Abstracta

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TRABALHOS ACEITOS PARA PUBLICAÇÃO

A 001- 07Electronic and Mechanical Properties of Super Carbon Nanotube Networks.
A 002- 07Elastic Properties of Normal and Binormal Helical Nanowires.
A 003- 07Molecular Dynamics Simulation of Single Wall Carbon Nanotubes Polymerization Under Compression.
A 004- 07Prediction of the Hydrogen Storage Capacity of Carbon Nanoscrolls.
A 005- 07Mechanical properties of carbon nanotube networks by molecular mechanics and impact molecular dynamics calculation.
A 006- 07Entanglement in the dispersive interaction of trapped ions with a quantized field.

TRABALHOS PUBLICADOS

Dezembro 2006 à Janeiro 2007

P 001-07 à P 038-07

Trabalhos Aceitos para Publicação

A 001- 07Electronic and Mechanical Properties of Super Carbon Nanotube Networks

Vitor R. Coluci, Socrates O. Dantas, Ado Jorio, and Douglas S. Galvao

Eletronic and mechanical properties of ordered carbon nanotube networks are studied using molecular dynamics simulations and tight-binding calculations. These networks are formed by single walled carbon nanotubes(SWNT) regularly connected by junctions.The use of different types of junctions ("Y"-, "X"-like junctions, for example) allows theconstruction of networks with different symmetries. These networks can be very flexible and the elastic deformation was associated with two main deformation mechanisms (bending and stretching) of the constituents SWNTs. Rolling up the networks, "super" carbon nanotubes can be constructed. These super-tubes share some of the main electronic features of the SWNT which form them but important changes are predicted (e.g. reduction of bandgap value). Simulations of their deformations under tensile stress have revealed that the super-tubes are softer than the corresponding SWNT and that their rupture occur in higher strain values.

Proceedings Material Research Symposia-Fall 2006, accepted on January 2007.

A 002- 07Elastic Properties of Normal and Binormal Helical Nanowires

A. F. da Fonseca, C. P. Malta and D. S. Galvao

A helical nanowire can be defined as being a nanoscopic rod whose axis follows a helical curve in space. In the case of a nanowire with asymmetric cross section, the helical nanostructure can be classified as normal or binormal helix, according to the orientation of the cross section with respect to the helical axis of the structure. In this work, we present a simple model to study the elastic properties of a helical nanowire with asymmetric cross section. We use the framework of the Kirchhoff rod model to obtain an expression relating the Hooke's constant, h, of normal and binormal nanohelices to their geometric features. We also obtain the Young's modulus values. These relations can be used by experimentalists to evaluate the elastic properties of helical nanostructures. We showed that the Hooke's constant of a normal nanohelix is higher than that of a binormal one. We illustrate our results using experimentally obtained nanohelices reported in the literature.

Proceedings Material Research Symposia-Fall 2006, accepted on January 2007.

A 003- 07Molecular Dynamics Simulation of Single Wall Carbon Nanotubes Polymerization Under Compression

S. F. Braga and D. S. Galvao

Single wall carbon nanotubes (SWCNTs) often aggregate into bundles of hundreds of weakly interacting tubes. Their cross-polymerization opens new possibilities for the creation of new super-hard materials. New mechanical and electronic properties are expected from these condensed structures, as well as novel potential applications. Previous theoretical results presented geometric modications involving changes in the radial section of the compressed tubes as the explanation to the experimental measurements of structural changes during tube compression. We report here results from molecular dynamics simulations of the SWCNTs polymerization for small diameter arm chair tubes under compression. Hydrostatic and piston-type compression of SWCNTs have been simulated for di erent temperatures and rates of compression. Our results indicate that large diameter tubes (10,10) are unlike to polymerize while small diameter ones (around 5A) polymerize even at room temperature. Other interesting results are the observation of the appearance of spontaneous scroll-like structures and also the so-called tubulane motifs, which were predicted in the literature more than a decade ago.

Journal of Computational Chemistry, accepted on January 2007.

A 004-07 Prediction of the Hydrogen Storage Capacity of Carbon Nanoscrolls

V. R. Coluci, S. F. Braga, R. H. Baughman, and D. S. Galvao

Classical grand canonical Monte Carlo simulations were performed to investigate the hydrogen storage capacity of carbon nanoscrolls. The results show that hydrogen molecules can be absorbed in the internal cavity as well as on the the external surface of the scroll when the interlayer spacing is less than 4.4 °A. When the interlayer spacing is increased to 6.4 °A, by assuming spacing increase due to intercalation of other species, the hydrogen molecules can also be incorporated in the interlayer galleries, doubling the gravimetric storage capacity and reaching 5.5 wt% hydrogen per weight carbon at 150 K and 1 MPa. Our results showed that intercalated carbon nanoscrolls may be a promissing material for hydrogen storage.

Physical Review B 2007, accepted on January 2007

A 005-07 Mechanical properties of carbon nanotube networks by molecular mechanics and impact molecular dynamics calculation.

V. R. Coluci, S. O. Dantas, A. Jorio, and D. S. Galvao.

We report a theoretical investigation of the mechanical properties of idealized networks formed by single walled carbon nanotubes showing crossbar and hexagonal architectures. The study was performed by using molecular mechanics calculations and impact dynamics simulations based on bond order empirical potential. The studied networks were predicted to have elasticity modulus 210−100 GPa and bulk modulus 210 GPa. The results show a transition from high to moderate flexibility during the deformation stages. This behavior was associated with the existence of two deformation mechanisms presented by the network related to the nanotube stretching and junction bending processes.

Physical Review B , accepted on February 2007.

