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Abstracta

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TRABALHO ACEITO PARA PUBLICAÇÃO

A 002-06 Nonlinear Charge Transport in III-N Semiconductors: Mobility, Diffusion and a Generalized Einstein Relation

A 003- 06 Pseudoscopic imaging in a double diffraction process with a slit: critical point properties

TRABALHOS PUBLICADOS FEVEREIRO/MARÇO 2006

P 042-06 à P 080-06

TRABALHO ACEITO PARA PUBLICAÇÃO

A 002-06 Nonlinear Charge Transport in III-N Semiconductors: Mobility, Diffusion and a Generalized Einstein Relation

Rodrigues, C. G., Vasconcellos, A. R., Luzzi, R.

A theoretical study of nonlinear charge transport in polar semiconductors is presented. It is based on a nonequilibrium statistical ensemble formalism which provides a generalized Boltzmann style nonlinear quantum kinetic theory. The mobility and the difffusio coefficients are obtained and, relating both, it is derived a Nernst-Townsend-Einstein relation extended to the nonlinear regime(i. e outside the Ohmic domain). Numerical calculations are performed considering the particular case of the strongly-polar III-Nitrides, which have application in blue-emitting diodes.

Journal of Applied Physics, accepted on February, 2006.

***A 003- 06* Pseudoscopic imaging in a double diffraction process with a slit: critical point properties**

Lunazzi, J. J. and Rivera, N. I. R.

Pseudoscopic (inverted depth) images that keep a continuous parallax were shown to be possible by use of a double diffraction process intermediated by a slit. One diffraction grating directing light to the slit acts as a wavelength encoder of views, while a second diffraction grating decodes the projected image. The process results in the enlargement of the image under common white light illumination up to infinite magnification at a critical point. We show that this point corresponds to another simple-symmetry object-observer system. Our treatment allows us to explain the experience by just dealing with main ray directions.

Journal of the Optical Society of America A, accepted on May, 2006.

TRABALHOS PUBLICADOS

P 042- 06 "A method to synchronise video cameras using the audio band"

de Barros, R. M. L., Russomanno, T. G., Brenzikofer, R., and Figueroa, P. J.

This paper proposes and evaluates a novel method for synchronisation of video cameras using the audio band. The method consists in generating and transmitting an audio signal through radio frequency for receivers connected to the microphone input of the cameras and inserting the signal in the audio band. In a software environment, the phase differences among the video signals are calculated and used to interpolate the synchronous 2D projections of the trajectories. The validation of the method was based on: (1) Analysis of the phase difference changes as a function of time of two video signals. (2) Comparison between the values measured with an oscilloscope and by the proposed method. (3) Estimation of the improvement in the accuracy in the measurements of the distance between two markers mounted on a rigid body during movement applying the method. The results showed that the phase difference changes in time slowly (0.150 ms/min) and linearly, even when the same model of cameras are used. The values measured by the proposed method and by oscilloscope showed equivalence (R-2 = 0.998), the root mean square of the difference between the measurements was 0.10 ins and the maximum difference found was 0.31 ms. Applying the new method, the accuracy of the 3D reconstruction had a statistically significant improvement. The accuracy, simplicity and wide applicability of the proposed method constitute the main contributions of this work.

Journal of Biomechanics **39[4], 776-780. 2006.**

P 043- 06 "A theoretical study on the photoionization of the valence orbitals of phosphine"

Nascimento, E. M., Machado, L. E., Ribeiro, E. M. S., Brescansin, L. M., and Lee, M. T.

We report a theoretical study on the photoionization of phosphine in the static-exchange level and frozen core approximation, using the method of continued fractions. The main subject of the present study is to investigate in which extent the Hartree-Fock description of the target applied to molecular photoionization is valid. Also, the role played by multichannel coupling is analysed. Our study shows that single-channel Hartree-Fock calculations can provide reliable results except for photon energies near the photoionization threshold

Journal of the Brazilian Chemical Society **17[1], 162-167. 2006.**

P 044- 06 "Al-based anodic oxide films structure observation using field emission gun scanning electron microscopy"

Regone, N. N., Freire, C. M. A., and Ballester, M.

In the present work, the anodic oxide films of Al, Al-Cu 4.5% and Al-Si 6.5% alloys are formed using direct and pulse current. In the case of Al-Cu and Al-Si alloys, the electrolyte used contains sulfuric acid and oxalic acid, meanwhile for Al the electrolyte contains sulfuric acid only. Al-Cu alloy was submitted to a heat treatment in order to decrease the effect of inter metallic phase theta upon the anodic film structure. Fractured samples were observed using a field emission gun scanning electron microscope JSM-6330F at (LME)/ Brazilian Synchrotron Light Laboratory (LNLS), Campinas, SP, Brazil. The oxide film images enable evaluation of the pore size and form with a resolution similar to the transmission electron microscope (TEM) resolution. It is also observed that the anodizing process using pulse current produces an irregular structure of pore walls, and by direct cur-rent it is produced a rectilinear pore wall.

