest. In our laboratory, we experiment more precisely the synthesis of nanophase conductive ceramics. Trials have led to interesting results on oxygen conductivity. However, several powders presented handling difficulties and bad densification rates, it was the case of Yttria Stabilised Zirconia (YSZ) powders. The present study deals with improved YSZ powder synthesis and encapsulation of the grains with a polymer in supercritical carbon dioxide, with the aim of preventing particle agglomeration and of facilitated handling. An encapsulation method has been studied based on the dispersion polymerisation of MMA in supercritical carbon dioxide. Surfactants were used as coupling molecules between the oxide surface and the polymer. The surfactant choice revealed to be a decisive parameter. Currently, experimentations are carried out on hydrocarbonated surfactants capable to be fully decomposed during the sintering phase.

Frequency Responses of Au Nanoparticles Embedded in Polyurethane Resin

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The frequency properties of Au nanoparticles imbedded in polyurethane have been investigated. The Au nanoparticles prepared by phase transfer method were added to polyurethane resin and hardened with polyisocyanate. The frequency reflective loss of the resultant nanocomposites were measured and calculated. From the experimental results, the frequency responses of the resultant composite resin have demonstrated to be affected with the little addition of Au nanoparticles. The electric and magnetic permittivities of Au-nanoparticle-imbedded resin arise from the cut-off frequencies of about 9.0Ч108 Hz. As a result, the reflective energy loss increased with the addition of Au nanoparticles. However, the magnitudes of those permitivities are not proportional to the amount of Au nanoparticles in the resin. The surface status of various morphologies might be the reason to explain the variation of electrical frequency response.

AFM CHARACTERIZATION OF SURFACE MORPHOLOGY OF NANOSTRUCTURED COPPER

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Atomic force microscopy (AFM) techniques are increasingly used for studies of materials surfaces on micro √ and nano - scales. AFM readily provides high resolution digitized images of surface features. In situ surface characterization helps to develop a better understanding of microstructure evolution of materials subjected to any kind of mechanical loading as well as to thermal treatment. The main objective of this study is to exploit the capabilities of AFM to accurately perform an analysis of the surface features of nano-structured copper and multiphase composites subjected to a plastic deformation to provide the basis necessary for the development of a model describing the evolution of the topography that can be used for explaining the specific mechanical properties of nano-materials and non- homogeneous structures. For this purpose, AFM and SEM (scanning electron microscopy) have been used for the investigations of (i) surface morphology of deformed materials; (ii) nucleation and formation of slip bands and protrusions in materials; (iii) crack propagation.

Synthesis and structure of bulk FeAl nanostructured materials by spray forming and spark plasma sintering

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Bulk FeAl Nanostructured Materials (NMs) were successfully synthesized by High Velocity Oxy-Fuel (HVOF) spray forming and Spark Plasma Sintering (SPS) processes using milled feedstock powder. The processing parameters of these two processes were optimized not only to retain the original nanostructure of the milled powder but also to obtain a high density of final products. The microstructures of initial powder and bulk materials were characterized by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) as well as Transmission Electron Microscopy (TEM). A comparison of the results indicates that both processes can effectively restrict grain growth because of very rapid thermal cycles applied during the whole treatment procedures; however, essentially different formation mechanisms result in very different structural features. Regardless of this fact, spray forming and SPS processes provide a promising way to produce bulk near-net-shape NMs for industrial applications.

Preparation and properties of self-assembled nanoparticles prepared from the cholesteryl derivative of didanosine

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Dideoxyinosine cholesteryl succinate (DICS) was synthesized by condensing dideoxyinosine (ddI, an anti-HIV agent) with cholesterol through succinyl moiety as a linker. DICS functions as an amphiphile. Homogeneous opalescent suspensions were obtained after DICS solution (5 mg/ml) and Poloxamer 188 solution (1 mg/ml) in tetrahydrofuran (THF) were injected into water. Based on negative-stained transmission electron microscopy, the self-assembled nanoparticles in suspensions showed various shapes that depended on DICS concentration in suspensions and whether THF was removed. Globe-like nanoparticles appeared when DICS concentration was less than 0.5 mg/ml; DICS with higher concentration gave ribbon-like nanoparticles before removing THF and rod-like nanoparticles (average size 200 nm) after removing THF. Hydrophobic interaction between cholesteryl moieties leads DICS to self-assemble bilayers and hydrogen bonding between inter-bilayer nucleobase moieties leads layer-by-layer aggregation. The self-assembled nanoparticles carrying anti-HIV agents would become novel drug delivery systems.

Cyclic Response of Nanostructured NiTi and NiTiHf Processed by Equal Channel Angular Extrusion

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In this study, we address the issue of thermomechanical cyclic instability (irrecoverable strain) in conventional NiTi and high temperature NiTiHf shape memory alloys and propose mechanisms for enhancing cyclic stability through ausforming, texture strengthening and grain refinement using a severe plastic deformation technique, i.e. Equal Channel Angular Extrusion (ECAE). Three different compositions (equiatomic NiTi, 50.8 at.% NiTi, NiTi-8 at.%Hf) were processed at temperatures above austenite finish temperature at which different deformation mechanisms were targeted. These are stress-induced martensitic transformation plus plastic deformation of martensite, deformation twinning in austenite and dislocation slip in austenite. The main cause of cyclic instability in shape memory alloys is defect production during transformation which acts as a barrier to parent-martensite interface motion. The consequences of this instability are change in transformation temperatures, decrease in transformation strain, increase in thermal hysteresis, and increase in irrecoverable strain. A possible solution is to reduce defect production during cycling by increasing the strength of parent phase. ECAE was shown to improve the strength of parent phase by increasing dislocation density and forming substructures, grain size refinement and formation of specific texture. The solutionized materials were extruded using a 90 ┌┘ ECAE die using various combinations of routes in order to tailor the microstructure and texture suitable for stable cyclic response. Thermal cycling at various stress levels and DSC analysis showed that stable cyclic response was achieved for 50.8 at.% NiTi processed at room temperature after one ECAE pass, equiatomic NiTI processed at 300 ┌┘C after one ECAE pass and NiTiHf alloy processed at 650 ╟ЖС after two ECAE passes using Route B. These materials have also demonstrated a large difference between the stress required for stress induced martensitic transformation and the stress for plastic deformation of martens
ite which also indicates possibility of cyclic stability. The former two alloys exhibited no irrecoverable strain when they underwent 1000 cycles at an applied strain level of 3%.In this presentation , stable cyclic response, pseudoelasticity, change in transformation temperatures, formation of R-phase and nanograins, effects of precipitates will be rationalized with the observations on microstructures and possible deformation mechanisms. The unique microstructural findings were: 1) the observation of a mixture of heavily deformed B2 (austenite) and B19╟ ├ (martensite) phases in the samples processed at room temperature although martensite stabilization was expected, 2) the observation of highly organized, twin-related nanograins in B2 phase of the samples deformed at room temperature, 3) simultaneous observation of B2 austenite and strain induced B19╟ ├ martensite, and (4) the observation of (112) type deformation twins in austenite as well as (113) and (114) type. Strain-induced martensite in NiTi alloys was reported for the first time. The formation of well-organized twin-related nanograins via severe plastic deformation opens a new opportunity for twinning induced grain boundary engineering in NiTi alloys.

Nanopowder Consolidation Using Equal Channel Angular Extrusion

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The present work is focused on the fabrication of near full density bulk nanocrystalline copper and stainless steel from powder precursors using equal channel angular extrusion (ECAE). The initial powder sizes used were 100 nm, 130 nm and 45 micron for copper and 100 nm for stainless steel. The evolution of the microstructure and the mechanical behavior of the consolidates were investigated and correlated with the processing route. Possible deformation mechanisms are proposed and compared to those in ECAE processed bulk materials. The effects of extrusion parameters for consolidation such as ECAE route, number of passes and extrusion rate are evaluated. Two extrusion passes were sufficient for obtaining full density. Combined high ultimate tensile stress (490 MPa) and ductility (~20% tensile fracture strain) with near elasto-plastic behavior was observed in consolidated √325 mesh Cu powder. On the other hand, early plastic instability took place leading to a continuous softening in flow stress of bulk ECAEd copper while this was not the case in stainless steel. Tensile strengths as high as 730 MPa and ductility of 6-10% were achieved in consolidated 130 nm copper powder. The average grain size of the consolidated 130 nm powder was about 90 nm. In this study, some of these experimental observations will be presented in comparison with microcrystalline consolidates and with severely deformed pure copper and stainless steel. This study helps to clarify the relationship between different ECAE processing parameters, mechanical properties and the microstructure of nanocrystalline metals with low and medium stacking fault energies.

Microstructure and Mechanical Behavior of Severely Deformed 316L Stainless Steel Polycrystals and Hadfield Steel Single Crystals

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The present work focuses on the microstructural evolution and deformation behavior of AISI 316L austenitic type stainless steel and high manganese Hadfield steel. Equal channel angular extrusion (ECAE) equipped with a 90 tool angle is utilized. While, bulk 316L stainless steel bars are processed at temperatures of 450 C, 550 C, 600 C, 700 C and 800 C; Hadfield steel single crystals were extruded at room temperature. Microstructure and mechanical properties of successfully extruded billets are investigated using light microscopy, electron microscopy, and mechanical testing. X-ray analysis is conducted to monitor macro-texture evolution in 316L stainless steel while orientation imaging microscopy (OIM) is used for tracking micro-texture evolution in Hadfield steel single crystals. High strength levels even in the 316L samples deformed at 800 ╟C was attributed to the relatively high volume fraction of nanoscale deformation twins formed during ECAE. Observed tension/compression asymmetry in the yield strength values and strain hardening was attributed to the deformation induced directional back stress. Activation of twinning at such high temperatures (0.65Tm) was attributed to the effect of the high stress levels on the stacking fault energy. The goal is to produce desired end microstructures where deformation twinning is stabilized at high temperatures forming nanostructured AISI 316L stainless steel, leading to improved mechanical properties. Single pass extrusions of Hadfield single crystals demonstrated that twinning was the main deformation mechanism. One objective of this study is to see the effect of initial orientation and severe deformation on the activation of mechanical twinning in single crystals and on the resulting mechanical properties.

Nanoscale Deformation Twinning in Difficult-To-Work Alloys at Unexpected Temperatures During Severe Plastic Deformation

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In this talk, we will report deformation twinning formed at unexpected conditions as a means of microstructural refinement and additional source for plasticity in selected difficult-to-work alloys during severe plastic deformation (SPD) through equal channel angular extrusion (ECAE). The selected materials were 316L austenitic stainless steel, a NiTi shape memory alloy (SMA) and Ti-6Al-4V. Extensive deformation twinning was observed in 316L stainless steel and Ti-6Al-4V at 800 ╟C after only one ECAE pass. The twinning activity at such high temperatures in stainless steel was attributed to the effect of high strength levels achieved on the partial dislocation separation. It was also speculated that a similar mechanism could be effective in Ti-6Al-4V. In NiTi with 50.8 at.% Ni, very high volume fraction of twin related nanograins formed in B2 phase after one pass at room temperature. This was thought to be a consequence of stress-induced martensitic transformation, deformation twinning in martensite and back transformation to B2 phase. The deformation twinning formation instead of well-known Type-I and Type-II transformation twinning in martensite was also because of high strength levels and high shears applied during deformation. In all these cases, twin thickness was smaller than 100 nm which is important for Hall-Petch strengthening. With the supporting evidence from recent studies on nanocrystalline aluminum and copper, it was concluded that deformation twinning can be one of the main modes of deformation in many metallic alloys in a wide range of temperatures when high strength levels are reached irrespective of the way in which they are achieved. The ramifications of twinning on the post-processing mechanical behavior will be discussed.

Processing and evaluation of X-ray line profiles measured from nanostructured materials produced by severe plastic deformation

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The classification of the micro-structure of nano-structured materials and their relation to macroscopic properties is essential for the development and application of nano-materials. X-ray line profile analysis is a non-destructive method yielding a series of interesting micro-structural parameters:The Bragg reflection of an ideal crystal is a narrow delta-function like peak. Distortions of the regular crystal lattice as well as a finite size of the coherently scattering domains leads to a significant broadening of the peak. By using physical models describing the individual types of broadening [1, 2] it is possible to relate the broadening of the peak to the micro-structure of the material. The most successful applications to date assume mainly size and strain broadening [3, 4]From these models various techniques have been developed making it possible to use the same dataset to evaluate the same physical quantities via individual methods thereby adding more reliability and robustness to the evaluation. Among these methods are the well known Williamson-Hall and Warren Averbach methods [5, 6], the so called modified Williamson-Hall and Warren Averbach methods [7] and multiple whole profile fitting/modeling [8, 9].Usually the measured data can not directly be used for the evaluation. Also in the case of simultaneous measurement of multiple profiles in individual detectors, the data needs to be joined for evaluation. It is thus necessary to have robust processes for a sensible removal of the background as well as peak-seperation, removal of artefacts etc.Several characteristic cases showing the individual problems are presented and solved via the same, general procedure.[1] M.A. Krivoglaz, X-ray and neutron diffraction in nonideal crystals, Springer 1996[2] B.E. Warren, X-ray diffraction, Dover 1990[3] T. Ungar, S. Ott, P.G. Sanders, A. Borbely, J.R. Weertman, Acata Mater. 46 (1998) 3693[4] A. Dubravina, M. Zehetbauer, E. Schafler, I. Alexandrov, Mater. Sci. Eng. (2004) in press[5] G.K. Williamson, W.H
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Effect of Viscous Grain-Boundary Sliding on High-Temperature Deformation of Nano-Sized Grains

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For steady-state deformation caused by grain-boundary diffusion, the macroscopic creep rate and the effect of viscous grain-boundary sliding in a polycrystal of nano-sized grains are analyzed by the energy-balance method in two and three dimensions. Furthermore, for a two-dimensional polycrystal of hexagonal microstructures, the stress distribution on grain boundaries and the effect of grain elongation are examined, while for a three-dimensional polycrystal consisting of space-filling polyhedral grains, the upper-bound and lower-bound creep rates causing by grain-size distribution are estimated. The grain-grain interactions in polycrystals increase the degree of symmetry of diffusional field, resulting in a decrease of the effective diffusion distance. Meanwhile, both the viscous grain-boundary sliding and the grain-size distribution are found to decrease the creep rate. At decreasing grain sizes, the influence of the viscous grain-boundary sliding becomes increasingly important, which explains the recent experimental observations that the creep rates of nano-sized grains are much lower than those predicted by grain-boundary diffusion. The present analysis reveals that the grain-size exponent is dependent on the grain size and the grain-boundary viscosity: the exponent becomes unity for small grain sizes and/or high viscosity, while it becomes three for large grain sizes and/or low viscosity.

Effects of interface on the physical properties of nanocomposites

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This study investigated the effects of interface between nanoparticle and matrix polymer on the rheological and other physical properties of polymer nanocomposites by properly combining polar/nonpolar nanoparticles and polar/nonpolar polymers.The nanoparticle-filled polymer systems at the low content of nanoparticles showed a notable influence of interface on physical properties but little influence was noticed at high content. The interface affinity between polymer and nanoparticle proved to have little effect on the tensile properties of nanocomposites.

Nanostructed metal oxide films as gas sensing elements

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Nano structured gas sensing films of InOx , ZnO and ZAO2 (ZnO/Al2O3 2wt%), in the thickness range of 10-110 nm, grown by dc magnetron sputtering are presented with respect to their structural, electrical, and O3 and NO2 sensing properties. The layers are analyzed at various temperatures and gas sensing environments. Structural investigations carried out by XRD and AFM showed a strong correlation between crystallinity, surface topology and gas sensitivity. Moreover, the electrical conductivity exhibited a change of three to six orders of magnitude during the processes of photoreduction and oxidation depending on preparation conditions. Films showing sensitivity levels towards O3 of < 50 ppb and NO2 of < 100 ppb, at temperatures from RT to100 ╟C are presented.