A 006-07 Entanglement in the dispersive interaction of trapped ions with a quantized field

F. L. Semião and K. Furuya

The mode-mode entanglement between trapped ions and cavity fields is investigated in the dispersive regime. We show how a simple initial preparation of Gaussian coherent states and a postselection may be used to generate motional non-local mesoscopic states (NLMS) involving ions in different traps. We also present a study of the entanglement induced by dynamical Stark-shifts considering a clusterof N-trapped ions. In this case, all entanglement is due to the dependence of the Stark-shifts on the ions' state of motion manifested as a cross-Kerr interaction between each ion and the field.

Physical Review A, accepted on February 2007.

Trabalhos Publicados

P 001- 07 "Amorphous carbon nitrogenated films prepared by plasma immersion ion implantation and deposition"

Rangel, E. C., Durrant, S. F., Rangel, R. C. C., Kayama, M. E., Landers, R., and da Cruz, N. C.

In this work, an investigation was conducted on amorphous hydrogenated-nitrogenated carbon films prepared by plasma immersion ion implantation and deposition. Glow discharge was excited by radiofrequency power (13.56 MHz, 40 W) whereas the substrate-holder was biased with 25 kV negative pulses. The films were deposited from benzene, nitrogen and argon mixtures. The proportion of nitrogen in the chamber feed (R-N) was varied against that of argon, while keeping the total pressure constant (1.3 Pa). From infrared reflectance-absorbance spectroscopy it was observed that the molecular structure of the benzene is not preserved in the film. Nitrogen was incorporated from the plasma while oxygen arose as a contaminant. X-ray photoelectron spectroscopy revealed that N/C and O/C atomic ratios change slightly with R-N. Water wettability decreased as the proportion of N in the gas phase increased while surface toughness underwent just small changes. Nanoindentation measurements showed that film deposition by means of ion bombardment was beneficial to the mechanical properties of the film-substrate interface. The intensity of the modifications correlates well with the degree of ion bombardment.

Thin Solid Films **515[4], 1561-1567. 2006.**

P 002- 07 "Analysis of an interatomic potential for the condensed phases of helium"

Ujevic, S. and Vitiello, S. A.

A recent interatomic potential, that includes two- and three-body interactions, is used to study the liquid and solid equations of state of He-4 and other properties of this system. The high-order contributions are explicitly computed by multi-weight diffusion Monte Carlo. It turns out that this is an excellent interatomic potential for the description of condensed phases of helium atoms systems

International Journal of Modern Physics B **20[30-31], 5103-5106. 2006.**

P 003- 07 "Angra dos reis reactor neutrino oscillation experiment"

Anjos, J. C., Barbosa, A. F., Bernstein, A., Bowden, N. S., Fulgione, W., Kemp, E., Magnin, J., Nunokawa, H., Peres, O. L. G., Reyna, D., Schilithz, A., Shellard, R. C., and Funchal, R. Z.

We present the status and plans of the Angra Project, a new reactor neutrino oscillation experiment, proposed to be built in Brazil at the Angra dos Reis nuclear complex. This experiment is aimed to measure 013, the last unknown of the three neutrino mixing angles, We propose a high sensitivity multi-detector experiment, able to reach a sensitivity to antineutrino disappearance down to sin(2) 2 theta(13) = 0.006 in a three years running period, by combining a high luminosity design, very low background from cosmic rays and careful control of systematic errors. We also intend to explore the possibility to use the neutrino detector for purposes of safeguards and non-proliferation of nuclear weapons

Brazilian Journal of Physics **36[4A], 1118-1123. 2006.**

P 004- 07 "Anisotropic spin transport in (110) GaAs quantum wells"

Couto, O. D. D., Iikawa, F., Rudolph, J., Hey, R., and Santos, P. V.

Mobile piezoelectric potentials are used to coherently transport electron spins in GaAs (110) quantum wells (QW) over distances exceeding 60 mu m. We demonstrate that the dynamics of mobile spins under external magnetic fields depends on the direction of motion in the QW plane. This transport anisotropy is an intrinsic property of moving spins associated with the bulk inversion asymmetry of the underlying GaAs lattice

Physical Review Letters **98[3]. 2007.**

P 006- 07"Beam-based alignment of the NuMI target station components at FNAL"

Zwaska, R., Bishai, M., Childress, S., Drake, G., Escobar, C., Gouffon, P., Harris, D. A., Hylen, J., Indurthy, D., Koizumi, G., Kopp, S., Lucas, P., Marchionni, A., Para, A., Pavlovic, Z., Smart, W., Talaga, R., and Viren, B.

The Neutrinos at the Main Injector (NuMI) facility is a conventional horn-focused neutrino beam which produces muon neutrinos from a beam of mesons directed into a long evacuated decay volume. The relative alignment of the primary proton beam, target, and focusing horns affects the neutrino energy spectrum delivered to experiments. This paper describes a check of the alignment of these components using the proton beam. (c) 2006 Elsevier B.V. All rights reserved

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment **568[2], 548-560. 2006.**

P 007- 07"Bismuth doping of hydrogenated amorphous germanium thin films"

Burmeister, F., Comedi, D., and Chambouleyron, I.

The optoelectronic properties of Bi-doped hydrogenated amorphous germanium (a-Ge:H), with relative impurity concentrations [N-imp/N-Ge] ranging between 8 x 10(-6) and 5.5 x 10(-3), are reported. The incorporation of Bi produces small changes in the dark conductivity of a-Ge:H. For a three orders of magnitude change in impurity concentration the room-temperature conductivity changes by just one order of magnitude. Within this doping range no, or small, changes were measured in the values of the pseudo-gap, the Urbach energy, and the hydrogen content. The Fermi level always remains far from the conduction band edge, shifting by only 0.1 eV for the sample with the largest doping concentration. The main conclusion is that Bi is a very inefficient active donor in a-Ge:H. The likely reasons for such behavior are discussed. (c) 2006 Elsevier B.V All rights reserved

Thin Solid Films **515[4], 2442-2446. 2006.**

P 008- 07"Dirac and normal fermions in graphite and graphene: Implications of the quantum hall effect"

Luk'yanchuk, I. A. and Kopelevich, Y.