Journal of Materials Processing Technology **172[1], 146-151. 2006.**

P 045- 06 "Annealing experiments on induced fission tracks in apatite: Measurements of horizontal-confined track lengths and track densities in basal sections and randomly oriented grains"

Tello, C. A., Palissari, R., Hadler, J. C., Iunes, P. J., Guedes, S., Curvo, E. A. C., and Paulo, S. R.

To improve kinetic models for apatite fission-track annealing, we present new experimental annealing data that complement previously published data. To determine the degree of annealing of induced tracks, surface density (p), and mean horizontal-confined track lengths (1). were measured, both for basal and randomly oriented faces. Our annealing data were obtained by submitting an apatite sample collected in Itambe, Bahia, Brazil, to 46 different isothermal treatments where temperature ranged from 150 to 600 degrees C (duration of 1, 10, 100, and 1000 h). To compare the behavior of Itambe to Durango apatite, the latter was also annealed for I h in 9 isothermal experiments at temperatures between 240 and 380 degrees C. Our results show that the l/l(0) values in Durango are systematically smaller than those in Itambe sample, both in basal and random faces. The curves depicting relative track density reduction, rho/rho(0), and relative mean confined track length reduction, l/l(0), as a function of time and temperature, are similar for rho/rho(0) > similar to 0.5, but different for rho/rho(0) < similar to 0.5. In this interval, rho/rho(0),can be measured but the measurement of l/l(0) is very difficult because the confined tracks become undetectable. Measurements of rho/rho(0) and l/l(0) for tracks revealed in basal surfaces are systematically lower (but this difference is < 3%) than those in randomly oriented ones.

American Mineralogist **91[2-3], 252-260. 2006.**

P 046- 06 "Barrier-induced carrier localization effects in ordered/disordered/ordered quaternary quantum wells grown on GaAs substrates"

Ribeiro, E., Bernussi, A. A., Maltez, R. L., Carvalho, W., Gobbi, A. L., and Ugarte, D.

Optical and micro-structural properties of ordered/disordered/ordered InGaAsP quantum wells grown on GaAs substrates were investigated by photoluminescence spectroscopy, high-resolution transmission electron microscopy and selective area diffraction. Strong evidence of carrier localization effects was obtained from low temperature photoluminescence experiments. Photoluminescence spectra of thinner quantum wells were dominated by a broad emission band located at energies below the bandgap of the well material. The energy peak position of this emission varied considerably with the laser excitation power. Carrier localization was attributed to potential fluctuations in the barrier and well layers, as a result of two coexisting effects: Spontaneously atomic ordering and, in a minor degree, alloy inhomogeneities. We show that a reduction of the ordering degree in the bottom barrier layer resulted in a considerable decrease of localization effects in quaternary quantum well heterostructures.

Physical Review B 73[7]. 2006.

P 047- 06 "Black-box model for the complete characterization of the spectral gain and noise in semiconductor optical amplifiers"

Gallep, C. M., Rieznik, A. A., Fragnito, H., Frateschi, N. C., and Conforti, E.

A Black Box Model for the quick complete characterization of the optical gain and amplified spontaneous emission noise in Semiconductor Optical Amplifiers is presented and verified experimentally. This model provides good accuracy, even neglecting third order terms in the spectral gain shift, and can provide cost reduction in SOA characterization and design as well as provide simple algorithms for hybrid integration in-package control. (c) 2006 Optical Society of America.

Optics Express 14[4], 1626-1631. 2006.

P 048- 06 "Comment on "Sequencing-independent delocalization in a DNA-like double chain with base pairing" - Reply"

Caetano, R. A. and Schulz, P. A.

Physical Review Letters 96[5]. 2006.

P 049- 06 "Corrosion protection of fluorzirconate glasses coated by a layer of surface modified tin oxide nanoparticles"

Hammer, P., Rizzato, A. P., Alvarez, F., Landers, R., Pulcinelli, S. H., and Santilli, C. V.