Hard cyclic viscoplastic (HCV) deformation - method for testing of the nanocrystalline metallic materials behavior

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The main objective of this study is to new nanocrystalline metallic materials testing method √ Hard Cyclic Viscoplastic (HCV) deformation. This testing method, HCV deformation, was used for study of nanocrystalline metallic materials physical and mechanical properties behavior, nano defects and cracks forming during testing in viscoplastic field of loading. For HCV deformations of specimens the Automated Materials Testing System INSTRON 8516 in strain control regime was used. This testing method includes axial deformation (tension-compression) in viscoplastic field of metal loading with amplitude up to 2-3% of strain and by 20-30 cycles number. The specimen test part (30 ╠0.2 mm long and 10 ╠0.05 mm in diameter) have length/diameter ratio up to 3. By this ratio of length/diameter the specimen don't lost the stability during compression cycle. A test part of specimen was stressed in low cyclic tension-compression by axial straining in viscoplastic field of three series: I √ 1% of deformation amplitude; II √ 1% deformed specimens were subjected to deformation by 2% of deformation amplitude; and III √ specimens deformed in two first series were again loaded to hard cyclic straining of 1% deformation amplitude. Tests were made in strain control of deformation amplitude and 30 cycles during 600 s were made in each series. In this work, as testing material, the nanocrystalline pure copper was produced by ECAP method in condition of SPD. For reference the coarse-grained copper was used.To investigate a materials nanostructure evolution, nano pores and cracks forming during HCV deformation the atomic force microscope (AFM), scanning electron microscope (SEM) Gemini, LEO, Supra 35, and X-ray diffractometer (XRD) D5005, Bruker were used. The materials mechanical and physical properties change were tested during HCV deformation on INSTRON and on universal hardness tester Zwick Z2.5/TS1S by Microindentation method use. During first series of HCV deformation the nanocrystalline metallic materials show hardening behavi
or during compression and softening behavior during tension. Heat treated nanomaterials show high stability of mechanical properties and show the approximately fully elastic behavior. HCV deformation causes a decrease in Young module up to three times. The differences in pores forming and fracture mechanism between the coarse- and nanograined metals are not only in the pores forming and fracture mode but in differences mechanisms of fracture, as well. The pores have walls with thickness about 40-60 nm of new ultra fine nano structure. The local mechanical properties in near pore areas are enhanced and yield stress is increased marking the microvoids coalescence and crack propagation from flaw energetically unprofitable.

Nanocrystalline metallic materials viscoplastic behavior characterization by HCV deformation

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Nanocrystalline metallic materials exhibit outstanding viscoplastic properties by High Cyclic Viscoplastic (HCV) deformation treatment. Test specimens of nanocrystalline pure copper were fabricated using Equal-Channel Angular Pressing (ECAP) method. Using route Bc of 10 ECAP passes; a crystallite size of the pure copper was about 40 nm.The HCV deformed of specimens were tested with Automated Materials Testing System INSTRON 8516 in strain control regime. Testing was carried out according to General Test Setup of conformation with Standard EN-10002/Metallic materials √ tensile testing. The process of the HCV deformation included three series: I √ 1% of tension/compression deformation amplitude; II √ specimens after the first series were subjected to deformation by 2% of deformation amplitude; and III √ specimens deformed in the two first series were again loaded to hard cyclic straining of 1% deformation amplitude. HCV deformation was used for studying the nano-metallic !
materials physical and mechanical properties in a viscoplastic field of loading. To investigate material nanostructure evolution during HCV deformation the atomic force microscope (AFM), scanning electron microscope (SEM) Gemini, LEO, Supra 35, and X-ray diffractometer (XRD) D5005, Bruker were used. Changes in the material (mechanical and physical) properties were tested during HCV deformation using the INSTRON and the universal hardness tester Zwick Z2.5/TS1S. The test result have show, that softening of the nanocrystalline metallic materials takes pace during tension at strain 1.77% of absolute deformation. The HCV deformed material shows softening behavior during a tension cycle and hardening behavior during a compression cycle. The reference coarse-grained cold-drawn pure copper shows softening only. The nanocrystalline material after low temperature heat treatment at 200-230 ╟C and heating rate 1-2 ╟C/min and reference material after annealing at 650 ╟C for 1.5h show!
the highest strain hardening during first series of HCV deformation.
After heat treatment, the HCV deformed nano-metallic material shows the highest stresses stability. It is approximately elastic behavior. HCV deformation influences physical and mechanical properties of nanocrystalline pure copper. The Young module decreases up to three times. Tension stress decreases up to 20-30% with plasticity increase up to 1.5 times. The true stress of heat treated nanocrystalline pure copper after HCV deformation increases up to 2 times.

Synthesize of the nano-size precursors for b-Al2O3 (Na and Ag) bulk nano-ceramic

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Synthesize nano-powders in systems of Ce2O3-ZrO2 and Y2O3-ZrO2

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Nano-materials for high-temperatures sensors

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Effects of the number of ECAP passes and ECAP route on the heterogeneity in mechanical properties across the sample from ultrafine copper

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Annealed copper was processed by eight passes of equal-channel angular pressing (ECAP) using two routes, BC and C. Pressed samples had a square section with a side length of 8 mm.Mechanical properties at tension (conventional yield strength, tensile strength, elongation and contraction) were determined at 9 points across the sample using small-size specimens, 1.5 mm in diameter, cut out along the pressing direction.Heterogeneity in the mechanical properties across the sample was determined based on the value of the relative variation coefficient.Heterogeneity in all mechanical properties after the first ECAP pass was found to increase dramatically. The heterogeneity then decreases, with the decrease being more active for route BC than for route C

Dynamic Study of Carbon Nanotubes Production by Chemical Vapor Deposition of Alcohol

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In this study the influence of carbon precursor during the chemical vapor deposition process over a catalyst is investigated. Specifically, alumina enriched with iron, were used as a catalyst and alcohol (ethanol or methanol) were used as a carbon precursor. The experiments were carried out in a thermogravimetric chemical vapor deposition reactor enabling the continuous monitoring of the evolution of the loading of carbon with time. We studied the deposition rate and the final product of the different processes. These are depended on the way that the catalyst was prepared, the process temperature, which is ranged between 550oC and 800oC, the carbon precursor that was used, and the use of hydrogen as a mean to reduce the catalyst, before or during the deposition. The final product was analyzed using Scanning Electron Microscopy and Raman Spectroscopy. The results showed that using the same catalytic substrate with different carbon sources we have different rate and yield of carbon deposited, but in each case both multi-walled and single-walled carbon nanotubes were produced.

Mechanical alloying of nickel aluminides with Ni and phase transformations during heating of milling product

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In this work, nanocrystalline powders with stoichiometrie Ni3Al composition were prepared by ball milling of AlNi or Al3Ni2 intermetallic compounds with addition of Ni powder. Differential scanning calorimetry was used for examining the thermal stability of the milling products. The structural changes occurring in the materials during mechanical alloying and during subsequent heating in a calorimeter were investigated with the use of X-ray diffraction. It was found that in both cases at the first stage of the milling process, a metastable Ni(Al) solid solution was formed, and this phase remained as the only milling product. Upon heating of these powders in the calorimeter, the Ni(Al) solid solution transformed into the ordered Ni3Al intermetallic compound. The results obtained show that during heating in the calorimeter, a limited growth of grains occurred however, nanocrystalline structure of powders was preserved. The microstructure of the Ni3Al intermetallic compound was examined using transmission electron microscopy.

Soft magnetic properties of nanocrystalline iron- and cobalt-based alloys at high temperature

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The nanocrystalline iron-based alloys, obtained by partial crystallisation of metallic glasses, exhibit very good soft magnetic properties: low coercivity and losses, high permeability and saturation induction. These are: FINEMET (Fe-Si-Cu-Nb-B) and NANOPERM (Fe-Zr-Cu-B). However, they may be applied only where the operation temperature does not exceed 250 ╟C, because the Curie temperature of an amorphous matrix is relatively low. To extend the application temperature range, iron is partially replaced by cobalt. This increases the Curie point of both phases, and thus increases the working temperature, although the soft magnetic properties are worse in comparison to the cobalt-free alloys. The highest available operation temperature, about 600 ╟C, was found for HITPERM alloys (Fe-Co-Zr-Nb-Cu-B). In this work, the magnetic properties of FINEMET and NANOPERM alloys (generic and Co-doped) are determined from hysteresis loops measured at room and elevated temperature. As the result, guidelines for selection of nanocrystalline alloys for various temperature ranges are suggested.

Characterisation of noble metal nano cluster

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Noble metal Pt, Pd and Rh nano cluster have been studied by Extended X-ray Absorption Fine Structure
(EXAFS) and X-ray Photoelectron Spectroscopy (XPS). The nano clusters are deposited onto substrates
(Si <100> and Ta thin films) by Gas condensation method, and the size of the cluster in diameter are controlled from 2nm to10nm.
The size of nano-cluster on Si and Ta surfaces are characterized by combining with scanning electron
microscope (SEM), atomic force microscopy (AFM) and transmission electron microscope (TEM). Figure
1 show the relative narrow size distribution of Pd cluster under two different experimental conditions A and
B for the cluster formation. The size distribution is obtained by counting the well dispersed clusters of
numbers more than 300 from the TEM images. The quantum size effect of Pd nanocluster has been observed by EXAFS and XPS studies.

COMPUTER MODELLING OF OPTICAL POLARIZABILITY OF COVALENT BONDED CONNED SINGLE-WALLED ZIGZAG CARBON NANOTUBE WITH AMINO-ACIDS PHENYLALANINE

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Computer modeling of linear optical polarizability of single-walled zigzag (n,0) carbon nanotube (SWCNT) with different diameter capped at one end by half of fullerene and conned at another end such that it is able to be connected with (3,3) armchair nanotube. But instead of (3,3) nanotube we covalently bonded zigzag (n,0) nanotubes with different n with 6 amino-acids Phenylalanine for preventing hanging bonds. So we have nanotube closed by hydrophobic cluster from Phe radicals for one end and by fullerene for another one. The geometry of conned tube was such as described by R. Saito et.al. [1]. The numerical calculation of the electronic and optical properties of nanotube with cups in framework of the Su-Schrieffer-Heeger (SSH) [2] model was carried out. The localized states demonstrate the nonlinear aspects of excited states in that system. It was found that the molecules with different radius have the strong oscillating dependence of optical polarizability on the incident light energy. The length decrease and uncapping fullerene shifts the peaks of the optical polarization spectrum to the relatively high-energy region and suppress the height of the peaks. The same conclusion is achieved for nanotube without biological molecule capped at both ends for capped/conned configuration.

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Photovoltaic cells based on dispersed polymer-carbon nanotube heterojunctions

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4.

We present a systematic study on the effects of processing conditions on the performance of photovoltaic devices that combine a donor-acceptor dispersed heterojunction system. Solar cells have been fabricated based on poly(3-octylthiophene) as donor and single-wall carbon nanotubes as the electron acceptor with a PEDOT:PSS hole transport layer. A post fabrication annealing treatment was carried out at a temperature range from 40-200oC, while different solvents were used for the dispersion. The best results were obtained at 120oC using chlorobenzene, the cell shows a short circuit current, Isc = 0.7 mA/cm2, an open circuit voltage, Voc = 0.75V, a fill factor, FF= 0.6, resulting in a power conversion efficiency of ɜ = 0.3% under white light illumination. The altering of the processing conditions led to an improvement in the power conversion efficiency by a factor of 3. This was attributed to a better charge carrier transport in the polymer matrix and a more effective charge separation and collection.

Chemical Purification and Characterization of Ultradisperse Diamond Powder

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Nanoscale diamond has been found in meteorites, protoplanetary nebulae, interstellar dust, residues of detonation and in diamond films (2-5 nm diameters) (1, 2). On Earth nanodiamonds can be produced by detonation and by CVD (Chemical Vapor Deposition) techniques. TNT (Trinitrotoluene) detonation yields among other carbon structures nanocrystalline diamonds with diameters around 10 nm. This detonation synthesis has been optimized and nanodiamond produced with this technique is commercially available. These nanodiamonds are called ultradisperse diamond (UDD) due to their very narrow size distribution (2). Purification of UDD is important because small amount of graphitic impurities and other carbon structures in diamond crystal can alter its most important properties. We performed UDD powder purification, of sample from Alit S.A. (Ukraine) that was produced by TNT detonation. The purification process was made by acid reflux using nitric acid at different concentrations to obtain a high purity UDD (3). The samples were characterized by XRD (X-ray Drifaction), XPS (X-Ray Photoelectron Spectroscopy), Raman Spectroscopy and TEM (Transmission Electron Microscopy)before and after purification. This purified UDD was electrophoretically deposited on silicon wafers to obtain a device that can be used in applications such as charge and energy storage, light emission, sensing and others. This technique is used because offers the possibility of engineering and continuous grading of materials (4, 5).References:1. C. F. Chen and C.C Wu, J. Chem Phys. 2002, 116, 1211-1214.2. Jean Yves and Giulia Galli, Nat. Mater., 2003, 2, 792-795.3. A. G. Reinzler et. al., Appl. Phys. A. 1998, 67, 29-37.4. A.M. Affoune et. al., Langmuir, 2001, 17,547-551. 5. A. N. Alimova et. al., J. Vac. Sci. Technol. B, 1999, 17, 715-718.

Organic conducting micro- and nanostructures

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Organic conducting materials, e.g. CT and RIS TCNQ complexes and polymers (polyaniline), have been prepared in our laboratory in the form of micro- and nanocrystals, nanolayers, nanospheres, nanofibrils and nanotubes [1-3,8,10]. Fabrication, properties, modifications and selected applications of such structures will be presented and discussed, including biosensors, FETs, LEDs, neural nanonetworks [4-6,9].

Some conducting CT TCNQ complex (with an alkaloid) have been obtained in the form of micro- and nanocrystals of unique helical morphology.

Polyaniline micro- and nanolayers were used in biosensors, FETs and LEDs [6,9]. Polyaniline nanofibrils and nanotubes were doped with fullerene and fullerene derivatives [7], but have also been modified with high temperature [8] and their structure was improved as a result of synthesis in microgravity conditions [10].

A controlled polyaniline nanofibril network was fabricated in our laboratory and successfuly tested as a physical model of the neural network.

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Mechanical Properties of Cryomilled Nanostructured Al alloys

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Mechanical attrition in liquid nitrogen (i.e., cryomilling) is one of several synthesis techniques that are capable of producing structural materials with grain sizes in the 10-500 nm range, in large quantities. In the present study, cryomilling fundamentals are reviewed briefly, followed by a discussion of mechanical behavior and the underlying mechanisms. Particular emphasis is placed on the issues of high strength and low ductility at room temperatures, in an effort to highlight strategies for improvement of ductility, and high-temperature mechanical behavior.

Surface modifications of nano-structured glasses under irradiation

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We are studying energy transfer processes in nanoporous materials under irradiation, hydrogen gas (H2) production related to structural modifications, especially as a function of the pore size. We have carried out experiments with Controlled Pore Glasses (CPG) having from 8 to 300 nm pore diameter, irradiated with the 10 MeV electron linear accelerator of the laboratory and with gamma radiation. A strong enhancement of the production of H2 is always observed, as compared to free water. The evolution of the production of hydrogen gas will be discussed as a function of the hydratation of silica. The evolution of the silica before and after irradiation is followed by means of IR spectroscopy. In the case of dry silica, the isolated silanol disappears under irradiation. In the case of wet silica, a deshydratation of the system is observed under radiation. The combination of NMR and EPR experiments helps to highlight the mechanisms in silica/water systems.

Novel Properties of Si and II-VI Nanowires and Nanoribbons

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High-phase purity semiconductor nanowires and nanoribbons are produced in large-quantity by using the metal-free oxide-assisted growth and metal-catalytic vapor-liquid-solid method. Systematic characterizations reveal the novel structural, optical, electronic, and chemical properties of silicon and II-VI (ZnO, ZnS, CdS, ZnSe, etc) nanowires and nanoribbons. Atomically-resolved scanning tunneling microscopy imaging gives detailed atomic structures of Si nanowire (SiNW) surfaces, while scanning tunneling spectroscopy measurements demonstrates the quantum-size effect in the bandgaps of SiNW. Regular intramolecular junctions in SiNW show sharp conductivity changes across junctions, suggesting transistor possibility. Semiconductor nanowires assembled in aluminum oxide templates or bundles exhibit highly polarized photoluminescence and lasing properties. Significantly, individual nanoribbon of II-VI semiconductors shows strong simulated emission along the long axis. Due to the large-size nanoribbons are easy to handle, manipulate, and have a large signal, thus they are ideal systems to study the structural and optoelectronic properties of single nano-objects. One-dimensional nanomaterials offer exciting opportunities for fundamental research and to realize unprecedented optoelectronic applications of Si and II-VI semiconductors.