Spectral analysis of the Shubnikov-de Haas magnetoresistance oscillations and the quantum Hall effect (QHE) measured in quasi-2D highly oriented pyrolytic graphite (HOPG) [Phys. Rev. Lett. 90, 156402 (2003)] reveals two types of carriers: normal (massive) electrons with Berry phase 0 and Dirac-like (massless) holes with Berry phase pi. We demonstrate that recently reported integer- and semi-integer QHEs for bilayer and single-layer graphenes take place simultaneously in HOPG samples

Physical Review Letters **97[25]. 2006.**

P 009- 07"Effective coupling between two Brownian particles"

Duarte, O. S. and Caldeira, A. O.

We use the system-plus-reservoir approach to study the dynamics of a system composed of two independent Brownian particles. We present an extension of the well-known model of a bath of oscillators which is capable of inducing an effective coupling between the two particles depending on the choice made for the spectral function of the bath oscillators. The coupling is nonlinear in the variables of interest, and an exponential dependence on these variables is imposed in order to guarantee the translational invariance of the model if the two particles are not subject to any external potential. The effective equations of motion for the particles are obtained by the Laplace transform method, and, besides recovering all the local dynamical properties for each particle, we end up with an effective interaction potential between them. We explicitly analyze one of its possible forms

Physical Review Letters **97[25]. 2006.**

P 010- 07 "Electromagnetic forces for an arbitrary optical trapping of a spherical dielectric"

Neves, A. A. R., Fontes, A., Pozzo, L. D. Y., de Thomaz, A. A., Chillce, E., Rodriguez, E., Barbosa, L. C., and Cesar, C. L

A double tweezers setup was employed to perform ultra sensitive force measurements and to obtain the full optical force curve as a function of radial position and wavelength. The light polarization was used to select either the transverse electric (TE), or transverse magnetic (TM), or both, modes excitation. Analytical solution for optical trapping force on a spherical dielectric particle for an arbitrary positioned focused beam is presented in a generalized Lorenz-Mie diffraction theory. The theoretical prediction of the theory agrees well with the experimental results. The algorithm presented here can be easily extended to other beam geometries and scattering particles.

Optics Express **14[26], 13101-13106. 2006.**

P 011-07 "Electron cyclotron plasma etching damage investigated by InGaAs/GaAs quantum well photoluminescence"

Mestanza, S. N. M. and Frateschi, N. C.

Photoluminescence (PL) was used to study the damage of (100) GaAs surfaces exposed to BCl3/Ar plasma generated by an electron cyclotron resonance system. With PL measurement of strained InGaAs/GaAs quantum wells within the etched top GaAs layer, our analysis shows that this technique assesses damages to the structure not detected by atomic force microscopy and photoreflectance. A transport model is used to show a 100 times reduction in the Debye length for a 100 nm layer underneath the etching surface. (c) 2006 American Vacuum Society

Journal of Vacuum Science & Technology B **24[6], 2726-2730. 2006.**

P 012 - 07 "Experimental realization of suspended atomic chains composed of different atomic species"

Bettini, J., Sato, F., Coura, P. Z., Dantas, S. O., Galvao, D. S., and Ugarte, D.

Research into nanostructured materials frequently relates to pure substances. This contrasts with industrial applications, where chemical doping or alloying is often used to enhance the electrical or mechanical properties of materials(1). However, the controlled preparation of doped nanomaterials has been much more difficult than expected because the increased surface-area-to-volume ratio can, for instance, lead to the expulsion of impurities (self-purification)(2). For nanostructured alloys, the influence of growth methods and the atomic structure on self-purification is still open to investigation(2,3). Here, we explore, experimentally and with molecular dynamics simulations, to what extent alloying persists in the limit that a binary metal is mechanically stretched to a linear chain of atoms. Our results reveal a gradual evolution of the arrangement of the different atomic elements in the narrowest region of the chain, where impurities may be expelled to the surface or enclosed during elongation

Nature Nanotechnology **1[3], 182-185. 2006.**

P 013-07 "Fixed holograms in iron-doped lithium niobate: simultaneous self-stabilized recording and compensation"

Frejlich, J., de Oliveira, I., Arizmendi, L., and Carrascosa, M.

We analyze the mechanisms leading to a highly diffractive fixed hologram in photorefractive Fe-doped lithium niobate crystals by simultaneous self-stabilized holographic recording and compensation at moderately high temperatures. We show that a partially compensated running hologram is produced during recording under this condition and discuss the performance of the process in terms of the operating temperature, the degree of oxidation ([Fe3+]/[Fe2+] ratio) of the sample, and the effect of the absorption grating arising from the spatial modulation of the Fe2+ concentration produced during photorefractive recording. We experimentally measure the evolution of the uncompensated remaining hologram during recording and the evolution of the diffraction efficiency of the fixed hologram during white-light development and show that the maximum fixed grating modulation to be achieved is roughly limited by Fe-dopant saturation. A reproducible eta approximate to 66% efficiency fixed grating was obtained on a sample exhibiting an otherwise maximum fixed eta approximate to 3% when using the classical three-step (recording at room temperature-compensating at high temperature-developing at room temperature) process.

Applied Optics 46[2], 227-233. 2007.

P 014-07 "Growth aspects of photochemically synthesized silver triangular nanoplates"

Rocha, T. C. R. and Zanchet, D.