The protection efficiency against water corrosion of fluorozirconate glass, ZBLAN, dip-coated by nanocrystalline tin oxide film containing the organic molecule Tirone (R) was investigated by X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM). The chemical bonding structure of the surface region and morphology were studied before and after two water exposure periods of 5 and 30 min. The results of the analysis for the as-grown sample revealed a SnO1.6 phase containing carbon and sulfur, related to Tiron (R), and traces of elements related to ZBLAN (Zr, F, Ba). This fact and the clear evidence of the presence of tin oxifluoride specie (SnOxFy) indicates a diffusion of the glass components into the porous coating. After water exposure, the increase of the oxygen concentration accompanied by a strong increase of Zr, F, Ba and Na content is interpreted as filling of the nanopores of the film by glass compounds. The formation of a compact protective layer is supported by the morphological changes observed by AFM. (c) 2005 Elsevier B.V. All rights reserved.

Thin Solid Films 502[1-2], 94-98. 2006.

P 050- 06 "Cross-sections for rotational excitations of C3H4 isomers by electron impact"

Lopes, A. R., Bettega, M. H. F., Varellai, M. T. N., and Lima, M. A. P.

We report elastic (rotationally summed) and rotationally resolved cross-sections for scattering of low-energy electrons by the C3H4 isomers allene, propyne, and cyclopropene, which belong to the D-2d, C-3v and C-2v groups respectively. We employed the Schwinger multichannel method with pseudopotentials at the static-exchange approximation, combined with the adiabatic-nuclei-rotation (ANR) approximation to calculate the rotational excitation cross-sections for energies ranging from 5 to 30 eV. Our rotational resolved cross-sections show the isomer effect more strongly related to scattering potentials of different molecular geometries and to transition selection rules than to differences in mass distribution which account for the energy spacing in the rotational spectra of the molecules.

European Physical Journal D 37[3], 385-392. 2006.

P 051- 06 "Crosstalk in double-pumped fiber optic parametric amplifiers for wavelength division multiplexing systems"

Boggio, J. M. C., Marconi, J. D., and Fragnito, H. L.

We study experimentally inter-channel crosstalk in double-pumped fiber optic parametric amplifiers constructed with conventional dispersion shifted fibers (DSFs) having different lengths (L-A = 13.8, L-B = 6.8, L-C = 4.3, and L-D = 0.8 km). For long fibers (L-A and L-B), eye diagram measurements in a 5-channel (100 GHz spacing) system show that in order to have negligible crosstalk, the output signal power per channel, P-s, should be limited to P-s < 0 dBm. By decreasing the fiber length (to L-C) it is possible to increase the output signal power and/or the number of signals while keeping the crosstalk on negligible levels. This trend was further confirmed by using a very short DSF (L-D = 0.8 km). Finally, we experimentally demonstrate that a general trend in 2P-FOPAs is that spurious FWM increases with the number of signal channels up to a given number of channels when a saturation regime is reached. This saturation of the generation of spurious tones occurs when the bandwidth occupied by the signals exceeds similar to 4-5 nm. (c) 2005 Elsevier B.V. All rights reserved.

Optics Communications 259[1], 94-103. 2006.

P 052- 06 "Dynamics of chiral oscillations: a comparative analysis with spin flipping"

Bernardini, A. E.

Chiral oscillation as well as spin flipping effects correspond to quantum phenomena of fundamental importance in the context of particle physics and, in particular, of neutrino physics. From the point of view of first quantized theories, we are specifically interested in pointing out the differences between chirality and helicity by obtaining their dynamic equations for a fermionic Dirac-type particle (neutrino). We also identify both effects when the nonminimal coupling with an external (electro)magnetic field in the neutrino interacting Lagrangian is taken into account. We demonstrate that, however, there is no constraint between chiral oscillations, when it takes place in vacuum, and the process of spin flipping related to the helicity quantum number, which does not take place in vacuum. To conclude, we show that the origin of chiral oscillations (in vacuum) can be interpreted as projections of very rapid oscillations of position onto the longitudinal direction of momentum.

Journal of Physics G-Nuclear and Particle Physics 32[1], 9-22.

P 053- 06 "Effects of non-parabolicity and in-plane magnetic fields on the cyclotron effective mass and g(perpendicular to)-factor in GaAs-(Ga,Al)As quantum wells"

Dios-Leyva, M., Reyes-Gomez, E., Perdomo-Leiva, C. A., and Oliveira, L. E.