Strain Hardenability of Ultrafine Grained Low Carbon Steels Processed by ECAP

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The structural use of ultrafine grained (UFG) and nanostructured alloys is limited at present primarily due to a lack of their strain hardenability. Several approaches have been suggested to improve it, such as a bimodal grain size distribution, uniform distribution of nano-sized second phase particles, strain gradient plasticity, etc. We processed three kinds of UFG low carbon steel via ECAP, UFG ferrite-pearlte steels without or with nano-sized vanadium precipitates and UFG ferrite-martensite dual phase steel, and compared their room temperature tensile properties, focusing on their strain hardenability. It was found that uniform distribution of nano-sized vanadium precipitates slightly improve strain hardenability, but UFG ferrite-martensite dual phase steel exhibited extensive strain hardening from the onset of plastic deformation, similar to coarse grained counterpart. The strain hardening behavior of the three UFG steels was characterized via the modified Crussard-Jaoul analysis and explained in terms of their microstuctures.

Synthesis and Optical Properties of Nanostructured Zinc Oxide

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In this research, a novel DC thermal plasma reactor was used to produce spherical, rod- and tetrapod-shaped ZnO nanopowders for photocatalytic as well as ultraviolet- (UV-) and near infrared- (NIR-) shielding applications. Visible light absorption of the nano-ZnO photocatalyst was achieved by doping up to a few thousands ppm of nitrogen into the material. And the extent of visible light absorption increased with doping concentration. Under visible light illumination, the N-doped ZnO phtocatalyst possessed excellent anti-microbial ability. In the study of light-absorbing property, we found that ZnO nanorods synthesized in a reduced atmosphere revealed a strong absorption of near-infrared (NIR) light in addition to ultraviolet (UV) light. UV absorption is attributed to the transfer of electrons from valence to conduction band while NIR absorption the effect of plasma resonance. Room-temperature photoluminescence spectroscopy of the ZnO nanorods showed a UV emission peak at 380 nm, a green emission peak at 520 nm, and a weak NIR emission peak at 750 nm. The UV emission was assigned to the near band-edge emission while the green and the NIR emissions corresponded to the deep-level emission from different defects. In addition, the green emission peak of the nanorods shifted when subjected to different annealing conditions, with blue-shift in a reductive annealing atmosphere and red-shift in an oxidative atmosphere. Finally, discrete UV lasing modes were observed in the random-packed nanorods at room temperature. This may be attributed to recurrent light scattering that provides coherent feedback for lasing.

Nano- and Micro-World of Block Copolymers - From Self-Assembly to Nanomechanical Devices

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Block copolymers self-assemble under appropriate conditions forming various mesophasic structures. The different domains of such mesophases can be crosslinked and/or degraded yielding nanostructures including hollow nanospheres, nanofibers, nanotubes, crosslinked polymer brushes (monolayers), and smart nanochannels in polymer thin films. The block copolymer nanostructures produced can be used as templates for synthesizing polymer-encapsulated inorganic nanostructures including superparamagnetic polymer/-Fe2O3 nanofibers. Polymer/inorganic hybrid nanostructures can be further coupled with other nano- or micro-structures yielding nanomechanical devices such as an ⌠optical magnetic nanohand■. Reviewed in my talk are the preparation, property, and application of nano-, micro-, and super-structures derived from block copolymers.

ANALYSIS OF STRUCTURE AND MECHANICAL PROPERTIES OF A 5083-F ALUMINIUM ALLOY PROCESSED BY ECAE AT DIFFERENT TEMPERATURES

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In order to alight a little more on the understanding of the mechanisms involved when severe plastic deformation is carried out by ECAP on ductile
alloys, routes R and A have been applied on a AA 5380 alloy at 150 and room temperature. Metallographic characterisation has been done by means of optical microscopy, scanning electron microscopy and high resolution transmission electron microscopy to investigate size, morphology and distribution evolution of the metallic matrix and the precipitates present in this type of aluminum alloy. Also, some mechanical properties have been studied using nanoindentation, US measurements and mechanical testing. From the results it is worth noting that the microstructure shows two observation levels. In one case, as expected, micrometric level does follow classical statements and thus properties are related to microstructure evolution, whereas in the nanometric scale these relationships do not seem to agreed.

Low-than-room temperature effect on the stability of CuO nanofluid

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This study involves the use of copper oxide nanofluid produced by the Submerged Arc Nanoparticle Synthesis System (SANSS) to investigate temperature effect on particle suspension of copper oxide nanofluid. The purpose is to understand the deposition state feature of copper oxide nanofluid in a lower-than-room-temperature work environment and to motion behavior of suspended nanoparticle and to analyze its size distribution. The amount of the nanoparticle was also varied. The relationship between temperature and particle size distribution was investigated. An analytical method to predict the results was introduced. It was concluded that particle size distribution change stable as the temperature decrease due to Brownian motion of retard. The change of environmental temperature can affect copper oxide nanofluid stability in application. Hence, the phenomenon is important when the copper oxide nanofluid in a lower-than-room-temperature of work environment.

Polymeric substrates and encapsulation for flexible electronics: Bonding structure, surface modification and functional nanolayer growth

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Nowadays, the production of flexible electronic devices by large scale manufacturing processes represents a rapidly growing sector and the development of functional (inorganic and/or organic) thin layers onto flexible polymeric substrates is one of the main research issues in nanotechnology. Therefore, the flexible substrate materials should meet specific and advanced demands, in order to be incorporated in a growing number of emerging applications, such as flexible displays, organic light emitting devices, photovoltaic cells and (opto)electronics, data storage and recording media, food and pharmaceutical packaging, etc. Among the other desirable properties of flexible substrate materials, the two most important ones are the optical transparency and high barrier – low permeability in specific gases such as oxygen and water vapour, in order to be used for the encapsulation of the flexible electronic devices, and which have a major affect on their performance, efficiency and lifetime. These properties are determined by the inorganic and the organic nanolayer's properties (developed on top of the flexible material) and the substrate and layers bonding and nanostructure.
In this work, we provide a detailed overview on the incorporation of polymeric substrates, such as Poly(Ethylene Terephthalate)-PET and Poly(Ethylene Naphthalate)-PEN films towards the production of future flexible electronics covering all aspects, from surface treatment to the growth mechanisms of transparent functional oxide nanolayers, (e.g. SiO2, SiO, SiOx, TiO2) in terms on their bonding structure, surface and interface morphology, stoichiometry, microstructure, optical and mechanical behavior. For this study we have used surface-sensitive, non-destructive characterization techniques, such as in-situ and real-time Spectroscopic Ellipsometry, in an extended spectral region from IR to Vis-farUV, Scanning Probe Microscopies and Nanoindentation in combination to advanced methodologies and modeling procedures.
The above contribute towards the optimization of the functional oxide nanolayers deposition on the polymeric materials that can dramatically increase their quality in order to be used for the encapsulation of flexible electronics. This methodology reveals the potentiality of in-situ and real-time monitoring of transparent functional nanolayers growth on transparent polymeric substrates, exhibiting desirable and functional properties, meeting specific demands in a growing field of flexible electronics applications.

Properties of the Aurivillius phases in the Bi4Ti3O12 √ BiFeO3 system

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Ferroelectric materials of the Aurivillius family with the general formula are currently being widely studied for potential uses in nonvolatile memory (FeRAM) applications. In the Bi4Ti3O12 √ BiFeO3 system the compounds with different layers number were synthesized. The compounds with big layers number (more than 8) and complex alternating with layers number were synthesized for the first time.X-ray diffraction study was carried out for phase determination and lattice parameter calculation.The microstructure and the phase composition were investigated by scanning electron microscopy (SEM) coupled with EDX.By using differential scanning calorimetry the Curie temperature and the decomposing temperature were determined. The results obtained indicate the gradual decrease in thermal stability of the compounds in the Bi4Ti3O12 √ BiFeO3 system on the increasing of Fe2O3 in the system.Thermomechanical properties were studied by dilatometry. The temperatures of the sintering activation and linear thermal expansion coefficients were determined.The microhardness of the compounds decreases gradually on the increasing of layers number in unit cells.The electrical properties of polycrystalline samples were investigated. The values of activation energies for the conductivity were calculated.

Bulk zirconia nanoceramics prepared by cold isostatic pressing and pressureless sintering

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Bulk zirconia ceramics (stabilized by 1.5 and 3mol.% of yttria) was prepared by cold isostatic pressing and pressureless sintering. After sintering at 1100 ╟C, the bodies had a density exceeding 99%t.d. and grain size below 60nm. The sintering kinetics of these nanoceramic materials was compared with sintering kinetics of submicrometric zirconia.

Thermoelectric power in nucleobases and DNA based molecular junctions

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The measurement of thermoelectric voltage over a molecule with two contacts at different temperature can provide new insights into electron transport in molecular systems. In fact, the extreme sensitivity of thermopower to finer details in the electronic structure allows one to gain valuable information regarding the location of the Fermi energy relative to the molecular levels. Thus, the thermoelectric voltage over guanine (G) molecules on a graphite substrate was measured by Poler et al. using a STM tip [1]. The obtained Seebeck coefficient value (+20 microvolts/K at room temperature) indicates a p-type conduction. A similar figure has been recently derived in a theoretical study considering a Phenyl-dithiol molecule chemisorbed on a gold surface. In addition, this study reveals that thermoelectric voltage should be relatively insensitive to the quality of the tip contact [2]. This result deserves further attention since strong contact effects are expected in the measurement of both electrical conductance and I-V curves of DNA molecules connected to metallic leads [3]. In this work we present a theoretical study of the thermoelectric power for several oligonucleotides of increasing complexity degree, described within the tight-binding approach. In order to perform a systematic comparative study, we start by considering the thermoelectric properties of single nucleotides G, C (cytosine), A (adenine) and T (thymine), dinucleotides and codon trinucleotides of biological relevance and, finally, a representative GACT tetranucleotide. To evaluate the thermoelectric voltage we make use of the transmission as a function of energy, according to the approach introduced by Paulsson and Datta [2]. To compute the transmission coefficient at zero bias the oligonucleotides are connected to two semi-infinite electrodes [3,4]. In this way, we obtain closed analytical expressions describing the temperature dependence of the Seebeck coefficient for a complete series of short DNA chains. By the light of the obtained results, t
he possible use of DNA based thermoelectric devices is discussed in the context of current search for novel thermoelectric materials [5]. References:[1] J. C. Poler, R., M. Zimmermann, and E. C. Cox, Langmuir 11 (1995) 2689.[2] M. Paulsson and S. Datta, Phys. Rev. B 67 (2003) 241403(R).[3] E. Macib, F. Triozon, and S. Roche, Phys. Rev. Lett. (submitted).[4] S. Roche, D. Bicout, E. Macib, and E. Kats, Phys. Rev. Lett. 91 (2003) 228101.[5] E. Macib, Nanotechnology (submitted).

Preparation of mixed WxMo1-xO3 nano crystalline powders using sol-gel method

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In this study nano - crystalline powders WxMo1-xO3 were obtained using peroxo-sol- gel method. Mixed sols of peroxotungsent and peroxomolidic acids were prepared after oxidizing reaction between metal powders of tungsten and molybdenum, and hydrogen peroxide solution. The sols have undergone slowly gelation at room temperature. The obtained gels were heat-treated at different temperatures (100-400oC). The structural and phase transformations were investigated by IR and XRD analysis. The precursor with ratio of W:Mo = 4:1 crystallized in W71Mo29O3 with excess of m-WO3. The sample with ratio of W:Mo = 1:1 crystallized in W0.53Mo0.47O3 with excess of m-WO3 while from the sample with initial ratio W:Mo = 1:4 crystallized in Mo7.568W1.432O25 and o-MoO3. The infrared spectra of the gels treated at 100 and 200oC show all bands typical of peroxo-complexes. The characteristic bands of WxMo1-xO3 solid solutions were observed in the IR spectra of the samples after heat-treatment at 300 and 400 oC .By this method powders are synthesized with particles dimension in the range of 30nm

Nanostructured Electrode Materials for High Rate, Large Format Lithium Ion Batteries

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Lithium ion batteries are superior to NiMH batteries in energy density, but have been excluded from the highest power density applications due safety and cost limitations. The cathode materials in conventional lithium ion cells are based on metal oxide materials, typically containing nickel or cobalt. Nickel and cobalt are expensive and reactive with the electrolyte. Metal oxides are electronic insulators, which can limit the rate performance of lithium ion cells. The open circuit potential of conventional metal oxide electrodes is relatively high. This limits the charge acceptance rate, since the polarization under high rate charging (> 10C) can exceed the potential limit of the electrolyte. Similarly, the open circuit potential of conventional graphitic anode materials is close to the lithium plating potential which also limits high charge rate acceptance. T/J Technologies has developed and demonstrated new bulk energy storage concepts based on nanostructured composite metal oxide anode and metal phosphate cathode electrodes. The composite design provides for high electronic conductivity, and the nanostructure limits the lithium transport distance. The open circuit potentials for these materials are displaced from the lithium plating and electrolyte decomposition potentials. These features contribute to high rate capability. In these systems, up to 40% of the C/10 capacity is retained at charge/discharge rates of >100 C. The data presented for these cells will include improved thermal stability and electrolyte oxidation resistance, excellent cycle life, and potentially low cost for high volume/large format applications. With much higher energy density than ultracapacitors or hybrid battery/capacitors, these ultra-high rate lithium batteries are ideally suited for hybrid electric vehicles.

GAS SENSING PROPERTIES OF NANOCRYSTALLINE NiO AND Co3O4 IN POROUS SILICA SOL-GEL FILMS

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Thin SiO2-NiO and SiO2-Co3O4 nanocomposite films consisting of either NiO or Co3O4 nanocrystals in a porous SiO2 matrix have been prepared using sol-gel methods. The morphology, crystalline phase and chemical composition of the films have been characterised using X-ray diffraction, transmission electron microscopy and Fourier transform infrared techniques. The sensor response to H2 (20 √ 850 ppm) and CO (10 √ 500 ppm) in dry air and different operating temperatures (50 ╟C√ 300 ╟C) has been investigated using both conductometric and, for CO, also with optical transmittance transduction methods. Both the NiO and Co3O4 doped films exhibit a conductometric p-type response, with a resistance increase upon exposure to the reducing gas. The nanocomposite films showed also a reversible change in the optical transmittance in the VIS-NIR range when exposed to CO (10 √ 10000 ppm) in dry air. SiO2-NiO films have shown the highest response to H2 at 300 ╟C operating temperature and good selectivity to the measure of H2 if CO is the interfering gas. SiO2-Co3O4, which to the best of our knowledge may represent a new p-type material for gas sensing applications, shows similar behaviour to the SiO2-NiO films. Detection limits of approximately 10 ppm CO and H2 are demonstrated.

Buried nano-layers prepared in single crystalline silicon by co-implantation of Cz-Si with hydrogen / helium and treatment under high hydrostatic pressure

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To prepare buried nano-structured layers in single crystalline Czochralski grown silicon (Cz-Si), 001 oriented Cz-Si was co-implanted with hydrogen (doses, D = 2.5 -5x10(16)cm(-2), energy, E = 135 keV) and helium (D = 2.5 - 5x10(16)cm(-2), energy, E = 50 - 150 keV) and subjected to high temperature (up to 1400 keV) – high pressure (up to 1.2 GPa) treatment in hydrostatic conditions (Ar ambient). Depending on the implantation and treatment conditions, the sponge – like buried layers composed of silicon nano – crystals and amorphous silicon, with hydrogen / helium filled cavities and platelets / bubbles, were created at about 0.75 micrometer depth. Such layers indicate specific properties in respect of hydrogen release (always increasing with temperature and sometimes also with pressure) and of gettering activity (for carbon, oxygen and some heavy metals). Perspective usefulness of such structures for microelectronics and similar applications will be discussed.