Aspects of the growth mechanism of silver triangular nanoplates by photochemical synthesis were addressed by detailed characterization using ultraviolet-visible spectroscopy, electron microscopies, and atomic force microscopy. The quantitative characterization of their size and thickness during the reaction showed that both increase with time as well as the aspect ratio. Samples irradiated by different wavelengths showed that the size of the nanoplates can be controlled by the incident wavelength and it is responsible for the increase of the aspect ratio, but the thickness seems to be determined by the conditions of the initial seeds. It was also found that irradiation with wavelength out of resonance with the surface plasmon of the initial seeds leads to a slower kinetics. The results suggested that rational exploration of the synthesis parameter such as the type of the initial seeds in combination with the wavelength irradiation may lead to a broader type of particles already obtained by this method

Journal of Nanoscience and Nanotechnology **7[2], 618-625. 2007.**

P 015-07 "Incipient orbital order in half-metallic Ba2FeReO6"

Azimonte, C., Cezar, J. C., Granado, E., Huang, Q., Lynn, J. W., Campoy, J. C. P., Gopalakrishnan, J., and Ramesha, K.

Largely unquenched Re 5d orbital magnetic moments in half-metallic Ba2FeReO6 drive a symmetry lowering transition from a cubic paramagnet to a compressed tetragonal (c/a < 1) ferrimagnet below T-C similar to 305 K, with a giant linear magnetoelastic constant and the spins lying spontaneously along the unique tetragonal axis. The large orbital magnetization and degree of structural deformation indicate proximity to a metal-insulator transition. These results point to an incipient orbitally ordered state in the metallic ferrimagnetic phase

Physical Review Letters **98[1]. 2007.**

P 016-07 "Influence of the microstructure on the electrochemical performance of thin film WO3 cathode"

Figueroa, R., Kleinke, M., Cruz, T. G. S., and Gorenstein, A.

In this work, WO3 thin films deposited at different powers and geometries have been evaluated for use as electrodes in thin film batteries. The potential profiles and cycling capacity in lithium electrolyte were investigated. The discharge capacity for samples strongly depends on the deposition conditions, and there is a clear correlation between microstructure and electrochemical performance. (c) 2006 Elsevier B.V. All rights reserved

Journal of Power Sources **162[2], 1351-1356. 2006.**

P 017-07 "Kondo effect in a quantum dot - the atomic approach"

Lobo, T., Figueira, M. S., and Foglio, M. E.

We describe the Kondo resonance in quantum dots employing the atomic approach for the Anderson impurity. The starting point of this approach is the exact solution of the Anderson impurity in the zero-bandwidth limit, and we choose the level of the atomic conduction band so that the completeness relation be satisfied. There are two or more solutions close to the chemical potential that satisfy this condition at low temperatures, and we choose the one with minimum Helmholtz free energy, considering that this corresponds to the Kondo solution. At low temperatures we obtain a density of states that characterizes well the structure of the Kondo peak. The results obtained for both the localized density of states at the chemical potential and for dynamical properties (like the conductance) agree very well with those obtained by the numerical renormalization group formalism and by the slave boson mean field approach, respectively. This result is a consequence of the satisfaction of the Friedel sum rule by the atomic approach in the Kondo limit. As a simple application we calculate the conductance of a side-coupled quantum dot

Nanotechnology **17[24], 6016-6026. 2006.**

P 018- 07"Lande g tensor in semiconductor nanostructures"

Alegre, T. P. M., Hernandez, F. G. G., Pereira, A. L. C., and Medeiros-Ribeiro, G.

Understanding the electronic structure of semiconductor nanostructures is not complete without a detailed description of their corresponding spin-related properties. Here we explore the response of the shell structure of InAs self-assembled quantum dots to magnetic fields oriented in several directions, allowing mapping of the g-tensor modulus for the s and p shells. We find that the g tensors for the s and p shells exhibit a very different behavior. The s state, being more localized, probes the confinement potential details by sweeping the magnetic-field orientation from the growth direction towards the in-plane direction. For the p state, the g-tensor modulus is closer to that of the surrounding GaAs, consistent with a larger delocalization. In addition to the assessment of the g tensor, these results reveal further details of the confining potentials of self-assembled quantum dots that have not yet been probed

Physical Review Letters **97[23]. 2006.**

P 019- 07"Limitations on the principle of stationary phase when it is applied to tunneling analysis"

Bernardini, A. E.

Using a recently developed procedure-multiple wave packet decomposition-here we study the phase time formulation for tunneling or reflecting particles colliding with a potential barrier. To partially overcome the analytical difficulties which frequently arise when the stationary phase method is employed for deriving phase (tunneling) time expressions, we present a theoretical exercise involving a symmetrical collision between two identical wave packets and an one-dimensional rectangular potential barrier. Summing the amplitudes of the reflected and transmitted waves-using a method we call multiple peak decomposition-is shown to allow reconstruction of the scattered wave packets in a way which allows the stationary phase principle to be recovered

Physical Review A **74[6]. 2006.**

P 020- 07"Magnetic interaction between manganese (2+) atoms through aquo bridges and bifurcated cyano groups"

Martinez-Garcia, R., Reguera, L., Knobel, M., and Reguera, E.