The envelope-function approach is used to theoretically study the effects of in-plane magnetic fields on the cyclotron effective mass and Lande g(perpendicular to)-factor associated to conduction electrons in single GaAs-(Ga,Al)As quantum wells. Non-parabolic and anisotropy effects are included in the calculations within the Ogg-McCombe effective Hamiltonian to describe the electron states in the semiconductor heterostructure. The electronic structure and both the cyclotron effective mass and Lande g(perpendicular to)-factor were obtained, by expanding the corresponding envelope wave functions in terms of harmonic-oscillator wave functions, as functions of the in-plane magnetic field, cyclotron orbit-center position, and quantum-well widths. This procedure allows us to consider the different terms in the Hamiltonian on equal footing, avoiding therefore the use of approximate methods to obtain the envelope wave functions and the corresponding energy spectrum. Results obtained for the Lande g(perpendicular to)-factor were found in quite good agreement with available experimental measurements

Physical Review B 73[8]. 2006.

P 054- 06 "Exciton g factor of type-II InP/GaAs single quantum dots"

de Godoy, M. P. F., Gomes, P. F., Nakaema, M. K. K., Iikawa, F., Brasil, M. J. S. P., Caetano, R. A., Madureira, J. R., Bortoleto, J. R. R., Cotta, M. A., Ribeiro, E., Marques, G. E., and Bittencourt, A. C. R.

We investigated the magneto-optical properties of type-II InP/GaAs quantum dots using single-dot spectroscopy. The emission energy from individual dots presents a quadratic diamagnetic shift and a linear Zeeman splitting as a function of magnetic fields up to 10 T, as previously observed for type-I systems. We analyzed the in-plane localization of the carriers using the diamagnetic shift results. The values for the exciton g factor obtained for a large number of a InP/GaAs dots are mainly constant, independent of the emission energy, and therefore, of the quantum dot dimensions. The result is attributed to the weak confinement of the holes in type-II InP/GaAs quantum dots.

Physical Review B 73[3]. 2006.

P 055- 06 "Exotic characteristics of Centauro-I (1) - Re-examination of Centauro-I"

Ohsawa, A., Shibuya, E. H., and Tamada, M.

Nuclear Physics B-Proceedings Supplements 151, 227-230. 2006.

P 056- 06 "Exotic characteristics of Centauro-I (2) - A model to describe Centauro-I"

Ohsawa, A., Shibuya, E. H., and Tamada, M.

Nuclear Physics B-Proceedings Supplements 151, 231-235. 2006.

P 057- 06 "Genuine multipartite entanglement in quantum phase transitions"

de Oliveira, T. R., Rigolin, G., and de Oliveira, M. C.

We demonstrate that the global-entanglement (GE) measure defined by Meyer and Wallach [J. Math. Phys. 43, 4273 (2002)] is maximal at the critical point for the Ising chain in a transverse magnetic field. Our analysis is based on the equivalence of GE to the averaged linear entropy, allowing an understanding of multipartite entanglement (ME) features through a generalization of GE for bipartite blocks of qubits. Moreover, in contrast to GE, the proposed ME measure can distinguish three paradigmatic entangled states: GHZ(N) (Greenberger-Horne-Zeilinger), W-N, and EPRcircle times N/2. As such the generalized measure can detect a genuine ME and is maximal at the critical point.

Physical Review A 73[1]. 2006.

P 058- 06 "Geometric and electronic structure of carbon nanotube networks: 'super'-carbon nanotubes"

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

Structures of the so-called super-carbon nanotubes are proposed. These structures are built from single walled carbon nanotubes connected by Y-like junctions forming a 'super'-sheet that is then rolled into a seamless cylinder. Such a procedure can be repeated several times, generating a fractal structure. This procedure is not limited to carbon nanotubes, and can be easily modified for application to other systems. Tight binding total energy and density of states calculations showed that the 'super'-sheets and tubes are stable and predicted to present metallic and semiconducting behaviour.

Nanotechnology **17[3], 617-621. 2006.**

P 059- 06 "Hydrostatic-pressure effects on the correlated electron-hole transition energies in GaAs-Ga1-xAlxAs semiconductor quantum wells"

Raigoza, N., Duque, C. A., Reyes-Gomez, E., and Oliveira, L. E.

The effects of hydrostatic pressure on the correlated e-h transition energies in single GaAs-Ga1-xAlxAs quantum wells are calculated via a variational procedure, in the framework of the effective-mass and nondegenerate parabolic-band approximations. The valence-band anisotropy is included in our theoretical model by using different hole masses in different spatial directions. Both heavy- and light-hole exciton energies are obtained, and correlated e-h transition energies are found in good agreement with available experimental measurements. (c) 2006 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Physica Status Solidi B-Basic Solid State Physics **243[3], 635-640. 2006.**

P 060- 06 "Interatomic potential for the condensed phases of helium atoms"

Ujevic, S. and Vitiello, S. A.