Formation and Characterization of Highly Interfacial Hybrid Nanocomposites

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The formation and characterization of highly interfacial hybrid nanocomposites is described. The nanocomposites are formed by a two step, near net-shape manufacturing process that includes nanoparticle formation via high energy ball-milling followed by consolidation via hot isostatic pressing. Two types of hybrid materials will be described; metal/ceramic nanocomposites, in which corrosion properties are highlighted; and polymer/ceramic nanocomposites, in which proton conductivity is described. The influence of processing parameters and interfacial characteristics of the nanocomposites on selected properties is being investigated. Recent advances in contamination control during nanoparticle formation and the effect of contaminants on nanocomposites properties are also described.

Study of the operating parameters on the production of carbon nanotubes using CVD

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The issue of this study is the production of carbon nanotubes using the chemical vapor deposition (CVD) method. Experiments have been carried out on a system assisted by a sensitive microbalance capable to measure the weight increase of the deposited material during the synthesis process. Results are presented concerning the effect of operating parameters on the rate of nanotubes growth and the properties of the nanotube materials produced. The catalytical substrate consists of precursor oxides of the metallic catalyst (e.g. Fe) and the support oxides (e.g. alumina). The experimental results show that the reduction temperature of the metallic catalyst affects the structure of the catalytical substrate modifying the deposition rate. The deposition rate as well as the form of the deposited carbon are also affected by the deposition temperature. Increase of the metallic catalyst concentration is found to lead to higher amounts of material deposited. The produced material is studied through scanning electron microscopy (SEM) and Raman spectroscopy revealing multiwall carbon nanotubes.

Characterization of barium strontium titanate for phase shifters applications

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Ultrathin films are currently gaining interest in many areas such as integrated optics, sensors, friction, reducing coatings or surface orientation layers. Polyelectrolytes are charged polymers. The approach consists of two parts: (a) the chemisorption of 11-mercaptoundecylamine to construct a self-assembled monolayer with the consequent protonation of the amine and (b) the deposition of sandwiches of opposite charged polyelectrolytes. Surface characterization of the modified barium strontium titanate (BSTO) substrates were done with atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared (FT-IR)specroscopy in specular reflectance mode. The approach has the advantage that ionic attraction between opposite charges is the driving force for the multilayer build up. For our purposes, the multilayer of polyelectrolytes depends on the quality of the surface needed to construct the phase shifter devices in a way that the roughness factor defects will be diminished. Electrical data of phase shifters will be presented including voltage and temperature cycling issues. The polyelectrolytes selected for the study are: polystyrene sulfonate sodium salt , polyvinylsulfate potassium salt , and polyallylamine hydrochloride.

Electrochemical deposition of PtMo and PtRuMo electrocatalysts on HOPG substrate and their behavior toward electrooxidation of methanol

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Sequential and simultaneous electrodeposition methods were applied to prepare PtMo and PtRuMo electrocatalysts on previously activated HOPG substrate. The influences of Mo and Ru concentration on the electrodeposits were showed by the electrochemical and surface science techniques. Catalysts deposited by sequential method showed to have better morphological and catalytic behavior and some properties that are wished to meet in the development of a catalyst and also, this method have some advantages over the simultaneous deposition. Morphological and microscopic characterization, carried out with (SEM), (AFM), showed that, in general, the deposits are clusters of aggregated particles XPS complemented with cyclic voltammograms of PtMo electrodes showed the presence of the different molybdenum oxidation states. Electrocatalytic examination of methanol oxidation, carried out by cyclic voltammetry, showed that the oxidation current densities for the PtRu and PtRuMo electrodes were enhanced compared to the pure Pt.

Fabrication and Microstructural Characterization of Nano-Crystalline ZrO2-Based Composite

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Ceramic materials are known to exhibit excellent mechanical properties when grain size is reduced to less than 100 nm. Since the lower mechanical properties such as fracture toughness, fracture strength and deformability have prevented ceramic materials from use in engineering applications, the nanocrystalline (nc) ceramic materials with grain sizes of <100 nm have received considerable attention. The present study was therefore performed to fabricate nc ZrO2-based ceramics.In order to synthesize nc ceramic materials, we have employed high-energy ball-milling (HEBM) and spark-plasma-sintering (SPS) techniques, that have been widely used for the synthesis of nc and amorphous ceramic materials. Using HEBM process, nc ZrO2-spinel powders can successfully be synthesize from the sub-micrometer sized powders of about 300 nm. After 400 h ball-milling, an amorphous-like phase was observed among nc ZrO2 and spinel particles of <10 nm. From the nc powders, a fully dense nc ZrO2-based composite with grain sizes of less than 100 nm can successfully be consolidated using the SPS technique. In this talk, we will discuss the mechanical properties of nc ZrO2-based composite.

Processing and Characterization of Nanoceramic Composites with Interesting Structural and Functional Properties

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Processing and characterization of alumina-based nanocomposites that produce nanostructures with attractive structural and functional properties have been emphasized. A three-phase alumina based nanoceramic composite demonstrated superplasticity at a lower temperature and at a higher strain rate. An alumina-carbon nanotube-niobium nanocomposite has a fracture toughness that is five times higher than that of pure alumina and an electrical conductivity that is thirteen orders of magnitude greater than that of pure nanocrystalline alumina. It also has excellent potential for use as a thermoelectric material. An alumina-spinel nanocomposite demonstrated optical transparency in the mid-infrared range. It also can be deformed superplastically at temperatures as low as 1000 ╟C. These structural and functional properties will be discussed in the context of microstructural investigations.

PECULIARITIES OF MANIFESTATION OF SIZE EFFECTS IN Bi NANOWIRES AT LOW TEMPERATURES

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For the first time glass covered single crystal bismuth nanowires with d<100 were studied. Glass covered single crystal Bi wires of strictly cylindrical form with d=100-50 nm were obtained by the liquid phase casting by the Ulitovsky-Tailor method. Orientation of the samples of all the diameters was the same: the wire axis made up an angle of ~20^0 with the bisector axis C2 in the bisector-trigonal plane. The diameter was controlled with the help of SEM and AFM microscopes.In the nanowires new effects were found, among them the following: Minimum of the negative magnetoresistance in the transverse magnetic field and presence of ⌠special■ points at T=4.2K-1,6K. Oscillating dependence of the resistance deformation curve R(ksi), where ksi=deltal/l, l is the sample length. Observation of oscillations with 3 period being equidistant by the direct field in strong magnetic fields (4-14 T). Anomaly of the temperature dependence of the resistance and thermopower and their change with elastic stretch. The results are interpreted from the viewpoint of manifestation of the confinement effect, Aaron-Boom effect and quantum size effects of size quantization.ACKNOWLEDGEMENTSThis work is supported by Civilian Research and Development Foundation (CRDF), CGP # MO-E1-2603-SI-04.

Nanocrystalline Mn-doped ZnO Prospective candidate for spintronic devices?

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Nanocrystalline Mn-doped ZnO has been synthesized by using a soft chemical route. X-ray diffraction study shows that as-prepared powders were amorphous in nature and crystallization into Mn-doped ZnO phase occurs after heating above the crystallization temperature. Rietveld analysis indicates that growth of crystalline phase is anisotropic and average particle size varies from 20 to 25 nm with doping concentration annealed at 650 C for 30 min. Analysis also indicates that Mn is not going into the structure, as lattice parameter remains unaltered with doping. Available magnetization data revealed a spin-glass like behavior with a magnetization about 0.2 emu/gm.

Magnetic and Structural Characterization of CoFe2O4 Nanoparticles Encapsulated within Block Copolymer Films

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Nanometer-size CoFe2O4 nanoparticles have been synthesized by self-assembly within diblock co-polymer films, through a novel room-temperature templating strategy, easily amenable to large scale fabrication processes. X-Ray diffraction, TEM, SQUID and Mцssbauer measurements are combined in order to explore the morphological, structural, micromagnetic and interfacial characteristics of this nanocomposite system. TEM micrographs indicate low polydispersity, with average particle size of 9.6 nm diameter. Low temperature Mцssbauer studies predict average sublattice saturation hyperfine magnetic fields Hsat (A) = 501 kOe and Hsat [B] = 527 kOe, respectively, for the tetrahedral and octahedral iron coordination sites of the ferrite spinel structure. Superparamagnetic relaxation processes, analyzed within a cubic magnetic anisotropy model, give an effective magnetic anisotropy density Keff = 3.23 x 105 J/m3, while SQUID magnetometry measurements predict a saturation coercivity Hc = 6.1 kOe. Deviations of the above parameters from those of bulk CoFe2O4 and unsupported CoFe2O4 nanoparticles of comparable size are discussed in terms of finite-size effects and interfacial interactions. The results indicate that particle-support interactions at the ferrite/polymer interface can be profitably utilized for the stabilization of non-equilibrium phases and manipulation of the magnetic properties of this nanocomposite system.

ENHANCEMENT OF MECHANICAL PROPERTIES OF EPOXY-BASED NANOCOMPOSITES USING HIGH MAGNETIC FIELDS

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In this paper we describe the results of recent experiments designed to investigate the influence of high uniform magnetic fields on the curing of a variety of composites comprising nanoparticles infused in simple epoxy resins. The particulate components include highly acicular carbon nanofibers and multi-walled carbon nanotubes. Significant improvements have been observed for various elastic moduli as well as for thermal characteristics to a degree that indicates magnetic field-assisted ordering of the nanoparticles within the epoxy matrix. The epoxy selected for these experiments, SC-15, is completely cured at room temperatures over several hours, with gel formation occurring after ~30 mins. The curing takes place in high-uniformity DC magnetic fields of up to 28 T. Significant field enhancement of mechanical properties such as strength and stiffness has been observed. A theoretical model, for field alignment of nanofibers and nanotubes, is also briefly described.

Organic-inorganic hybrid nanostructures by sol-gel process for biomedical applications

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Organic-inorganic hybrid materials can offer multifunctional properties tailoring from submicrometer to nanometer length scales in various applications such as micro and nano photonic devices including, waveguides, light emitting devices, quantum dot devices, photonic band gaps and holographic materials. In the present investigation, hybrid materials based on polydimethoxy silane and fluorine based polymer were spin coated on to different substrates glass, quartz, and polycarbonate substrates at room temperature. The deposited films have been cured under UV irradiation for better polymerisation followed by annealing at 100oC (polycarbonate), 200oC and 300oC for 30 minutes. UV-visible spectroscopy (UV-vis), Fourier transform infrared (FTIR) spectroscopy and X-ray diffraction (XRD) have been used for optical absorbance, vibrational and stretching bands, and phase formation of the deposited of the films, respectively. The deposited films are transparent, hard, scratch resistance and in particular hydrophobic. Adhesion strength failure and hardness measurements on plastic substrates were examined by using scratch resistance tester and nanohardness tester, respectively.

Synthesis of nanostructured-MoS2 / Ag2S multilayered coatings by sol-gel for solar energy storage aapplications

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In the present investigation, in order to have quantum confinement effect, thin nanostructured single MoS2 and Ag2S as well as multilayered films of MoS2 / Ag2S have been synthesised by simple and cost effective sol-gel dip coating technique. The films were deposited on to glass, quartz substrates at room temperature. The deposited nanostructured films MoS2 (5-6 nm) and Ag2S (5-8 nm) were subjected to annealing treatment from 100oC to 400oC and the effect of annealing on structural, optical and electrical properties has been studied in detailed. UV-vis and Fourier transform infrared (FTIR) spectroscopes have been employed in order to study the optical absorption as well as band gap of the individual films and multilayered films and vibrational and stretching bands, respectively. Electrical resistivity of the films have been measured using four-probe sheet resistance technique. Thermoemf measuremnts indicated that the deposited films were p-type in case of MoS2 and n-type in case of Ag2S.

Nanoscale pH responsive block copolymer micelles with potential use in water purification methodologies

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A series of well-defined poly(hydroxy styrene-block-methacrylic acid) (PHS-PMAA) diblock copolymers have been prepared by a combination of anionic polymerization high vacuum techniques and post polymerization hydrolysis. Molecular characterization of these polymers by size exclusion chromatography, FT-IR and NMR has shown the homogeneity of the samples in terms of composition and molecular weight and has given their detailed molecular characteristics. The self-organization of these copolymers in aqueous solutions has been studied by conductivity, turbidity, light scattering and ж-potential measurements as a function of concentration and pH. The block block copolymers self-assemble in nanometer scale core-shell micelles with PHS cores and PMAA coronas at intermediate pHs. At low pH precipitation occurs from aqueous solutions due to neutralization of the PMAA coronas. Fluorescence spectroscopy measurements showed that encapsulation of pyrene is possible in these micelles. The potential use of these micellar aggregates in nanotechnological water purification methodologies is discussed.

Comparative assessment of different sacrificial materials for releasing SU-8 structures

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In recent years SU-8 has become a very attractive negative working photoresist for high-aspect-ratio structures and thick resist layers. It is commonly used in a wide range of applications of micro-nano-fabrication because of its physical properties, thermal and chemical stability, biocompatibility, and its low cost fabrication. Releasing cured SU-8 structures from the substrate in the final fabrication step has become very important because of crucial effects on the integrity of microstructures and because of undesirable long and time-consuming release processes – especially for microstructures with large contact surface. In the past, research was carried out in order to investigate the performance of individual sacrificial layers for releasing SU-8 structures. In this paper, a comparative investigation is carried out in order to critically assess the characteristics of different materials, metals and polymers for realizing SU-8 structures of different size. For this reason, a number of samples were prepared and their properties were assessed using SEM by examination of structures before and after their release. Additionally, the release time was compared. The materials that have been investigated are chromium, copper, aluminium, PMMA, OmniCoatTM(MicroChem Inc.), polyimide, and polystyrene. The experimental results showed that metals are better sacrificial layers for small SU-8 structures (500 nm – 100 □m). However, polymers can be produced as very thin films which can be detached from the silicon wafer and allow the release of small cured SU-8 structures.

STRENGTH OF MICRO- AND NANO-STRUCTURED MATERIALS: UNIFIED INFLUENCE OF COMPOSITION, GRAIN SIZE AND STRUCTURAL DIMENSION

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The strength of micro- and nano-structured grained materials is extensively analysed, assuming the key role played by the interfaces. A fractal approach (that assumes a self-similar grain size distribution) is proposed, without assuming ad hoc hypotheses, to unify the influences on the strength of grain and structural sizes as well as of volumetric grain content. Different assumptions on the statistical distribution of grain sizes, e.g., a Gaussian distribution, show that the results are more general than expected, being reproduced by a particular value of the fractal exponent. As a matter of fact, we report a detailed experimental comparison on WC-Co alloy and Poly-Crystalline Diamond (PCD), showing that the theoretical fractal predictions are in clear agreement with the experimentally observed strengths. In particular, the finding on grain size effect represents an extension of the well-known empirical Hall-Petch relationship for material strength. Finally, a fractal structural parameter, representing an extension of the Gurland's structural parameter, is proposed to investigate or design micro- and nano-structured material with a specified strength.

FRACTURE STRENGTH OF NANOTUBES: EXPERIMENTS AND THEORY

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In this paper we report detailed experimental and theoretical investigations on fracture strength of multi-walled carbon nanotubes (MWCNTs). The fracture strengths of MWCNTs were measured with a nanostressing stage located within a Scanning Electron Microscope (SEM). The MWCNT was gripped and then stretched between two opposing Atomic Force Microscope (AFM) tips. The MWCNTs broke in the outermost layer so that the fracture strengths (as well as the Young▒s moduli and the failure strains) of the external layers were obtained. Transmission Electron Microscopic (TEM) examination of the broken nanotube fragments revealed interesting fracture topologies. The experimental data set has been analysed by applying a new theory, Quantized Fracture Mechanics (QFM), which accounts for the quantized crack propagation in nanostructures (broken chemical bonds). For large enough data sets, the statistics of fracture strength distributions could also be derived.The experimental-theoretical comparison suggests that: (i) the experimental method is a useful tool for nanoscale tensile tests, (ii) the observed fracture strengths are quantized, (iii) few defects were responsible for the fracture of the tested MWCNTs and, (iv) QFM is a useful theory for predicting the strength of defective nanostructures. We gratefully acknowledge the grant support from the NSF grant ⌠Mechanics of Nanoropes■ (NSF #0200797, Ken Chong and Oscar Dillon, program managers), and the NSF grants NIRT: Electrical and Mechanical Properties of Boron and Metal and Nanoscale Devices Built from them (NSF #0210120) and NIRT: Synthesis, Characterization and Modeling of Aligned Nanotube Arrays for Nanoscale Devices and Composites (NSF #030450); and from the Office of Naval Research "Mechanics of Nanostructures" grant under award No. N000140210870 and the NASA University Research, Engineering and Technology Institute on Bio Inspired Materials (BIMat) under award No. NCC-1-02037(Jeff Jordan, program manager).