The magnetic interaction between adjacent manganese atoms through aquo double bridges in Mn-2[M(CN)(6)] center dot xH(2)O where x = 8 and 2 and M= Fe, Ru, Os, was studied. Through these bridges a relatively weak antiferromagnetic interaction is established with an estimated Curie-Weiss temperature, vertical bar theta(CW)vertical bar, close to 4 K and a super exchange constant, vertical bar J vertical bar, of 0.27 cm(-1). When these materials are dehydrated the antiferromagnetic interaction between the Mn atoms undergoes a dramatic increase, with estimated values for vertical bar theta(CW)vertical bar and vertical bar J vertical bar of 61 K and 4.11 cm(-1), respectively. Such reinforcement in the magnetic interaction is accompanied by a shift of 32 cm(-1) for the. (CN) vibration towards the low frequency region while for the iron compound the Mossbauer spectrum, initially a single line, becomes a quadrupole splitting doublet of relatively low isomer shift (delta) value. The Curie constant of the involved Mn atoms shows a negative correlation with the observed shifts in. (CN) and d on dehydration. From the observed magnetic behaviour and the spectroscopic data a double coordination of an N end of the CN ligand to two Mn atoms is proposed. Such strong magnetic interaction through the N atom of the CN ligand could be used as a prototypical bridge to obtain high T-c molecular magnets.

Journal of Physics-Condensed Matter **19[5]. 2007.**

P 021-07 "Magnetic structure and enhanced T-N of the rare-earth intermetallic compound TbRhIn5: Experiments and mean-field model"

Lora-Serrano, R., Giles, C., Granado, E., Garcia, D. J., Miranda, E., Aguero, O., Ferreira, L. M., Duque, J. G. S., and Pagliuso, P. G.

In this work the physical properties of the intermetallic compound TbRhIn5 were investigated by means of temperature-dependent magnetic susceptibility, electrical resistivity, heat-capacity, and resonant x-ray magnetic diffraction experiments. TbRhIn5 is an intermetallic compound that orders antiferromagnetically at T-N=45.5 K, the highest ordering temperature among the existing RRhIn5 (1-1-5, R=rare earth) materials, which in contrast to what is expected from a de Gennes scaling along the RRhIn5 series. The x-ray resonant diffraction data have allowed us to solve the magnetic structure of TbRhIn5. Below T-N, we found a commensurate antiferromagnetic structure with a propagation vector (1/2,0,1/2) and the Tb moments oriented along the c axis. Strong (over two orders of magnitude) dipolar enhancements of the magnetic Bragg peaks were observed at both Tb absorption edges L-II and L-III, indicating a fairly high polarization of the Tb 5d levels. Using a mean-field model including an isotropic first-neighbor exchange interaction (J(R-R)) and the tetragonal crystalline electrical field (CEF), we evaluate the influence of the CEF effects in the physical properties of TbRhIn5. The results reported here seem to corroborate a general trend of CEF-driven effects on T-N along the RRhIn5 series

Physical Review B **74[21]. 2006.**

P 022- 07"Magnetic structure and critical behavior of GdRhIn5: Resonant x-ray diffraction and renormalization group analysis"

Granado, E., Uchoa, B., Malachias, A., Lora-Serrano, R., Pagliuso, P. G., and Westfahl, H.

The magnetic structure and fluctuations of tetragonal GdRhIn5 were studied by resonant x-ray diffraction at the Gd L-II and L-III edges, followed by a renormalization group analysis for this and other related Gd-based compounds, namely Gd2IrIn8 and GdIn3. These compounds are spin-only analogs of the isostructural Ce-based heavy-fermion superconductors. The ground state of GdRhIn5 shows a commensurate antiferromagnetic spin structure with propagation vector (tau) over right arrow=(0,(1)/(2),(1)/(2)), corresponding to a parallel spin propagation along the (a)over-right-arrow direction and antiparallel propagation along (b)over-right-arrow and (c)over-right-arrow. The spin direction lies along (a)over-right-arrow. A comparison between this magnetic structure and those of other members of the R-m(Co,Rh,Ir)(n)In3m+2n family (R=rare earth, n=0,1; m=1,2) indicates that, in general, (tau)over-right-arrow is determined by a competition between first- (J(1)) and second-neighbor (J(2)) antiferromagnetic (AFM) interactions. While a large J(1)/J(2) ratio favors an antiparallel alignment along the three directions (the G-AFM structure), a smaller ratio favors the magnetic structure of GdRhIn5 (C-AFM). In particular, it is inferred that the heavy-fermion superconductor CeRhIn5 is in the frontier between these two ground states, which may explain its noncollinear spiral magnetic structure. The critical behavior of GdRhIn5 close to the paramagnetic transition at T-N=39 K was also studied in detail. A typical second-order transition with the ordered magnetization critical parameter beta=0.35 was experimentally found, and theoretically investigated by means of a renormalization group analysis. Although the Gd 4f(7) electrons define a half-filled, spherically symmetrical shell, leading to a nearly isotropic spin system, it is argued that a significant spin anisotropy must be claimed to understand the second order of the paramagnetic transition of GdRhIn5 and the related compound Gd2IrIn8

Physical Review B **74[21]. 2006.**

P 023 -07"Magnetic study of Mg0.95Mn0.05Fe2O4 ferrite nanoparticles"

Sharma, S. K., Kumar, R., Kumar, S., Kumar, V. V. S., Knobel, M., Reddy, V. R., Banerjee, A., and Singh, M.