Results from diffusion Monte Carlo have been used in fits of a damping function of the triple dipole and of the intensity of the exchange three-body interactions. The equations of state obtained considering this three-body potential are in excellent agreement with experiment both at the solid and liquid phases. The calculations show that exchange nonadditivities that contribute less than 0.2% of the two-body potential energy in the solid phase are needed to describe the properties of a system of helium atoms.

Physical Review B **73[1]. 2006.**

P 061- 06 "Investigations of intrinsic strain and structural ordering in a-Si : H using synchrotron radiation diffraction"

Harting, M., Britton, D. T., Minani, E., Ntsoane, T. P., Topic, M., Thovhogi, T., Osiele, O. M., Knoesen, D., Harindintwari, S., Furlan, F., and Giles, C.

The residual strain in a-Si:H layers has been determined directly using synchrotron radiation diffraction, at LNLS in Brazil, by two different methodologies. Using a method previously presented using laboratory X-ray sources, the height and length of side of the Si-Si-4 tetrahedron are determined from variations in the diffraction angle of the first two amorphous peaks. In a more extensive calculation, the spatially dependent pair correlation from changes in the bond length and the bond angle. Two different layers, deposited by HW-CVD oil glass substrates at growth temperatures of 300 and 500 degrees C, have been studied to investigate the effect of growth temperature on residual stress. (c) 2005 Elsevier B.V. All rights reserved

Thin Solid Films **501[1-2], 75-78. 2006.**

P 062- 06 "Kinetic model for the annealing of fission tracks in minerals and its application to apatite"

Guedes, S., Hadler, N. J. C., Oliveira, K. M. G., Moreira, P. A. F. P., Lunes, P. J., and Tello, S. C. A.

Fission tracks are formed in apatite and other minerals after the passage of fission fragments, which deliver locally intense amounts of energy to the crystal lattice. It is well known that the observable mean track lengths are reduced due to thermal treatment. If the annealing kinetics are known, it is sometimes possible to infer the thermal history a given sample experienced. Given the present lack of appropriate information on track formation, annealing and etching, researchers have used empirical models fitted to laboratory data on annealing to describe the annealing kinetics. In this work, a kinetic model is presented to describe the annealing process. It is based upon some experimental evidence. Instead of furnishing a complete and detailed description, it is intended to relate the observable quantities, namely, etched confined fission tracks, time and temperature based on simple hypotheses using a simplified view of the track. A kinetic model equation for the reduced mean track length, L/L-0, as a function of temperature, T, and heating duration, t, which fits quite well the available literature, has been derived and is given by (L/L-0) =exp{-n exp[-w'(U-0 - A(1) ln(t) + A(2) ln-2 (t) - k(B)T)(1/2)]} in which n is a parameter related to etching and track geometry, w' and U-0 are the width and the energy of a newly hypothesized potential barrier, respectively. A(1) and A(2) account for the dependence of the energy barrier on the duration of heating. Correlations with cell parameters of compositionally different apatites show that the barrier energy is the principal model descriptor for annealing. (c) 2005 Elsevier Ltd. All rights reserved

Radiation Measurements **41[4], 392-398. 2006.**

P 063- 06 "Local detection of entanglement"

Rigolin, G. and Escobar, C. O.

We construct an explicit model where it can be established if a two mode pure Gaussian system is entangled or not by acting only on one of the parts that constitute the system. Measuring the dispersion in momentum and the time evolution of the dispersion in position of one particle we can tell if entanglement is present as well as the degree of entanglement of the system

European Physical Journal D **37[2], 291-296. 2006.**

P 064- 06 "Local structure reconstruction in hydrogenated amorphous silicon from angular correlation and synchrotron diffraction studies"

Britton, D. T., Minani, E., Knoesen, D., Schut, H., Eijt, S. W. H., Furlan, F., Giles, C., and Harting, M.

Hydrogenated amorphous silicon (a-Si:H) is a widely used thin film semiconductor material which is still incompletely understood. It is generally assumed to form a continuous random network, with a high concentration of coordination defects (dangling bonds), which are hydrogen terminated. Neither the exact nature of these sites nor the degree of medium range order has been fully determined. In this paper, we present the first results for the local structure, from a combined study using angular correlation of positron annihilation radiation (ACAR) and synchrotron radiation diffraction. Reciprocal space information is obtained directly, for the mesoscale structure and the local defect structure, from the orientation dependent diffraction and 2D-ACAR patterns, respectively. Furthermore, inversion of both patterns yields a comparison of real space information through maps of the silicon-silicon pair correlation function and the electron-positron autocorrelation function B-2 gamma(r). From this information, it is possible to identify the dominant structural defect as a vacancy-size dangling bond cluster, around which the network strain is fully relaxed. (c) 2005 Published by Elsevier B.V.