Contact angle studies on Porous Alumina Templates

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Nanoscale materials have being widely studied because of their particular properties and potential applications. In particular, one dimensional nanoscale materials have attracted much attention, in recent years. One of the most important methods for the preparation of the one dimensional nanoscale materials is the template method, which use the membranes with nanopore channels as the template. In the template method, anodic aluminium oxide membranes AAO, prepared by electrochemical etching aluminum foil in oxalic, sulphuric and phosphoric acid solutions are the most popular membranes used. For example, the fabrication of semiconductor nanowires, superconductor nanowire arrays, carbon nanotube arrays, etc. On this examples the force who make the nanomaterials go into the pores of the membrane, is the electrochemical one; but, when is tried to do otherwise, is necessary to use vacuum or high temperatures. The immersion of the AAO in a saturated solution of the material you need to grow in, is not enough. That is why; in this paper we present the study of the interaction of different solvents with the sulphuric and oxalic AAOs, in order to explain this fact.We present the results of contact angle measurements by Langmuir balance and goniometer determinations of fourteen different solvents with different polarities and superficial tension properties.

Attachment of Single-Wall Carbon Nanotubes on Platinum Surfaces by Self-Assembling Techniques

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Single-wall carbon nanotubes (SWNTs) have a very interesting combination of properties as their structure, morphology, dimension (high length-to-diameter ratio), and electronic properties. The properties suggest potential applications as chemical sensors, reinforcement material in polymer composites, tips for scanning probe microscopy, membrane material for fuel cells, and metal catalysts support. These bring the possibility of using nanotubes as nanosized container systems or as templates for fabrication of novel nanomaterials. In this work, self-assembled monolayers (SAMs) technique was used to adsorb 4-aminothiophenol (4-ATP) on platinum electrodes, in order to obtain an amino-terminated SAM as the base for the attachment of SWNTs. Previously purified SWNTs were oxidized with strong acids to obtain open ended nanotubes terminated with carboxylic acid groups. These acid-treated SWNTs were attached by a condensation reaction through the amino terminated SAM on Pt surface. The 4-ATP/SWNTs electrodes were characterized by scanning electron microscopy (SEM), reflection absorption infrared (RAIR) spectroscopy, and X-ray photoelectron spectroscopy (XPS). High resolution XPS studies and RAIR spectrum for platinum electrodes modified with 4-ATP indicate that molecules are sulfur-bonded to the platinum surface, producing the amino-terminated SAM as was expected. XPS and IR spectroscopy characterization was employ to follow SWNTs functionalization (formation of oxygen containing groups) throughout purification and acid-treatment steps. The results obtained from the characterization of SWNTs attachment suggest the successful bonded of SWNTs through the formation of amide bonds between carboxyl-SWNTs and the amino-terminated SAM.

Phonon Confinement and Surface Phonon Modes in CdSe-CdS Core-Shell Nanocrystals

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We have investigated the vibrational properties of bare and CdS shelled CdSe nanocrystalline particles. From the line profile analysis of the high resolution transmission electron microscopy (HRTEM) images the core-shell structure in the particles has been confirmed. We have observed the unique characteristics of the nanocrystals (which are absent in the corresponding bulk material), such as confinement of optical phonons and the appearance of surface phonons, in these systems. Making use of the dielectric response function model we are able to match the experimental and theoretical values of the frequencies of the surface phonons. We believe that our studies using optical probes provide further evidence on the existence of core-shell structures in CdSe-CdS type materials.

Preparation of New Layered Double Hydroxide, Co-V LDH

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The layered double hydroxide (LDH) is one of the nano ordered layered compounds and well known for its ability to intercalate anionic compounds. Most popular LDH is prepared conventionally only with divalent and trivalent cations. In this study, Co-V LDH consisting of divalent and tetravalent cations was prepared and reacted with monocarboxylic acids at room temperature. The Co-V LDH and intercalated compounds characterized by chemical analysis (C,H,N analysis, ICP and ESCA), X-ray diffraction, IR spectra, thermal analysis and Scanning electron microscope (SEM). The insertion of cyanate and carbonate anions into LDH was confirmed by chemical analysis and IR spectra. XRD patterns of the prepared Co-V LDH showed that the interlayer spacing of the LDH is 0.78 nm. The spacing is similar to that of usual LDH in which chloride, carbonate or bromide anion is the guest. SEM images showed that the morphology of Co-V LDH before and after intercalation reactions is plate-like structure.

Far from equilibrium processing of dense nanocomposite ceramics

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A two step process has been developed to fabricate a ceramic nanocomposite from commercially available raw material, which involves (a) synthesis of metastable ceramic powder via plasma melting and rapid quenching, (b) consolidation of the metastable powder to a dense ceramic via controlled phase decomposition during sintering. Powder compositions were spray dried and then heat-treated to ensure the integrity of the powder during the injection into a plasma jet. The powders melt and homogenize in the high temperature zone of the plasma and are quenched and collected in water. All melted particles showed a homogeneous metastable phase either with respect to crystal structure and/or extensive solid solubility. These powders decompose to equilibrium phases during subsequent Hot Isostatically Pressing and produce dense (<0.5 vol% porosity) ceramic parts. Hardness and toughness of different biphasic and triphasic compositions based on zirconia, alumina and spinel will be presented.

Characterization and properties of nanocrystal-forming Zr-based bulk metallic glasses

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Recently, a number of bulk metallic glasses with extremely high glass-forming ability (GFA) were reported in Zr-based multicomponent alloy systems. They have attracted much attention in the aspects of the scientific interests in a high stability of glassy state. More recently, it is found that various nanocrystalline phases are formed as a primary precipitation phase from a glassy state. Especially, formation of metastable phase such as icosahedral quasicrystalline phase is important for the investigation of mechanism of high GFA as well as the improvement of mechanical properties. In the previous studies, the unique local structure, which is different from those in the stable crystalline phases, is pointed out in the metallic glasses with high GFA. The authors have suggested that the primary metastable phase is correlated with the local structure in the glassy state. In this paper, we report the characterization such as structure, composition and kinetics of nanostructured alloys based on Zr-Al-Ni-Cu metallic glasses by nanoscale analysis of XRD and TEM. In these studies, we intend to investigate the formation mechanism of metastable nanocrystalline phases correlated with their high stability of glassy state. Moreover, the improvement of mechanical properties with the formation of nanocrystal will be reported. These results lead us to the conclusion that it is very useful for the formation of new nanostructured materials based on the metallic glasses.

The Characteristics of Giant Magnetoresistance in Co/Cu/Co Nanostructures and Their Dependent on Film Thickness, Annealing Temperature, Bilayer and Gas Rate

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The characteristics of giant magnetoresistance (GMR) in Co/Cu/Co nanostructures are investigated in association with different sets of experimental conditions. The samples were fabricated using a magnetron sputtering method with varying Co layer thicknesses in vacuum and were later subjected to post-deposition annealing at temperatures 200-450 ╟C for 150 minutes. GMR measurements were made using a specially design circuit in magnetic fields of ╠ 2500 Gauss. Apparently, a rapid 10% rise in GMR with Co layer thickness was observed between 2 - 6 nm, followed by a gradual drop along the thickness up to 20 nm. Annealing temperature has similar effect when its ascending mode attains a 24% GMR peak point at 400 ╟C beyond which the GMR starts to fall steadily and finally reaches 20% at 450 ╟C. It is predicted that, the Co and Cu species become soluble to each other as they reach 400 ╟C and a solubility process is initiated between them with Co atoms gradually precipitated from the Cu matrix, thus forming the Co clusters. Due to ferromagnetic interaction occurring at temperature exceeding 400 ╟C an anti-parallel structure is established in the sample that causes degrading in GMR values. For the as-prepared samples, the GMR increases linearly with the number of bilayer, n except for (Co/Cu) x 8 due tendency of the curve to decrease between n = 5 - 8. However, the GMR starts to rise again along the n > 8 bilayers until 12.5% GMR is reached for (Co/Cu) x 15. This up-down variation is somewhat similar to periodicity, possibly due to the [Co/Cu]n acting as a parallel shunt resistance to the sandwich structure which may results in lower GMR. For a 400 ╟C annealed sample plotted on similar axes the GMR shows an upward shift and much better improvement, preferably as high as 33%, with the mode of the graph remains unchanged. The effect of argon gas rate injected into the deposition chamber was also studied. Initially, a small rise and fall in GMR was observed resulting in a 11% peak between the Ar gas rates 8-15 sccm, with the curve
sloping down gradually until the upper limit of 30 sccm. Such a variation may be attributed to the improvement of Co and Cu crystals formed during the 10 sccm Ar rate. GMR is also observed to increase with annealing times up to 90 minutes for a temperature of 300 ╟C prior to saturation at 18%. All these results are indicative of GMR dependency on selected experimental parameters.

Gold nanoparticles supported on SiO2 and TiO2: synthesis and characterization

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In recent years, it was found that gold nanoparticles (< 5 nm) supported on metallic oxides are catalytically active for different oxidation and hydrogenation reactions. The catalytic activity of gold nanoparticles depends on particle size and shape, and of the nature of the support. It was propossed that reducible supports lead to more active catalyst than inert support, but some authors claim that supported gold particle with the same size present similar activities in both reducible and inert supports. We have prepared small gold particles on Au/SiO2 and Au/TiO2 by deposition-precipitation, and cation and anion adsorption methods. The substrates used were commercial TiO2 (Degussa) and SiO2 prepared by ultrasonic assisted sol-gel method. Au/SiO2 was prepared from a TEOS/HCl4Au mixture submmited to ultrasonic irradiation. Characterizations of Au/SiO2 and Au/TiO2 materials by TEM, HRTEM, DTA-TGA and by FT-IR, Raman spectroscopies will be presented.

Enhanced antibacterial and photcatalytical properties of Fe+3 doped TiO2 sol-gel thin films deposited on carbon nanotubes

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Fe+3 doped TiO2 based nanostructured thin films have been prepared by the sol-gel process and applied on to previously carbon nanotubes coated quartz substrates. The as deposited films and annealed films have been characterized for structural and morphological properties by employing X-ray diffraction and field emission scanning electron microscopy techniques. The antibacterial activity against E-coli and S. aures has been examined applying the so-called antibacterial drop test. The bactericidal activity for the above bacteria cells was estimated by relative number of bacteria survived calculated from the number of viable cells, which form colonies on the plates. The films exhibited enhanced antibacterial properties when compared to carbon nanotubes films filled with Fe+3 alone. The influences of Fe+3 dopant concentration, annealing temperature on the films structure, thickness of thin films, have been investigated.

Characterization of nanostructured materials by X-ray Line Profile Analysis

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For the characterisation of micro- and nanostructures in bulk as well as in loose powder materials the X-ray Line Profile Analysis (XPA) has proven to be an excellent method. In the last two decades not only the evaluation procedures have been improved extensively, but also the instrumentation like X-ray generators, monochromators and detectors have been developed furthermore, not to forget the unique properties of Synchrotron radiation.An ideal diffraction profile is a narrow, symmetrical, delta-function like peak at a particular position in reciprocal space and corresponds to a well defined unit cell. Different irregularities in the microstructure of the material usually cause deviations from the ideal shape: (i) shift of peak, peak broadening and asymmetry. Here we will focus on size and strain broadening as these are the most important regarding nanomaterials and their production.According to the kinematical theory of scattering, diffraction profiles are the convolution of the size and distortion profiles. After Fourier transformation the Warren-Averbach equation results [1]. Size broadened profiles can be described by assuming (i) a size distribution function and (ii) the shape of crystallites or of coherently scattering domains. From a log-normal size distribution function f(x), which is given by the median m and the variance s, the arithmetic-, the area- and the volume weighted average crystallite diameters can be evaluated [2].In the case of strain broadening the major task is the description of the mean square strain. Phenomenological and also dislocation models have been designed to describe the diffraction vector dependence of the mean square strain [3, 4]. This way the density and distribution of dislocations can be determined even for very high densities.The universal character of the method are documented by several examples, ranging from sintered ceramic powder to electrodeposited Ni, the main focus is dedicated to the microstructural characterization of nanostructured materials produc
ed by severe plastic deformation (SPD).[1] Warren, B. E., Progr. Metal Phys. 1959, 8, 147.[2] Hinds, W. C., Aerosol Technology: Properties, Behavior and Measurement of Airbone Particles, Wiley, New York, 1982.[3] Ungár, T.; Borbély, A., Appl. Phys. Letters, 1996, 69, 3173.[4] Ungár, T.; Ott, S.; Sanders, P. G.; Borbély, A.; Weertman, J. R., Acta Mater. 1998, 10, 3693.

Prototype Commercial Devices from Piezoelectric Nanotubes: Ink-Jet Print Heads and Self-trenched 200:1 Aspect-ratio Capacitors for DRAMs

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We have designed and fabricated high-dielectric piezoelectric nanotubeswith concentric cylindrical electrodes. A discussion is given on the electroding, comparing Pd-acetate, AgBr, and Ru-DER deposition. Applications include ink-jet print heads capable of sub-picolitre droplet delivery, drug-delivery systems, (monodisperse asthma inhalers), and a variety of micro-fluidic activators, plus very high aspect-ratio DRAM capacitor trenching. This work has been carried out with and funded by industry partners in the UK and USA. As a result much of it remains proprietary. The details disclosed will depend upon the timing of patent disclosures in late 2004 and early 2005.

Plasma Coating and Magnetic Alignment of Carbon Nano Fibers in Polymer Composites

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In order to well disperse carbon nanotubes in polymer composites, they have been coated by a unique plasma polymerization method. In this presentation, we will present our recent experimental results on the plasma coating of carbon nanotubes. An extremely thin layer of polymer film has been coated onto both outer and inner surfaces of the nanotubes. Due to surface modification, the dispersion of nanotubes in the polymer matrix is significantly enhanced. HRTEM images, SIMS results of coated surface films on nanotubes, and mechanical properties of the composites will be presented. For fundamental study and novel engineering applications, carbon nanotubes also need to be aligned along certain specified directions. Single wall carbon nanotubes, due to small amount of catalyst elements such as Ni and Co, can be well aligned in a magnetic field. However, the extremely small magnetic susceptibility of multi wall carbon nanotubes is not sufficient to induce a magnetic alignment. In this study, we present a novel method by which these nanotubes can be well aligned in a polymer matrix at moderate magnetic field. Both TEM and SEM results show clear evidence of well aligned nanotubes in the polymer composite. Mechanical testing results have also shown pronounced anisotropy in tensile strength in directions normal and parallel to the applied field, confirming an alignment of the nanotubes in the sample matrix. The magnetic alignment mechanism is discussed.