The magnetic properties of Mg0.95Mn0.05Fe2O4 ferrite samples with an average particle size of similar to 6.0 +/- 0.6 nm have been studied using X-ray diffraction, Mossbauer spectroscopy, dc magnetization and frequency dependent real chi'(T) and imaginary chi"(T) parts of ac susceptibility measurements. A magnetic transition to an ordered state is observed at about 195 K from Mossbauer measurements. The zero-field-cooled (ZFC) and field-cooled (FC) magnetization have been recorded at low field and show the typical behavior of a small particle system. The ZFC curve displays a broad maximum at T-mean = 195 +/- 5 K, a temperature which depends upon the distribution of particle volumes in the sample. The FC curve was nearly flat below T-mean, as compared with monotonically increasing characteristics of non-interacting superparamagnetic systems indicating the existence of strong interactions among the nanoparticles. A frequency-dependent peak observed in chi'(T) is well described by Vogel-Fulcher law, yielding a relaxation time tau(0) = 5.8 x 10(-12) s and an interaction parameter T-0 = 195 +/- 3 K. Such values show the strong interactions and rule out the possibility of spin-glass (SG) features among the nanoparticle system. On the other hand fitting with the Neel-Brown model and the power law yields an unphysical large value of tau(0) (similar to 6 x 10(-69) and 1.2 x 10(-22) s respectively). (c) 2006 Elsevier Ltd. All rights reserved

Solid State Communications **141[4], 203-208. 2007.**

P 024- 07"Measurement of pressure effects on the magnetic and the magnetocaloric properties of the intermetallic compounds DyCo2 and Er(Co1-xSix)(2)"

Singh, N. K., Kumar, P., Suresh, K. G., Nigam, A. K., Coelho, A. A., and Gama, S.

The effect of external pressure on the magnetic properties and magnetocaloric effect of polycrystalline compounds DyCo2 and Er(Co1-xSix)(2) (x = 0, 0.025 and 0.05) has been studied. The ordering temperatures of both the parent and the Si-substituted compounds are found to decrease with pressure. In all the compounds, the critical field for metamagnetic transition increases with pressure. It is seen that the magnetocaloric effect in the parent compounds is almost insensitive to pressure, while there is considerable enhancement in the case of Si-substituted compounds. Spin fluctuations arising from the magnetovolume effect play a crucial role in determining the pressure dependence of the magnetocaloric effect in these compounds. The variation of the magnetocaloric effect is explained on the basis of the Landau theory of magnetic phase transitions

Journal of Physics-Condensed Matter **19[3]. 2007.**

P 025- 07"Microstructured-core optical fibre for evanescent sensing applications"

Cordeiro, C. M. B., Franco, M. A. R., Chesini, G., Barretto, E. C. S., Lwin, R., Cruz, C. H. B., and Large, M. C. J.

The development of microstructured fibres offers the prospect of improved fibre sensing for low refractive index materials such as liquids and gases. A number of approaches are possible. Here we present a new approach to evanescent field sensing, in which both core and cladding are microstructured. The fibre was fabricated and tested, and simulations and experimental results are shown in the visible region to demonstrate the utility of this approach for sensing. (c) 2006 Optical Society of America

Optics Express **14[26], 13056-13066. 2006.**

P 026- 07"Modelling dynamics of samples exposed to free-electron-laser radiation with Boltzmann equations"

Ziaja, B., de Castro, A. R. B., Weckert, E., and Moller, T.

We apply Boltzmann equations for modelling the radiation damage in samples irradiated by photons from free electron lasers (FELs). We test this method in a study case of a spherically symmetric xenon cluster irradiated with VUV FEL photons. Qualitative agreement between the model predictions and experimental data is found. The results obtained demonstrate the potential of the Boltzmann method for describing the complex and non-equilibrium dynamics of samples exposed to FEL radiation

European Physical Journal D **40[3], 465-480. 2006.**

P 027-07 "Neutrino physics: the roadmap for precision physics"

Peres, O. L. G.

In the last years, we experienced a complete change of the view of weak interaction physics. Robust results from many experiments as Super-Kamiokande, KamLAND, SNO, K2K, show us that the neutrinos have the remarkable phenomena of oscillations, a quantum interference mechanism that operates to distances as large as 100 km and even bigger distances. From this we know that neutrinos change identity from one flavor to another, as was demonstrated by the joints results of SNO and Super-Kamiokande experiments. We show here the review of latest results of neutrino physics, as for example, the first evidence of neutrinos produced in the core of the earth and the updated results of KamLAND and others. Our understating of all experimental results will completed by the state-of-art of the theoretical effort to understand such phenomena. For the near future, we expect the new generation of precision physics, like the running experiments of MINOS and Double CHOOZ, and the proposals of SADO and ANGRA shed light on unresolved issues such as the CP-violation for neutrinos and the relative magnitude of solar and atmospheric scales

Brazilian Journal of Physics **36[4A], 1178-1183. 2006.**

P 028- 07"On the hydrogen etching mechanism in plasma nitriding of metals"

Figueroa, C. A. and Alvarez, F.

Iron alloys and aluminum were nitrogen implanted in a controlled oxygen atmosphere and the role of hydrogen on the surface etching mechanisms studied. The surface composition was analyzed by in situ photoemission electron spectroscopy (XPS). In iron alloys, hydrogen strongly etches oxygen, improving nitrogen retention on the surface. On the other hand, hydrogen removes nitrogen from aluminum surfaces, with a deleterious effect on the nitriding effectiveness. The oxygen removal in iron alloys is associated with the catalytic effect of electrons in d-orbitals and the nitrogen removal in aluminum is associated with a steric effect. (c) 2006 Elsevier B.V. All rights reserved

Applied Surface Science **253[4], 1806-1809. 2006.**

P 029- 07"Photochromism, bleaching and photorefractive recording in undoped Bi12TiO20 crystals in the visible and near infrared wavelength range"

dos Santos, P. V., Carvalho, J. F., and Frejlich, J.

We describe the effect of radiation of different wavelengths in the visible and near infrared range over photochromism, bleaching and photorefractive recording on undoped Bi12TiO20 crystals. These experiments lead to a phenomenological description of the relevant photoactive centers in this material. At least an empty donor level 0.42 eV below the conduction band, some deeper donor levels up to 1.6 eV below the conduction band and an acceptor level 1 eV above the valence band were identified. (c) 2005 Elsevier B.V. All rights reserved

Optical Materials **29[5], 462-467. 2007.**

P 030-07 "Quantum channels in random spin chains"

Hoyos, J. A. and Rigolin, G.