Applied Surface Science 252 (9): 3194-3200 Feb 28 2006

P 065- 06 "Open photoacoustic cell: Applications in plant photosynthesis studies"

Mesquita, R. C., Mansanares, A. M., da Silva, E. C., Barja, P. R., Miranda, L. C. M., and Vargas, H.

In this article, we review the applications of the open photoacoustic cell (OPC) technique in studies of photosynthetic activity in plant leaves. The ability to perform in vivo and in situ measurements makes this technique particularly suitable for monitoring photosynthesis of plants subjected to specific treatments. Therefore, our objective in the present article is to describe, in more detail, the principles of the OPC technique and to follow the historical path of its applications related to the study of plants and photosynthesis, including recent results. It will be shown that the technique has been used to observe spectroscopic responses to herbicide application and to soil toxicity, in the study of photosynthesis induction, gas exchange, photochemical loss, photoinhibition, photosynthesis saturation, and photosynthetic responses to changes in parameters such as temperature, atmospheric conditions, and nutrient availability. Recent results have demonstrated its usefulness in the determination of the action spectrum directly from oxygen evolution measurements.

Instrumentation Science & Technology **34[1-2], 33-58. 2006.**

P 066- 06 "Orientational defects in ice Ih: An interpretation of electrical conductivity measurements"

de Koning, M., Antonelli, A., da Silva, A. J. R., and Fazzio, A

We present a first-principles study of the structure and energetics of Bjerrum defects in ice Ih and compare the results to experimental electrical conductivity data. While the DFT result for the activation energy is in good agreement with experiment, we find that its two components have quite different values. Aside from providing new insight into the fundamental parameters of the microscopic electrical theory of ice, our results suggest the activity of traps in doped ice in the temperature regime typically assumed to be controlled by the free migration of L defects.

Physical Review Letters **96[7]. 2006.**

P 067- 06 "Oxygen clamps in gold nanowires"

Novaes, F. D., da Silva, A. J. R., da Silva, E. Z., and Fazzio, A.

We investigate how the insertion of an oxygen atom in an atomically thin gold nanowire can affect its rupture. We find, using ab initio total energy density functional theory calculations, that O atoms when inserted in gold nanowires form not only stable but also very strong bonds, in such a way that they can extract atoms from a stable tip, serving in this way as a clamp that could be used to pull a string of gold atoms.

Physical Review Letters **96[1]. 2006.**

P 068- 06 "Oxygen, hydrogen, and deuterium effects on plasma nitriding of metal alloys"

Figueroa, C. A., Weber, S., Czerwiec, T., and Alvarez, F.

We report the oxygen, hydrogen, and deuterium effects on nitrogen implantation of stainless steel. Oxygen is absorbed on the surface creating a potential barrier and diminishing the nitrogen retention. Deuterium removes more oxygen from the surface than hydrogen, augmenting the nitrogen chemical potential and yielding faster nitrogen diffusion into the bulk material. (c) 2006 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Scripta Materialia **54[7], 1335-1338. 2006.**

P 069- 06 "Phase constraint for the waves diffracted by lossless symmetrical gratings at Littrow mount"

Cordeiro, C. M. B., de Carvalho, E. J., Cescato, L., Freschi, A. A., and Li, L. F.

The energy conservation of grating diffraction is analyzed in a particular condition of incidence in which two incident waves reach a symmetrical grating from the two sides of the grating normal at the first-order Littrow mounting. In such a situation the incident waves generate an interference pattern with the same period as the grating. Thus in each direction of diffraction, interference occurs between two consecutive diffractive orders of the symmetrical incident waves. By applying only energy conservation and the geometrical symmetry of the grating profile to this problem it is possible to establish a general constraint for the phases and amplitudes of the diffracted orders of the same incident wave. Experimental and theoretical results are presented confirming the obtained relations. (c) 2006 Optical Society of America.

Journal of the Optical Society of America A-Optics Image Science and Vision **23[1], 166-171. 2006.**

P 070- 06 "Single wall carbon nanotubes polymerization under compression: An atomistic molecular dynamics study"

Braga, S. F. and Galvao, D. S.