Enhanced mechanical behaviour in nanometric layers of zirconia

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Pure zirconia is an interesting technological material because of its outstanding mechanical and electrical properties. This material possesses an high melting point which allows its use as thermal barrier in airplane reactors. Moreover, its important dielectric constant (about 12) makes this compound a good high-k nanomaterial candidate for high-end electronic devices. However, zirconia single crystals undergo a disruptive tetragonal to monoclinic first order phase transition at about 1200 K, preventing the manufacturing of dense and resistant samples. Nevertheless, a tetragonal phase is generally observed in zirconia nanoparticles at room temperature and under atmospheric pressure. Understanding the quenching mechanism of this tetragonal phase is a key issue for elaborating the dense samples of pure zirconia required for these mechanical and electronic applications. Starting from experimental observations (neutron scattering, electron diffraction, spectroscopic tecniques, ...) a comprehensive model, within the Landau theory, is developed to describe the microscopic mechanisms responsible for the modificatons of the phase diagram. This model suggests an unusual strong coupling between the atomic displacements (phonons) and the mechanical strain field. The model actually predicts the quenching mechanism of the tetragonal phase observed in zirconia nanocrystals but it also explains the behaviour of zirconia samples submitted to intense ion radiation. The predictions of this model are not only important for understanding the behaviour of zirconia in nuclear reactors but they also also the stability of nanometric zirconia thin films in electronic devices operating in spacecrafts or in the high atomosphere. These results clearly suggest that ion irradiation seems to be an efficient way to produce dense nanometric layers of tetragonal zirconia.

MECHANICAL AND CREEP PROPERTIES OF ELECTRODEPOSITED NICKEL AND ITS PARTICLE-REINFORCED NANOCOMPOSITE

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The main objective of this work is to report the results of a study of microstructure-mechanical and creep property relationships of electrodeposited nanostructured unreinforced nickel and its composite (monolithic nickel reinforced by laser-generated SiO2 nanoparticles). The results of tensile tests at room temperature showed no substantial improvement in yield strength and modulus of elasticity for electrodeposits compared to conventional polycrystalline Ni. On the other hand, the electrodeposits exhibited higher values of the ultimate tensile strength than their coarse-grained counterpart. The results of tensile creep testing of both the electrodeposits at room temperature and 473K indicated that under these loading conditions power-law creep becomes the predominant deformation mechanism instead of diffusion creep. Creep resistance of a composite is higher than that for a monolithic electrodeposited nickel.

NANOCOMPOSITES ON BASIC SYSTEM ⌠THERMOSTABLE HIGLY-DISPERSED METAL (-Fe) √ SILICA■ AND REGULATION OF THEIR HEAT STABILITY

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The following oxides obtained at 280C and reduced by H2 at 450C to produce metal on the surface of silica were compared: · samples with iron-oxygen monolayers (1, 2, and 4, 3√15 Å thick) deposited on silica √ series 1; · samples with iron oxide on silica (microcrystals not greater than 200Å) on silica √ series 2;
Increase in temperature of reduction (higher than 450C) yielded in a remarkable sintering of iron and in decreased specific surface area (from 540 to 200 m2/gFe). To avoid crystallization of metal at higher temperature we tried to stabilize iron atoms obtained by reduction by the element-oxygen monolayer (sublayer) of a difficultly reduced element (Al, W). It was found that for the samples of series 1 with the sublayer till 800C specific surface area of metallic iron is high and almost constant (500 m2/gFe).

3D Numerical Simulations of the ECAE Process

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Numerical simulations of ECAE process carried using DRACON code (VNIIEF) based on variation-difference method of solving continuum mechanics equations have shown that satisfactory agreement between experimental and numerical data on deformed billet state can be achieved by using experimental data in the development of physical model. Issued analysis of billet shape influence on uniform state in ECAE

Development of ceramic molecular membranes to separate hydrogen from high temperature CO-containing flow for fuel cell-based plant application

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The current power machines where solid polymer electrolyte –based fuel cells are applied need materials that would be able to separate H2/CO mixtures at the temperatures ranging 800 to 9000C. The existing techniques to separate these gases employ only the palladium metal molecular membranes which constraints the gas mixture separation temperature (500-5500C). The paper provides findings of tests of ceramic molecular membranes with meso-porous structure of the mean diameter 7 nm, these membranes allowing separation of high temperature H2/CO gas mixtures. The initial experimental models of the disc ceramic molecular membranes were manufactured on the basis of zeolite ZSM-5 with formation of nano pores over the entire volume with sizes required to separate CO and H2. Tests of the membranes were carried out on a special purpose experimental "hydrogen" test bed where the flow temperatures up to 8000C and higher with pressure up to 2 MPa could be achieved, the water vapor effect on the membrane material could be studied, etc. On the basis of the developed and tested membranes, membrane devices can be designed, manufactured and studied which will allow expansion of application of solid polymer fuel cells to industry at the expense of use of natural gas instead of pure hydrogen both as independent power sources and at application of solid polymer fuel cells as a part of hybrid engines through which the efficiency of the power systems can amount to 55-65% and higher.

Microstructural evolution in commercial aluminium alloys during ECA pressing and subsequent heat treatment

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The microstructures of an Al-2024 (Al-Cu-Mg) alloy and a spray-cast Al-7034 (Al-Zn-Mg-Cu) alloy, processed through equal-channel angular pressing (ECAP), were studied using electron back-scatter diffraction (EBSD) and differential scanning calorimetry (DSC). The solutionising and age hardening and recrystallisation softening post-ECAP were studied by hardness testing and DSC. The EBSD results demonstrate there is a relatively rapid increase in the fraction of high-angle boundaries during the initial ECAP passes and a subsequent more gradual increase in further passes. The hardness and DSC results provide evidence for the solutionising and ageing behaviour of the two heat-treatable alloys. The crystallographic textures and their rotations during ECAP are analysed through EBSD.

Nanostructured ZnO and ZAO transparent thin films for gas sensing applications √ Surface Characterization

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Zinc oxide (ZnO) and aluminum zinc oxide (ZAO) transparent thin films with different thickness were prepared by dc magnetron sputtering technique using metallic and ceramic targets onto silicon and Corning glass substrates. Surface investigations carried out by Atomic Force Microscopy (AFM) and X-ray Diffraction (XRD) shown a strong influence of deposition technique parameters on the film surface topography. Film roughness (RMS), grain shape and dimensions were found to correlate with the deposition technique parameters as well as with the material. The results revealed also that the target composition has a radical effect on ZnO and ZAO film characteristics. XRD measurements proved that the films grown by dc magnetron sputtered are amorphous. The thin films sputtered from ceramic target AFM analysis shown a completely different surface behavior compared with the films grown from metallic target and the presence of hexagonal shaped grains of about 25 nm for the case of Zn. This work is demonstrating that the film surface characteristics are determined by the growth conditions. The gas sensing characteristics of these films are strongly influenced and consequently may be enhanced by the control of the film growth parameters.

Ni-Fe nanowire arrays and their magnetic properties

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One-dimensional (1D) nanomaterials have attracted great interest and research, because of their unique properties relative to the bulk ones and potential practical applications in the areas such as nanoscale electronic and optoelectronic devices, high-density magnetic memories. In this work, we report on magnetic properties of highly uniform Ni-Fe nanowire arrays fabricated using electrochemical deposition into the nanochannels of porous anodic aluminum oxide (AAO) template. The crystal structure, morphology and filling degree of AAO pores was evidenced by X-ray diffraction (XRD), scanning and transmission electron microscope (SEM, TEM), X-ray energy dispersive spectroscopy (EDS) and electron diffraction (ED). The magnetization measurements of the nanowire arrays were carried out at room temperature on a vibrating sample magnetometer (VSM) with the applied field either perpendicular or parallel to the surface of the samples. The coercivity was obtained from the hysteresis loop. The pores of AAO template are uniform and approximately 90 % of the pores are filled with nanowires. The Ni-Fe nanowires have polycrystalline structure and their diameter is about 50 nm. Magnetic measurements show that the magnetic coercivity for the applied field parallel to the nanowires is larger than that for the applied field perpendicular to the nanowires.

Calcium - poly (9,9-dioctylfluorene) interaction, a theoretical study

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The geometric and electronic structures of poly (9,9-dioctylfluorene) (PFO) oligomer interacting with Ca atoms have been studied using a Mшller-Plesset Perturbation Theory. A weak interaction with little charge transfer and with a pretty long Ca-C distance (about 4.0 E) is found when only one Ca atom attaching to a PFO unit. However, when two Ca atoms are adsorbed at a PFO unit, a strong interaction with a shorter Ca-C distance (about 2.67 E) takes place with considerable charge transfer from the Ca atom to the PFO and with significant deformation in the backbone of PFO oligomer. In the latter case, the frontier orbitals of PFO are modified. However, the deformed PFO and its modified frontier orbitals can be recovered when oxygen is added, in good agreement with experimental observation.

Peculiarity of nanolevel structuring in synthesis of novel functional solids and nanostructured materials

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The central conception of the communication consists in the idea that the most promising approach to use untapped reserves of property improving of the most advanced materials, specifically of structured composites, is based on the molecular level control of structuring chemical processes. Present state and perspectives of investigations in the field of high precision solid state chemical synthesis of highly organized nanostructured solids and solid materials of various levels of macroscopic organization are discussed. An accuracy of the synthesis is ╠ 0.1 nm. The notion of ⌠topology■ is proposed to describe solid compounds. The use of the notion allows to take into account various space distributions of atoms of synthesizing substance. We give an example of nanostructured materials: magnetic materials, adsorbents, nanostructured metallic materials √ of highly-organized structures of ⌠a frame-within-a frame■ (iron based composites reinforced by regulating carbide frame).

LOW TEMPERATURE MECHANICAL PROPERTIES OF NANOSTRUCTURED TITANIUM OF DIFFERENT COMMERCIAL PURITY PRODUCED BY EQUAL CHANNEL ANGULAR PRESSING

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Low temperature yield stress and strength have been studied of the nanostructured Ti (average grain size d~0.3 ─) of the different commercial purity: Grade 2 (O2 ┘ 0.16 % weight), VT1-0 (O2 ┘ 0.17 % weight), and Grade 4 (O2 ┘ 0.34 % weight) under uniaxial tension and compression (with the 0.0004 s-1 strain-rate) at 300, 77 and 4.2 K. Specimens for mechanical testing were cut from bars both parallel (||) and perpendicular (^) to the ECAP axis. High low temperature yield stress and strength at 300-4.2 K are obtained, which are dependent on the oxygen content. Increasing of the oxygen content from 0.16 % to 0.34% increases the strength on 13 % at 300 and on 9% at 77 K, with retaining high ultimate plastic deformation. Plastic deformation values to neck formation under tension (─neck) increase with temperature decreasing from 300 to 77 K and depend on the purity of the nanostructured Ti (30% for Grade 2 and 8% for Grade 4 at 77 K). Deformation was of a serrated character at 4,2 ─. The yield stress ─0 asymmetry at 300 and 77 K has been observed: the ─0 values of Ti Grade 2 under compression are 1.38 (300 K) and 1.22 (77 K) times larger comparing to the tension results. Under the compression of the different type of Ti at 77 and 4.2 ─ the failure took place by the catastrophic plastic shear sliding-off of one part of the sample relative to another.

SOLUBLE FUNCTIONALIZED CARBON NANOTUBES

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The organic functionalization of carbon nanotubes (CNT) has opened new avenues with opportunities to fabricate novel nanostructures by improving both their solubility and processibility. Our recent success in CNT functionalization based on the 1,3-dipolar cycloaddition of azomethine ylides, led us to pursue the covalent linkage of various functionalities. A central aspect of nanotube chemistry, which yet awaits exploration, is its function and performance in donor-acceptor ensembles.We report on intramolecular electron transfer reactions in single-walled carbon nanotube (SWNT)-based donor-acceptor ensembles by studying a novel SWNT√ferrocene (Fc) nanohybrid. This result opens the way to use the current examples of SWNT-Fc nanohybrids as integrative components in solar energy conversion. Furthermore, these systems can be used as chemical sensors and biosensors for the selective recognition and detection of H2PO4√ in organic solutions and the amperometric detection of glucose, respectively.

Test and analyze UV absorbance of TiO2 nanofluid with novel process

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We propose a novel TiO2 nanofluids preparation system (SANSS)*; using de-ionzed water as a medium without any of additives, those indicates the UV-absorbance much higher than any of the traditional TiO2 nanofluids preparation in the same medium condition.*SANSS (Submerged Arc Nanoparticle Synthesis System)1.Tsing-Tshih Tsung,Ho Chang, Liang-Chia Chen, Lee-Long Han, Chih-Hung Lo, Ming-Kun Liu, Development of Pressure Control Technique of An Arc Submerged nanoparticle Synthesis System (ASNSS) for Copper Nanoparticle Fabrication(Materials Transactions, Vol.44.No.6(2003) pp.1 to 5, C2003 The Japan Institute of Metals). (SCI).2.Tsing-Tshih Tsung, Ho Chang,Liang-Chia Chen,Ming-Kun Liu,Hong-Ming Lin, Chung-Kwei Lin, Process Development of a Novel Arc Spray Nanoparticle Synthesis System (ASNSS) for Preparation of TiO2 Nanoparticle Suspension, accepted and will be published in International Journal of Advanced Manufacturing Technology,#2060. (SCI)

Experimental study on the thermal properties of the brines with nanoparticles

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The major objective of this paper is to study thermal properties of brine with nanoparticles. There are two kinds of nanofluids that are produced by Submerged Arc Nanoparticle Synthesis System (SANSS). Water and ethylene glycol are used as based solvent. The nanofluids, i.e. aqueous solutions of ethylene glycol are made with different concentrations in volume fraction. Both coefficients of thermal conductivity and diffusivity of the solution are measured with transient hot-wire method. Comparison of the thermal properties between solution with and without nanoparticles is made. Experimental result shows that average thermal conductivity is improved by 6.8% for brine that is made of 1% wt of copper dioxide - ethylene glycol solution. 2.8% improvement if 1% wt is instead of 0.1% wt. of copper. No significant difference is found when thermal diffusivity and specific heat are concerned. Based on our study and analysis, better thermal conductivity of brines with nanoparticles can be expected.

Nanocrystallization of Carbon Steels by Shot Peening and Drilling

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Nanocrystalline (NC) structure in carbon steels were formed by various severe plastic deformation (SPD) processes, i.e. shot peening and drilling. The structural change during nanocrystallization was investigated using SEM and TEM. It was found that the NC structure formed in the specimen surface where the SPD with true strain larger than 7 was applied. The boundary between the NC and work-hardened regions is quite sharp, and the intermediate structure between there regions was not observed. High density of dislocations was observed in the work-hardened region, while the dislocation density in the NC region was low. This suggests that there exist a critical dislocation density at which dislocation-cell structure changes to grain-boundary structure.The detailed structure and properties of the NC structure will be shown and the nanocrystallization mechanism by SPD will be discussed.

Structural and optical properties of BN/Ag/BN and Si3N4/Ag/Si3N4 nanocermet thin films : a comparative study

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Composite media including metallic nanoclusters embedded in a dielectric matrix, also known as ⌠nanocermets■, exhibit a strong absorption band at the surface plasmon resonance (SPR). Optical filters, selective solar absorbers, ultrafast optical switches (due to the enhancement of the third-order non-linear susceptibility at the SPR) are the common technological applications brought up for such materials. The position of the SPR depends on the optical properties of the metal and the matrix but also on the size (weakly) and shape (strongly) of the clusters. In order to tailor the position of the SPR for a given metal and matrix, it is therefore desirable to elaborate nanocermets including clusters of the desired shape.In this study, thin films consisting of silver nanoclusters sandwiched between two dielectric layers are elaborated by ion beam alternate sputtering deposition of the metal and dielectric species. A dielectric layer is deposited first on the substrate. Then, deposition of silver leads to the formation of clusters (Volmer-Weber growth), which are finally covered by a second layer of the same dielectric material.The clusters morphology is then studied as a function of the dielectric compound (Si3N4 or BN, which exhibit similar optical properties) and as a function of the deposited amount of silver, with the help of HRTEM (plane-view and cross-section) and Grazing Incidence Small Angle X-ray Scattering (GISAXS). The main results of this structural study can be summarized as follows: 1 - For a given matrix, clusters can be described as truncated spheroids, which axis ratio (height/diameter) decreases when the deposited amount of silver increases. The coalescence regime has already been reached for the lowest deposited amount of silver.2 - For a given deposited amount of silver, the axis ratio of the clusters is always higher when they are embedded in a BN matrix (BN/Ag/BN films) than in a Si3N4 matrix (Si3N4/Ag/Si3N4 films).The differences between BN/Ag/BN and Si3N4/Ag/Si3N4 films are then discussed on the basis of thermodynamics, growth and coalescence kinetics, with the help of additional experimental results (structural studies of Si3N4/Ag/BN and Si3N4/Ag/BN films, influence of a delay before deposition of the second dielectric layer...).The optical properties of these samples are studied by transmittance measurements. A correlation between structural parameters and optical properties can be made.