We study the entanglement between pairs of qubits in a random antiferromagnetic spin-1/2 chain at zero temperature. We show that some very distant pairs of qubits are highly entangled, being almost pure Bell states. Furthermore, the probability to obtain such spin pairs is proportional to the chain disorder strength and inversely proportional to the square of their separation

Physical Review A 74[6]. 2006.

P 031-07 "SiO2 single layer for reduction of the standing wave effects in the interference lithography of deep photoresist structures on Si"

Carvalho, E. J., Alves, M. A. R., Braga, E. S., and Cescato, L.

We demonstrate that the use of a single SiO2 film, with thickness corresponding to one standing wave (SW) period allows the recording of deep photoresist structures on silicon substrates by laser interference, without use of any additional antireflecting coating. This condition corresponds just to the opposite thickness (half SW period) previously proposed for using the SiO2 films for phase-shifting the SW pattern. Theoretical and experimental results demonstrated that for the lithography of deep structures, the contrast of the SW pattern, the minimum light intensity of the SW pattern and the photoresist adhesion are the most important parameters of the process. (c) 2006 Elsevier Ltd. All rights reserved

Microelectronics Journal 37[11], 1265-1270. 2006.

P 032-07 "Size dependent magnetic behaviour of nanocrystalline spinel ferrite Mg0.95Mn0.05Fe2O4"

Sharma, S. K., Kumar, R., Kumar, V. V. S., and Dolia, S. N

Mg0.95Mn(0.05)Fe(2)O(4) ferrite nanoparticles having dimensions varying from 4.7-12 nm, have been synthesized by using solid-state reaction technique followed by high-energy ball milling for different times. An X-ray diffraction study indicates the presence of single-phase cubic spinel structure. The particle sizes were estimated from the X-ray line broadening of the (311) reflection using Debye-Scherrer's formula. The size-dependent magnetic properties of Mg0.95Mn0.05Fe2O4 nanoparticies were studied using SQUID magnetometry techniques. The saturation magnetization M, at 5 K obtained by extrapolating M versus 1/H plot to 1/H = 0 were decreased with the decrease in the particle size. The coercive force of the nanoparticles has a clear size-dependence below the blocking temperature. The calculated anisotropy constant was found to be rather large for nanoparticle samples. All these results can be explained on the basis of single-domain superparamagnetic effects

Indian Journal of Pure & Applied Physics 45[1], 16-20. 2007

P 033-07 "Structure and morphology of poly(epsilon-caprolactone)/chlorinated polyethylene (PCL/PECl) blends investigated by DSC, simultaneous SAXS/WAXD, and elemental mapping by ESI-TEM"

Plivelic, T. S., Cassu, S. N., Goncalves, M. D., and Torriani, I. L.

In this work, the structure and morphology of miscible blends of poly(epsilon-caprolactone) and chlorinated polyethylene with 48% chlorine weight content (PCL/PECl) were studied by differential scanning calorimetry (DSC), simultaneous small and wide-angle X-ray scattering (SAXS/WAXD), and electron spectroscopy imaging in the transmission electron microscope (ESI-TEM). A unique glass transition temperature was obtained in each blend. In addition to this, the heat capacity and the width of the glass transition did not have a linear behavior with blend compositions. These facts correlate with the presence of microheterogeneities originated from different local compositions and densities of interactions in each blend. A consistent picture of the mode of segregation of PECl in the blend was obtained. For higher concentration of PCL, the volume fraction of lamellar stacks in the samples decreased as a function of the PECl content, indicating preferential interfibrillar localization of the amorphous component. For lower PCL concentration, interespherulitic segregation was the dominant mode. Elemental maps of chlorine confirmed these results and also revealed changes in the concentration of this element depending on its localization in the microstructure of the system. Gradients of chlorine concentration were measured in larger amorphous regions of the 40/60 and 20/80 PCL/PECl blends. Calculations of the one-dimensional correlation function probed the reduction of the lamellar thickness of PCL when the quantity of PECl in the blend was increased. Such a tendency could be rationalized if the reduction of the fold surface free energy was a dominant factor in terms of the reduction of the degree of supercooling in the final crystal thickness

Macromolecules 40[2], 253-264. 2007.

P 034-07 "Synthesis and density functional calculations of the new molecule-based magnet precursor [Fe(H(2)opba-i)(dmso)(2)]Cl"

Souza, G. P., Konzen, C., Ardisson, J. D., De Abreu, H. A., Duarte, H. A., Alcantara, A. F. C., Nunes, W. C., Macedo, W. A. A., Knobel, M., and Stumpf, H. O.

A new precursor of molecule-based magnetic systems, [Fe(H-2 opba- i)(dmso)(2)]Cl (1), with opba = ortho-phenylenebis(oxamato) in an iminoalcohol tautomeric form, was obtained as a product from the reaction between H-4 opba and FeCl3. Data from elemental analysis, IR and Mossbauer spectroscopies and magnetic measurements indicate that this precursor is composed of a mixture of trans (83%) and cis (17%) isomers. The. M T value at 298K (2.1 emu K mol(-1)) corresponds to Fe-III with spin state (S) between 3/2 and 5/2. Theoretical calculations (PBE/DZVP2) of trans- and cis-[Fe(H-2 opba-i)(dmso)(2)](+) show that both isomers have spin S = 1/2 in the ground state and S = 3/2 for the trans and S = 5/2 for the cis in the first excited state. The combination of these results leads to chi T-M values of 0.375 and 2.3 emu K mol(-1), at low and high temperature respectively, which are in accordance with the experimental data for 1

Journal of the Brazilian Chemical Society 17[8], 1534-1539. 2006.