Recently, it was reported experimental observations of crosslinking between carbon nanotubes (CNTs) under pressure. Similarly to CNT growth formation the details of these polymerization processes are still unclear. In this work, we report a molecular dynamics simulation of the polymerization of a bundle of single-wall carbon nanotubes under compression using Brenner reactive potentials. Our results show that for small tube diameters extensive crosslinking formation can occur. For larger tube diameter, we obtained the first theoretical evidences that scroll-like structures (recently experimentally obtained) can be formed from SWCNTs. (c) 2005 Elsevier B.V. All rights reserved

Chemical Physics Letters **419[4-6], 394-399. 2006.**

P 071- 06 "Solution conformation and heparin-induced dimerization of the full-length extracellular domain of the human amyloid precursor protein"

Gralle, M., Oliveira, C. L. P., Guerreiro, L. H., McKinstry, W. J., Galatis, D., Masters, C. L., Cappai, R., Parker, M. W., Ramos, C. H. I., Torriani, I., and Ferreira, S. T.

Proteolytic cleavage of the amyloid precursor protein (APP) by beta and gamma-secretases gives rise to the beta-amyloid peptide, considered to be a causal factor in Alzheimer's disease. Conversely, the soluble extracellular domain of APP (sAPP alpha), released upon its cleavage by alpha-secretase, plays a number of important physiological functions. Several APP fragments have been structurally characterized at atomic resolution, but the structures of intact APP and of full-length sAPP alpha have not been determined. Here, ab initio reconstruction of molecular models from high-resolution solution X-ray scattering (SAXS) data for the two main isoforms of sAPP alpha (sAPP alpha(695) and sAPP alpha(770)) provided models of sufficiently high resolution to identify distinct structural domains of APP. The fragments for which structures are known at atomic resolution were fitted within the solution models of full-length sAPPa, allowing localization of important functional sites (i.e. glycosylation, protease inhibitory and heparin-binding sites). Furthermore, combined results from SAXS, analytical ultracentrifugation (AUC) and size-exclusion chromatography (SEC) analysis indicate that both sAPP alpha isoforms are monomeric in solution. On the other hand, SEC, bis-ANS fluorescence, AUC and SAXS measurements showed that sAPPa forms a 2:1 complex with heparin. A conformational model for the sAPP alpha:heparin complex was also derived from the SAXS data. Possible implications of such complex formation for the physiological dimerization of APP and biological signaling are discussed in terms of the structural models proposed.

Journal of Molecular Biology **357[2], 493-508. 2006.**

P 072- 06 "Structural changes in amorphous carbon nitride films due to bias voltage"

Champi, A. and Marques, F. C.

The effect of bias voltage on the structural properties of amorphous carbon nitride films deposited by plasma decomposition of methane (CH4) and nitrogen (N-2) is investigated. A series of films was deposited under conditions in which diamond-like a-C:H films are obtained, i.e., bias of -200 V, and pressure of 1.0 Pa. Another series of films was deposited under conditions where graphite-like films are obtained, i.e., bias of -800 V, and pressure of 12 Pa. To investigate the effect of these conditions on the properties of the films, FTIR, Raman, nanohardness, and ESR measurements were undertaken. It was observed that the incorporation of nitrogen and the investigated properties depend on the base structure (diamond-like vs. graphite-like).

Thin Solid Films **501[1-2], 362-365. 2006.**

P 073- 06 "Study of Co2+ in different crystal field environments"

Foglio, M. E. and Barberis, G. E.

We consider the ESR of Co2+ in different environments: in an regular octahedron (Co2+ in a MgO crystal), in a deformed octahedron (Co2+ in single crystals and powder samples of NH4NiPO4 center dot 6H(2)O) or in a trigonal bipyramid (Co2+ in powders of Co-2(OH)PO4 and Co-2(OH)AsO4). We Study the effect of the non-cubic crystal fields in the ESR of Co2+ in the deformed octahedron, by employing the normal modes of this structure to simplify the systematic study of the effect of these fields. A similar study was done for the deformed trigonal bipiramid, and it was necessary to derive the normal modes of this complex that are relevant to our problem

Brazilian Journal of Physics **36[1A], 40-54. 2006.**

P 074- 06 "The Pyrococcus exosome complex - Structural and functional characterization"

Ramos, C. R. R., Oliveira, C. L. P., Torriani, I. L., and Oliveira, C. C.