Deformation behaviour of nanocrystalline Mg studied at elevated temperatures

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Nanocrystalline Mg samples were prepared by milling procedure in an inert atmosphere and subsequent compacted and hot extruded. The linear grain size of specimens used was estimated by X-ray line profile analysis to be about 100 nm. Compression testing was performed at temperatures from room temperature up to 300 ╟C. Rapid decrease of the yield stress as well as the maximum stress with temperature was estimated. This decrease and the flat character of the stress strain curves at elevated temperatures indicate possible contribution of diffusion process/es. Stress relaxation tests were conducted in order to analyse thermally activated processes occurring during plastic deformation.

Magnetic Properties of Mesoporus Oxides

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The elaboration of materials with regular pore structures on the nanometer level is one of the most active areas of modern materials science. By manipulating synthesis conditions it is now possible to create continuous inorganic structures with regularly spaced voids while also controlling the overall topology of the porous matrix. Mesoporous materials could be at the basis of fundamental discoveries based on nanostructured materials and the interaction on the nanometer scale of very different chemical species. The discovery of stable mesoporous transition metal oxides further expands the potential range for host-guest inclusion reactions that could lead to a near metallic materials through the reduction of the pores structure. Although very little is known about the properties of these materials, recent work has shown that the inorganic framework of mesoporous niobium oxide acts as an electron acceptor, making it the first reducible molecular sieve. Moreover, with a surface area as high as 495 m2/g for meso tantalum oxide and 700 m2/g for meso niobium oxide, these new metal oxide structures differ substantially from other metallic systems which normally have a much reduced surface area. Recently we studied the intrinsic magnetic properties of mesoporous Ta and Nb oxide. Because of the high specific surface of these materials they are very sensitive of environment impurities such as water molecule, CO2 or other adsorbed species present during the synthesis processes. Due to this high surface area, these mesoporous materials can be greatly affected by these adsorbed species, and because of the charge transfer between these species and the wall structure of the mesopores, produce composite materials with very unique and interesting properties. In this presentation we will discussed some of our recent results for these materials and correlated them with thermal analysis using TG/DSC coupled with residual gas analysis as well as with XPS surface chemical analysis using in situ thermal annealing.

SYNTHESIS, CHARACTERISATION AND ADOSRBTION PROPERTIES OF TITANIA BASED ONE-DIMENSIONAL NANOSTRUCTURES

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Nanostructured materials have received a lot of attention because of their novel properties, which differ from those of the bulk materials. One-dimensional materials are an important category of nanostructured materials and have been widely researched yielding various special structures like nanotubes, nanorods, nanobelts and nanowires [1]. The materials in the nanotube form can be prepared from carbon, MoO3, Al2O3, MoS2, WS3, ZrO2 and NB, of which titania (TiO2), is one of the most extensively researched materials.Titania as a semiconductor, shows high photocatalitic activity and it is widely used as a catalyst and carrier of catalyst [2]. In addition, titania finds applications in the fileds of sensors, new type of solar cells, electrochromic devices, and antifogging and self-cleaning devices. The performance of titania in various applications depends on its dimensions, morphology and crystalline phase state. In recent years the materials has also been extensively studied as photocatalyst to deal with pollution, water purification, wastewater treatment, hazardous waste control, and air purification. Titania based 1D nanostructures were prepared hydrothermally treating anatase TiO2 powder with a NaOH solution. Figure 1 a) is a TEM image of as prepared TiO2 based nanotubes. From the TEM image is evident that both, open and closed end nanotubes were obtained. Titania based nanotubes prepared in our process have a diameter between 10-20 nm and in length can reach up to 500 nm. Figure 1 b) is an AFM image of TiO2 based nanowires. Nanowires are in comparison much longer and they can reach in length up to 4 μm, respectively. Their diameter is found to be between 25-35 nm.FIGURE 1. A) TEM image of TiO2 based nanotubes. The estimated diameter of tubular nanostructures is found to be between 10 to 20 n. B) AFM image of TiO2 based nanowires.NO2 is a primary component of NOx gases, which are beside CO and SO2 considered as greenhouse gases. As a very reactive gas NO2 in the air reacts readily with common o
rganic chemicals and even ozone, to form a wide variety of toxic products [3]. In view of that, we decided to investigate the adsorption properties of recently discovered TiO2 based nanotubes toward NO2. 1D nanostructures on the base of TiO2 were exposed to NO2 gas. A stronger adsorption of NO2 gas was observed in the case of nanotubes. A stronger adsorption was expected in the case of nanotubes since their specific surface area is for factor 10 higher that one of nanowires. The adsorption of NO2 was investigated with ESR technique, which enabled us to bild a picture of the surface properties of the TiO2 based nanotubes and nanowires and the way NO2 molecules are adsorbed. ESEEM experiments clearly demonstrate that the surface of nanotubes and nanowires must be hydrated. On the other hand the EPR lineshape anaylisis seems to be consistent with the oxygen attached to the surface. The average distance between the paramagnetic centreandhe hydrogen atom abtained from the ESEEM experiments suggest that the oxygen atom in the NO2 gas relatively strongly attach to the site Ti-OH.References:[1] M. Graetzel M., Nature 353 (1991)736.[2] R. Wang, K. Hashimoto, A. Fujishima, Nature 388 (1997) 431.[3] F. A. Cotton, G. Willkinson, Advanced Inorga

The New SPD Processing Routes to Fabricate Bulk Nanostructured Materials

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Keywords: severe plastic deformation, bulk nanostructured materials, nanocrystallization

Since the mid-1990's the fabrication of bulk nanostructured metals and alloys using severe plastic deformation (SPD) has been evolving as a rapidly advancing direction of modern materials science that is aimed at developing materials with new mechanical and functional properties for advanced applications. The principle of these developments is based on grain refinement down to the nanoscale level by various SPD techniques. However, within recent years SPD techniques have been applied for producing bulk nanomaterials using some other principles, namely, SPD-consolidation of powders, including nanostructured ones, as well as SPD-induced nanocrystallization of initially amorphous alloys. This paper is focused on investigations and development of these new SPD processing routes enabling fabrication of fully dense nanocrystalline metals and alloys with a mean grain size of 20-30 nm and homogenous microstructures. We consider physical principles of these routes and present results on the microstructural characterization of several nanocrystalline materials produced as well as on studies of their unique properties.

ORGANIZED ARCHITECTURES OF CARBON NANOTUBES FOR APPLICATIONS

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After more than one decade of extensive and fruitful investigation, carbon nanotubes and the nano- and micro-structures tailored from them still remain one of the most promising, interesting and challenging structures in nanotechnology. This fact is a consequence of the lack of full knowledge of the physical and chemical properties of these systems, and the lack of well-defined macroscale samples. In this talk I will describe our efforts and results on the directed assembly of carbon nanotubes using different approaches, namely chemical vapor deposition of single and multiwalled structures on planar substrates, growth of nanotube links between pillars and template based growth of multiwalled nanotubes. I will also describe our experiences for modifying carbon nanotube structures with focused ion beam irradiation and solvent treatment of singlewalled and multiwalled structures, respectively.
I will also talk about several characterization methods and applications of nanotube architectures. I will show our result on electrical, optical and thermal characterization of different nanotube structures. I also will present an application, where an as grown carbon nanotube large structure was used as a filter, applicable to filter different chemicals as well as biological contamination from water.

Nanostructured metal oxides prepared by aqueous solution routes

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The research presented here is focussed on entirely aqueous synthesis routes for (multi)metal oxides as thin films and nanoparticles. Chemical solution routes have the advantage of being very flexible since the synthesis parameters can easily be modified in order to achieve a more precise control of composition, shape, size and desired end properties. Moreover, the use of water as a solvent, the relatively cheap starting materials and the low cost equipment are significant additional ecological and economical advantages.
In this presentation the influence of synthesis parameters on the end properties and characteristics of diverse nanostructured multimetal oxides that have been prepared by aqueous solution routes will be exemplified. Research areas include a. o.
- nanoparticles of ZnO, ITO, Al2O3, Y-stabilised ZrO2
- Nanocomposites with improved mechanical properties and gas permeability.
- Nanocoatings
- Inorganic (TiO2) and hybrid photovoltaic devices (dye sensitized solar cells)
- ferroelectric capacitors with thin films of SrBi2Ta2O9 (SBT), SrBi2Nb2O9 (SBN), Pb(Zr0.53,Ti0.47)O3 (PZT) and (Bi,La)4Ti3O12 (BLT)
- RuO2 and SrRuO3 thin films as conductive oxides

The focus will be put on the potential of the solution synthesis methods in nanotechnology: rapid screening of different material compositions for nanostructured multimetal oxides, the possibility of preparation of both films/coatings and nanoparticles, easy technology transfer, etc.

Structural and magnetic studies of Mn3O4 nanoparticles

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Nanocrystalline Mn3O4 hausmannite has been prepared by a simple dissolution of manganese(II) acetate salt in a solvent mixture of N,N▒-dimethylformamide (DMF) and water (10%) at room temperature, without post-treatment of heating. The stability of the Mn3O4 colloidal dispersion was monitored by UV-visible electronic absorption spectroscopy. X-ray powder diffraction (XRD) pattern demonstrate its good phase purity. Transmission electron microscopy (TEM) image shows homogeneous nanorods with a narrow size distribution. The average diameter and length are 6.58 nm and 17.44 nm respectively. Magnetic properties of the Mn3O4 nanoparticles were studied by using a superconducting quantum interference device (SQUID), finding a ferromagnetic behavior at low temperatures, whereas they were paramagnetic at room temperature. Under zero√field cooling (ZFC) measurement at 100 Oe, the observed blocking temperature TB was 37 K.

Recent Progress in Superhard Nanocomposites

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After a brief overview of earlier work I shall show the differences in the properties of coatings where the superhardness results from energetic bombardment during their deposition, and superhard nanocomposites with high thermal and oxidation stability which were prepared according to our generic design principle. This principle will be explained with reference to the thermodynamic and kinetic constrains required for the successful reproduction of the results1. The second part of my talk will be devoted to the presently ongoing discussion regarding the possible reason of the lack of reproducibility of our results, as claimed and published by other workers. On the basis of several recently published papers I shall show that the reason of the lack of the reproducibility was either an inappropriate choice of the deposition conditions, such as too low nitrogen pressure and/or deposition temperature in contradiction to our recipes described and justified in 1, or impurities, as also published some time ago2. After clarifying these issues I shall concentrate on, a) the recent studies of the phase segregation during the deposition and, b) on the modelling of the mechanical properties of these materials by means of advanced finite element method (FEM).

a) The thermally activated relaxation phenomena within the grain boundaries were studied by means of internal friction measurements. It was shown that superhard nanocomposites that were deposited according to our design principle have a stable nanostructure and, therefore, show no internal friction peak. In contrast, coatings in which the phase segregation was not complete during the deposition because of inappropriate choice of the conditions show internal friction peak associated with the relaxation of the nanostructure towards the stable state upon post-annealing. Recent thermodynamic calculations and experimental results confirmed the spinodal nature of the phase segregation in the TiN-Si3N4 as suggested earlier.

b) An advanced FEM based on a new constitutional material model that accounts for the pressure dependence of elastic moduli and flow stress (as suggested recently3) allows us to model the non-linear behaviour of these materials the operate under extreme conditions. It is shown that the conventional linear mechanics that uses constant moduli and yield stress cannot describe such behaviour. This calls also for the development of new concepts for the evaluation of correct values of hardness from the load-depth-sensing indentation technique.

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MULTISCALE SIMULATIONS AND EXPERIMENTS OF ZEOLITE NANOPARTICLE SELF-ASSEMBLY AND GROWTH

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Understanding hierarchical supramolecular-precursor assembly to form complex organic-inorganic nanostructures with crystalline order is central in synthetic efforts for new materials ranging from substrates for quantum confinement and laser applications to biomaterial implants with controlled porosity and microstructure. The synthesis of pure silica zeolites in the presence of organic cations is one of the simplest examples of such a hierarchical assembly process. It involves cooperative weak interactions (e.g., van der Waals forces between the inorganic fragments and the organic ions) directing the formation of a covalently linked periodic oxide framework. Despite intensive work devoted to zeolite growth, the nucleation and growth mechanisms remain poorly understood. In this talk, the nucleation and growth mechanisms of zeolite nanoparticles will be discussed. First, experimental results of the silica phase behavior driven by self-assembly processes will be discussed ranging from small angle neutron scattering (SANS) and x-ray scattering (SAXS) to NMR to dynamic light scattering (DLS) to microscopy and XRD. It is shown that nanoparticles of silica in the range of 2-5 nm form that have a core of silica and a monolayer shell of template. Then, a variety of ab initio, molecular dynamics and continuum scale simulations will be presented to analyze these experiments and predict templating effects. For example, we are able to show that the templates stabilize silica nanostructures by shielding the Si-O-Si bonds. Results will be presented for the silicalite-1 (the purely siliceous form of zeolite ZSM-5).

Well Aliened and Size Controlled Fabrication of ZnS Nanowires on AAO Templates and Their Lasing Properties

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High-density and uniform-sized gold particle arrays have been prepared electrochemically on anodic aluminum oxide (AAO) templates. The gold particles were used as catalysts to synthesize ZnS nanowires. The as-grown nanowires had a wurtzite single-crystal structure and were aligned perpendicularly to the AAO template. The diameter of the nanowires can be controlled by the size of gold particles embed in AAO. Under high-power density optical excitation (266 nm), the nanowire array showed an intense, narrow [full width at half maximum (FWHM) of 2.2 nm] photoluminescent peak at 338 nm composed of a superposition of optical resonant modes (FWHM similar to0.3 nm) resulting from the collective emission of a large number of nanowires. These results indicate that the ZnS nanowires act as optical waveguide resonators.

DISPERSION OF NANOPHASE TITANIA IN POLY-LACTIDE-CO-GLYCOLIDE PROMOTES OSTEOBLAST FUNCTIONS: ORTHOPEDIC COMMERICAL APPLICATIONS

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Nanotechnology offers exciting alternatives to traditional bone implants since bone itself is a nanostructured material composed of nanofibered hydroxyapatite well-dispersed in a mostly collagen matrix. For this purpose, nanometer grain size titania was dispersed in a poly-lactide-co-glycolide (PLGA) matrix by various sonication powers from 0 W to 332.5 W. Osteoblast (bone-forming cell) adhesion and subsequent functions on nanophase titania/PLGA composites were investigated in vitro. Results demonstrated that the dispersion of nanophase titania in PLGA was enhanced by increasing the intensity of sonication and that greater osteoblast function leading to bone regeneration was correlated with improved nanophase titania dispersion in PLGA. In this manner, the present study demonstrated that PLGA composites with well-dispersed nanophase titania can improve osteoblast functions necessary for increased orthopedic implant efficacy. Commercial applications of such materials in the orthopedic industry will also be presented.

Nanocrystalline gamma-TiAl based microalloyed coatings as gas corrosion barriers

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ɼ-titanium aluminide is a promising structural material for use in automotive and aircraft applications due to its low density and creep and a relatively high strength even at the temperature as high as 1200 K, however its resistance to gas corrosion at high temperatures still needs to be improved. It has been proved in the work by means of SEM, EDS, EBSD, X Ray and microthermo-gravimetric analyses at 1173 K that a great improvement of this resistance has been achieved due to Ag or Cr or Nb or Mo or Si or Ta microalloyed gamma-TiAl based magnetron sputtered coatings: the parabolic rate constant of the oxidation of some nanocrystalline coatings is six orders of magnitude less than that of the bare gamma-TiAl substrate.