P 035-07 "The theory of irreversible processes: Foundations of a non-equilibrium statistical ensemble formalism"

Luzzi, R., Vasconcellos, A. R., and Ramos, J. G.

A general overview on the construction of a non-equilibrium statistical mechanics ensemble formalism is presented. Such construction has been approached along the recently past twentieth century by a pleiad of distinguished scientists, their work being subsumed in a large systematization in the form of a physically sound, general and useful, theoretical framework. It includes their contributions and also incorporates some extensions and generalizations. The present contribution has been organized in sixteen items and five appendices where the main questions associated to such construction are considered and discussed. Among them are the relevant ones of choice of the basic variables, the questions of historicity and irreversibility and the approach to equilibrium. The derivation of a non-equilibrium grand-canonical statistical operator is presented. In terms of it a statistical irreversible thermodynamics can be built, which provides microscopic (mechano-statistical) foundations to phenomenological extended irreversible thermodynamics. It also provides a statistical non-linear higher-order hydrodynamics, including fluctuations, thus providing a unification of the kinetics and hydrodynamic approaches. Moreover, a brief description of an all-important accompanying non-linear quantum kinetic theory of relaxation processes is presented, as well as a response function theory and a fluctuation-dissipation theorem for far-from-equilibrium systems. The aspect of validation of the theory (comparison of theory and experiment) is reviewed in compact form. Furthermore, the derivation of the formalism is briefly discussed within the scope of a variational principle in an approach associated to information theory. Considerations on the question of the use of the formalism for dealing with systems with complex structure, small systems, and other particular situations, are presented

Rivista del Nuovo Cimento 29[2], 1-82. 2006.

P 036-07 "Thin film of copper hexacyanoferrate dispersed on the surface of a conducting carbon ceramic material, SiO2/ZrO2/C-graphite: Characteristics and electrochemical studies"

Marafon, E., Lucho, A. M. S., Francisco, M. S. P., Landers, R., and Gushikem, Y

SiO2/ZrO2/C-graphite materials (SZC) were prepared by the sol-gel method presenting two compositions and designated as: (a) SZC30 (SiO2 = 50%, ZrO2 = 20%, C = 30%) and (b) SZC20 (SiO2 = 60%, ZrO2 = 20%, C = 20%) in wt.%. The material structure was investigated by X-ray diffraction (XRD), high resolution transmission electron microscopy (HR-TEM) and X-ray photoelectron spectroscopy (XPS). The electrical conductivities obtained for the pressed disks of these materials were 4 and 18 S cm(-1) for SZC20 and SZC30, and the specific surface areas (determined by the BET method) of the carbon ceramic composites were 45 and 12 m(2) g(-1), respectively. A copper hexacyanoferrate thin film was grown in situ on the material surface containing 30 wt.% C (SZC30). The thickness of the film was estimated as 110 nm. The midpoint potential for the redox process was dependent on the KCl supporting electrolyte concentrations in the range between 0.1 and 1.0 mol L-1 and the charge transfer resistance determined by electrochemical impedance spectroscopy experiment was 23.8 ohm cm(2)

Journal of the Brazilian Chemical Society 17[8], 1605-1611. 2006.

P 037-07 "Unique coordination of copper in hexacyanometallates"

Reguera, E., Rodriguez-Hernandez, J., Champi, A., Duque, J. G., Granado, E., and Rettori, C.

Within divalent transition metals hexacyanometallates (III) the copper (2+) salts show unique features. To the copper (2+) salts correspond the shortest unit cell edges, the highest v(CN) vibration frequencies, the lowest hydration degree and dehydration temperatures, the lowest Mossbauer isomer shift value, and the strongest magnetic exchange interaction (J) between the metal centers. Such unique features were attributed to a particularly strong bond of the copper atom to the N ends of the CN groups. The driving force for such behaviour was ascribed to a combined effect where the copper (2+) shows a high ability to receive electrons in its 3d hole favouring an electronic configuration close to 3d(10) and the CN group complements such ability donating electrons through its 5 sigma orbital which has certain anti-bonding character. This hypothesis is supported by the obtained structural and spectroscopic data. The occurrence of a cooperative Jahn-Teller effect in this family of materials was discarded. In the pseudo-octahedral coordination for the copper (2+) atom the e(g) orbital degeneration is initially removed. The collected EPR spectra are characteristic of a cubic environment (isotropic g-values). Analogue evidence was obtained from high resolution X-ray powder patterns recorded in the 12-300 K temperature range. All the patterns correspond to a cubic unit cell

Zeitschrift fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics 220[12], 1609-1619. 2006.

P 038-07 "X-ray multiple diffraction in the characterization of TiNO and TiO2 thin films grown on Si(001)"

Chiaramonte, T., Abramof, E., Fabreguette, F., Sacilotti, M., and Cardoso, L. P.

TiO2 and TiNxOy thin films grown by low pressure metal-organic chemical vapor deposition (LP-MOCVD) on top of Si(001) substrate were characterized by X-ray multiple diffraction. X-ray reflectivity analysis of TiO2[1 1 0] and TiNO[1 0 0] polycrystalline layers allowed to determine the growth rate (-80 angstrom/min) of TiO2 and (-40 angstrom/min) of TiNO films. X-ray multiple diffraction through the Renninger scans, i.e., phi-scans for (0 0 2)Si substrate primary reflection is used as a non-conventional method to obtain the substrate lattice parameter distortion due to the thin film conventional deposition, from where the information on film strain type is obtained.

Applied Surface Science 253[3], 1590-1594. 2006.

Abstracta

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