Surface reaction of (CH3)2S on Rh nanohole surface

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We have investigated the adsorption behavior of (CH3)2S on Rh nanohole surface by S K-edge NEXAFS (Near-Edge X-ray Absorption Fine Structure) and XPS (X-ray Photoelectron Spectroscopy) measurements. The Rh nanohole surface is synthesized by use of the spin coating technique and annealing at high temperature. The nanohole structure depends on annealing temperature. We have measured the nanohole size by means of AFM (Atomic Force Microscopy). The diameter of the nanoholes are from several 10nm to 100nm. It seems that this surface has a high reactivity for the desulfurization of the sulfur-including molecule. In this study we have investigated the interaction between molecular (CH3)2S and Rh nanohole surface at from 80K to 1000K by NEXAFS and XPS techniques.

Highly Preferred Oriented Lead Barium Titanate Thin Films using Acetylacetone as Chelating Agent in a Sol-Gel Process

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Ferroelectric (Pb1-x,Bax)TiO3 (PBT) materials can be synthesized by a sol-gel process incorporating acetylacetone as a chelating agent to form ligand with titanium isopropoxide. It was found that at a lower content of water, a slower rate of hydrolyzation occurred, which caused to a slower shift rate in the condensation. Therefore, a less cross-linking gel that pyrolyzed easily was observed. This less cross-linking gel could be converted to perovskite phase at temperatures as low as 450 oC. A high purity of (Pb0.5,Ba0.5)TiO3 powder was obtained at 500 oC, with a nano-meteric size of about 30-50 nm the specific surface area of 21.91 m2/g. Furthermore, a highly oriented PBT thin films were obtained by utilizing the as-prepared sol spin-coating on (100) MgO substrate. The oriented films were synthesized from all compositions between x = 0.2 and x = 0.8, at a crystallization temperature of 600 oC. In particular, for the Ba content in the range of x = 0.5~0.6, highly preferred (001)/(100) planes were observed.
Keywords: (Pb1-xBax)TiO3, sol-gel, acetylacetone, preferred oriented, thin films.

Free Volume Control of the Cast Zr-Cu-Al Glassy Alloys

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Relative difference of free volume of bulk glassy alloy (BGA) can be estimated by density measurement using the same rod shape.In order to decide the standard (as crystalline state), we use ideal solution with close packed structure as mixed faced centered cubic and hexagonal close packed structures. We define the free volume to be a volume expansion ratio from the ideal solution to glassy state. Therefore, the free volume as cast state can be divided into two factors, one is the minimum required free volume for amorphization, and the other is the excess free volume. | @ | @The origins of the strength and toughness in Zr-Cu-Al ternary BGAs are considered as Zr-Al networks and excess free volume, respectively. Therefore, we controlled excess free volume in glassy alloys by small additive elements to enhance the toughness. Especially, the increase of excess free volume brings about significant improvement of fatigue properties.

Synthesis and characterization of SiC nanowires and SiC/ZnO nano-heterostructures

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SiC is a suitable material for the fabrication of electronic devices operating at high power, high temperature and high frequency due to its unique physical, mechanical and electronic properties. Cubic phase SiC nanowires were synthesized in large quantity by simply heating NiO catalyzed Si substrates in the growth temperature of 1000 √ 1100 ╟C. A carbothermal reduction of WO3 provided reductive environment and carbon source to synthesize crystalline SiC nanowires. SiC nanowires were 20-50 nm in diameter and the as-grown nanowires were coated with SiO2 sheath of 20 nm thick. The grown nanowires were characterized using SEM, TEM, EDX and XRD. Also, the electron field emission of the SiC nanowires and core-shell SiC-SiO2 nanowires was investigated and the results showed excellent field emission properties. The turn on field at the emission current density of 10 mA/cm2 was below 4 V/мm and it showed uniform emission image. Heterostructures of ZnO nanorods(NR)/SiC nanowires(NW) were also produced using metal-organic chemical vapor deposition. Atomically abrupt interface was observed at the heterojunction of ZnO NR/SiC NW. The photoluminescence (PL) of aligned ZnO nanorods will be discussed as well.

Growth and characterization of Hf-silicate nanofilms

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Hf-silicate is a promising alternative gate dielectric for replacing SiO2, a conventional gate oxide for CMOS (complementary metal oxide semiconductor) device. In this work we present the growth of Hf-silicate nanofilms by atomic layer chemical vapor deposition (ALCVD) using TDEAHf(tetrakis-diethylamido-hafnium, Hf(N(C2H5)2)4) and TBOS(tetra-n-butyl-orthosilicate, Si(OBu)4) as source materials. The physical and chemical properties of the nanofilms were characterized using x-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), and transmission electron microscopy (TEM). Also, the capacitance √ voltage (C-V) and leakage current √ voltage (I-V) properties of the films were characterized.

New Electrode Materials for Direct Methanol Fuel Cell Using Hierarchical Nanoporous carbon with Mesoporous Wall

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Synthesis of macrostructurally patterned highly ordered fully interconnected hierarchical nanoporous carbons with uniform mesoporous walls has been demonstrated by template replication of aggregates of the small silica particles as molds, which were also templated by self-assembled ordered lattice of larger monodisperse polystyrene spheres. The size of the large macropores can be manipulated by controlling the diameter of the polystyrene spheres, while the size of the small mesopores and the overall specific surface area are determined by the silica particles. The mesopores can be easily regulated in the full mesopore range by proper size control of the silica particles. Due to unique structural properties of the nanoporous carbon with fully interconnected ordered uniform bimodal porosity and high surface area, the carbon could work as an excellent catalyst support, resulting in great improvement for methanol oxidation activity in direct methanol fuel cell.

Synthesis and Sintering Behavior of Oxide Coated Iron Nanopowder by Plasma Arc Discharge Process

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Oxide phase coated Fe nanopowders were fabricated by plasma arc discharge process and their sintering behavior has been investigated in this study. The surface passivated PADed Fe nanopowder by ~5 nm thickness of iron oxide layer has 20~200 nm in size and was completely dispersed without particle agglomeration. The oxide layer was removed during the initial sintering stage in hydrogen atmosphere and the hydrogen reduction of oxide layer enhanced the initial densification rate by the volume shrinkage for oxide to metal phase transformation. After hydrogen reduction, the densification rate was slightly retarded even at high temperature. The densification process of PADed Fe nanopowder was studied by means of thermal analyses and microstructural development.

Fabrication of Bimodal Porous Silica With Zeolite Core/Mesoporous Shell and Corresponding Nonspherical Hollow Carbon Capsules

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There has been great deal of interest in creating core-shell composite materials and capsules with tailored structural, optical and surface properties using spherical nanoparticles as molds. Various procedures have been applied to fabricate uniform coated and stable colloidal particles. Herein we would like to report the fabrication of dual porous silica with ZSM-5 zeolite core/mesoporous shell by forming a uniform mesoporuos shell over the respective psedo-hexagonal prismatic zeolite crystal core. The carbon capsules with hollow core/mesoporous shells were also fabricated using the dual porous zeolite core/mesoporous shell silica as sacrificial templates. The resulting carbon capsules have bimodal pore systems consisting of a uniform psedo-hexagonal prismatic hollow core and of a mesoporous shell with uniform thickness of 40 √ 50 nm. The dual porous silica with zeolite core/mesoporous shell and the corresponding nonspherical hollow carbon capsules will have potential for wide range of applications including catalysts, adsorbents, electrode materials, and advanced storage materials.

Preparation of magnetic glass-ceramics containing SrFe12O19 nanoparticles

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The samples of glass in systems SrO-Fe2O3-SiO2, SrO-Fe2O3-B2O3, SrO-Fe2O3-B2O3-Bi2O3, SrO-Fe2O3-B2O3-Al2O3 were prepared by a melt-quenching technique. The samples of magnetic glass-ceramics with nano- and submicronsized particles of SrFe12O19 were obtained by the glass heat treatment at temperatures 450-1250 C. It was shown that SrFe12O19 crystallized as plate-like particles with the aspect ratio dependent on the glass chemical composition and thermal treatment conditions. With increasing the annealing temperature the particle size increased, while the aspect ratio demonstrated the tendency to decrease. The particles were observed with aspect ratio from 1.4 to 7.4 and mean size from  10 nm to 1 μm. The thicker grains were characterized by a higher coercive force. Coercive force of the samples grew with the increasing of the annealing temperature reaching a maximum of 2000 - 7300 Oe dependent on the glass composition. That corresponded to nucleation and growth of monodomain particles.

Optical properties of small size semiconductor nanocrystals

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The Optical properties of small Si , Ge and mixed SiGe nanocrystals, are critically reviewed and the latest and more accurate results obtained recently by high level ab initio calculations in Patras are presented and discussed. These calculations have been performed in the framework of time dependent density functional theory (TDDFT) using the hybrid nonlocal exchange and correlation functional of Becke and Lee, Yang and Parr (B3LYP), as well as the sophisticated multi-reference second order perturbation theory (MR-MP2). The accuracy of the MR-MP2 calculations, and by comparison of the TDDFT/B3LYP results, is very high. The estimated largest possible error margin for the optical gap is of the order of 0.3 eV. This level of accuracy allows safe conclusions and interpretations about the origin of the gap, the role of surface oxygen or hydrogen and the critical dimensions for visible photoluminescence of the nanocrystals. The agreement of our theoretical predictions with accurate experimental results is excellent. We demonstrate that the disagreement between experimental results is mainly due to oxygen contamination and/or experimental uncertainties in the determination of the nanocrystal diameter. We also illustrate that the discrepancies between different theoretical results are either due to poor treatment of exchange (and correlation) or to erroneous fitting of empirical theoretical parameters describing the small nanocrytstals to bulk values.Finally, we demonstrate that the study of the optical gap as a function of the size of all three types (Si, Ge, SixGey) of nanocrystals at various concentrations of surface hydrogen and oxygen, is very promising for future gap and optical gap ⌠engineering■.

On pure bending of nanocrystals

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The investigation of elastic properties of such nanostructures as nanocrystals is very important to constructing of the adequate physical models. The moment interaction of particles of nanostructures plays a significant role to determination of elastic modulus [1]. In this paper the nonlinear problem of pure bending of prismatic beam with couple stresses is considered within framework of exact three-dimensional equations of nonlinear micropolar elastic theory [2].The initial three-dimensional problem for Cosserat continuum is reduced into a two-dimensional nonlinear boundary-value problem on cross-section of beam by using Saint-Venant semi-inverse method. The alternative set up of two-dimensional problem is proposed on the base of stress-functions and the variational formulation is given. The analysis of influence of taking into account of couple stresses and comparison with the problem of pure bending of prismatic beam made of simple nonlinear material [3] are given. The obtained results are useful to experimental investigations of nanostructures. References1. E. A. Ivanova, A. M. Krivtsov, N. F. Morozov, and A. D. Firsova. Inclusion of the Moment Interaction in the Calculationof the Flexural Rigidity of Nanostructures. Doklady Physics, Vol. 48, No. 8, 2003, pp. 455√458.2. A.C. Eringen Microcontinuum Field Theories. I. Foundations and Solids. Berlin, Heidelberg, New-York et al, 1999. 325 pp.3. A.A. Zelenina and L.M. Zubov, The Nonlinear Theory of the Pure Bending of Prismatic Elastic Solids. Prikl. Mat. Mekh. Vol. 64, No 3, 2000, pp. 416-423.

Synthesis of well aligned ZnO nanowires without catalysts

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Well aligned ZnO nanowires were synthesized by simple PVD approach using c-axis directed ZnO thin films as substrate without any catalysts or additives. The synthesized nanowires have two typical average diameters: 60nm in majority and 120nm in minority. The ZnO nanowires are about 4μm in length and well aligned along the normal direction of the substrate. Most of the ZnO nanowires are single crystalline with a hexagonal structure and grow along the [001] direction. PL spectrum shows that the ZnO nanowires have a single strong UV emission at 380nm, indicating that the ZnO nanowire arrays can be used in optoelectronic devices.

Deformation Mechanisms of Nanostructured Materials

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Nanostructured materials deform via mechanisms not accessible to their coarse-grained counterparts. Partial dislocation emission from grain boundaries, stacking faults and deformation twinning may occur in metals such as Al, which does not deform by twinning in its coarse-grained state. In this presentation I?ll discuss several deformation mechanisms in nanomaterials as well as their formation conditions. Specifically, I shall first give a brief overview on the deformation mechanisms, observed by both molecular dynamic simulations and experiments. I shall then present a dislocation-based model to describe the nucleation and growth of deformation twins in fcc metals. I shall also discuss other nanocrystalline-related deformation features such as wide stacking faults and five-fold twins.

Structure evolution during severe warm plastic deformation of carbon steel

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Intensive plastic straining of a number of steel grades in conjunction with a controlled thermal process yields very fine microstructures and favourable mechanical properties. This article focuses on the results from recent experimental of severe plastic deformation of medium carbon steel containing 0.45 wt pct carbon. In preliminary step of straining very fine microstructure with high degree of strengthening has been achieved by means of a multistep open die forming processing. Uniform and fine dynamically recrystallized structure of ferrite-pearlite mixture with grain size of about 1-2 μm resulted from performed hot press forging. Cementite within nest-like pearlite colonies retained rod-like morphology. During performed forming the total effective strain, imposed to specimen was of ~ 4. The further grain refinement was obtained during severe warm deformation of preliminary processed specimens using equal channel angular pressing (ECAP). The steel was subjected to three pressings. Employment of this processing route resulted in further refinement of ferrite grains. The submicrometer order ferrite grains enclosed by serrated and low angle boundaries were formed within the former ferrite grains. Fractured cementite particles modified the constitution of newly born substructure. Transmission electron microscopy of thin foils revealed that three executed passes was not enough to form fully fine grained structure with high angle grain boundaries.

Preparation of polymer nanocomposites through solvent casting and melt extrusion: A comparative study in the case of biodegradable and biocompatible polymer matrices

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Polymer nanocomposites are of great scientific and technological value due to their improved properties compared with the pristine polymers. Many routes for their preparation have been attempted in the lab. In this work, two such routes are examined and compared: The solvent casting method and the melt blending one. The first relies on slow-rate diffusion, while the second uses the shear stresses developed in a micro-extruder to speed up the whole process of preparation. Polycaprolactone (PCL) and montmorillonite (MMT) and poly(lactic acid) (PLA) and MMT were the two systems chosen for the comparative study. Both polymers are biodegradable and biocompatible, while MMT is an additive known to improve the thermo-mechanical properties of the hybrid material. Using the proper designs for our experiments and statistical analysis (Response Surface Methodology), we find the ⌠sweet spots■ for the preparation of the nanocomposites for both methods and compare them, while we emphasize on their difference regarding their environmental impact.

Thermo-mechanical and morphological properties of biodegradable and biocompatible inorganic/organic nanohybrid materials

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Recently, polymer clay nanocomposites have received significant scientific and industrial interest, because they often exhibit properties superior to virgin polymers and conventional composites. In the present study, hybrids were prepared by poly(lactic acid) (PLA) and various contents of organophilic montmorillonite (MMT) in order to improve thermal and mechanical features of the polymer. PLA is a polyester synthesized by renewable resources. It is environmentally friendly and is widely used in biomedical applications.Nanocomposites were produced by solvent casting technique and melt blending. The dispersibility of the organoclay in PLA matrix was investigated by XRD and TEM. TGA and DSC were performed to determine the thermal behavior of the prepared composites. According to the results, homogeneous dispersion of layered silicates delays the onset of thermal degradation of the PLA matrix. The mechanical properties were studied in tensile loading conditions where hybrid materials showed improved strength up to a specific clay content and increased Young's Modulus.

Quantum Entanglment in Quantum-Dot Molecules made of self-assembled InAs/GaAs

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Entanglment of electrons in dot-molecules is one of the most promissing routs to achieve Quantum Entanglment needed for Quantum Computers.However,it is not known experimentally (1) What are the optical signatures of entanglment (i,e.how is the number and energies of excitonic peaks related to the degree of entanglment) ,and (2) Can dot-molecules produce large enough entanglment,and if so,at what inter-dot separation.We have addressed these questions theoretically modelling InAs/GaAs dot molecules atomistically using a combination of pseudopotential theory (for the one-electron structure) with many-body expansion (for multi-particle effects).We predict the optical signature of entanglment,and quantify its degree.We show the critical separation where entanglment is maximal. This Work was done in collaboration with G.Bester and J.Shumway,and was recently published in Physical Review LettersVol 93, 047401 (2004).