The exosome is a conserved eukaryotic enzymatic complex that plays an essential role in many pathways of RNA processing and degradation. Here, we describe the structural characterization of the predicted archaeal exosome in solution using small angle x-ray scattering. The structure model calculated from the small angle x-ray scattering pattern provides an indication of the existence of a disk-shaped structure, corresponding to the "RNases PH ring" complex formed by the proteins aRrp41 and aRrp42. The RNases PH ring complex corresponds to the core of the exosome, binds RNA, and has phosphorolytic and polymerization activities. Three additional molecules of the RNA-binding protein aRrp4 are attached to the core as extended and flexible arms that may direct the substrates to the active sites of the exosome. In the presence of aRrp4, the activity of the core complex is enhanced, suggesting a regulatory role for this protein. The results shown here also indicate the participation of the exosome in RNA metabolism in Archaea, as was established in Eukarya

Journal of Biological Chemistry **281[10], 6751-6759. 2006.**

P 075- 06 "Theoretical description of the colossal entropic magnetocaloric effect: Application to MnAs"

von Ranke, P. J., Gama, S., Coelho, A. A., de Campos, A., Carvalho, A. M. G., Gandra, F. C. G., and de Oliveira, N. A.

We report on the theoretical investigations into the recently discovered colossal entropy change in MnAs under magnetic-field change in an isothermal process. The phenomenological model takes into account the exchange-Zeeman interactions, magnetoelastic interactions, the external pressure effect, and the magnetic-field dependence of the lattice entropy. The results show the fundamental role of the lattice entropy in the colossal entropy change for the MnAs compound. The best model parameters and their variation with pressure were determined

Physical Review B **73[1]. 2006.**

P 076- 06 "Theoretical modelling of low band-gap organic oligomers"

Amazonas, J. G., Guimaraes, J. R., Costa, S. C. S., Laks, B., and Del Nero, J.

Two low band-gap polymers (gap energy similar to 1 eV) based on carbon-bridged dithienyl monomers have been investigated by density functional theory (B3LYP/6-31G) and semiempirical/CI methods. Theoretical absorption spectra from monomers to pentamers were obtained and showed good agreement with the experimental spectra of the polymers. Comparison with data for oligomers of CDM and BDT (dithiophene derivatives indicated that the new polymers have a small band gap and could fulfill the conditions for n-dopability.

Journal of Molecular Structure-Theochem **759[1-3], 87-91. 2006.**

P 077- 06 "Thermo-statistics of irreversible processes: a Boltzmann-Gibbs-style ensemble formalism"

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

The area of Physics indicated in the title is nowadays of quite relevant interest, not only from the purely scientific point of view, but specially for its applied aspects associated to the present-time point-first-technologies. A particular research trend in the theory of irreversible processes, which are evolving in time in systems arbitrarily departed from equilibrium, is here briefly described. It consists in the construction of a Gibbs-style nonequilibrium ensemble formalism. The derivation of a nonequilibrium statistical operator is described (the variational approach of Predictive Statistical Mechanics is used). The main questions involved are presented and applications are briefly mentioned

Brazilian Journal of Physics 36[1A], 97-106. 2006.

P 078- 06 "Thermodynamic modeling of phase separation in manganites"

Sacanell, J., Parisi, F., Campoy, J. C. P., and Ghivelder, L.

We present a phenomenological model based on the thermodynamics of the phase separated state of manganites, accounting for its static and dynamic properties. Through calorimetric measurements on La0.225Pr0.4Ca0.375MnO3 the low temperature free energies of the coexisting ferromagnetic and charge ordered phases are evaluated. The phase separated state is modeled by free energy densities uniformly spread over the sample volume. The calculations contemplate the out of equilibrium features of the coexisting phase regime, to allow a comparison between magnetic measurements and the predictions of the model. A phase diagram including the static and dynamic properties of the system is constructed, showing the existence of blocked and unblocked regimes which are characteristics of the phase separated state in manganites

Physical Review B 73[1]. 2006.

P 079- 06 "Two-photon anisotropy: Analytical description and molecular modeling for symmetrical and asymmetrical organic dyes"

Fu, J., Przhonska, O. V., Padilha, L. A., Hagan, D. J., Van Stryland, E. W., Belfield, K. D., Bondar, M. V., Slominsky, Y. L., and Kachkovski, A. D.

One- and two-photon anisotropy spectra of a series of symmetrical and asymmetrical polymethine (PD) and fluorene molecules were measured experimentally and discussed theoretically within the framework of three-state and four-state models. For all the molecules discussed in this paper, the experimental two-photon anisotropy values, r(2PA), lie in the relatively narrow range from 0.47 to 0.57 and remain almost independent of wavelength over at least two electronic transitions. This is in contrast with their one-photon anisotropy, which shows strong wavelength dependence, typically varying from approximate to 0 to 0.38 over the same transitions. A detailed analysis of the two-photon absorption (2PA) processes allows us to conclude that a three-state model can explain the 2PA anisotropy spectra of most asymmetrical PDs and fluorenes. However, this model is inadequate for all the symmetrical molecules. Experimental values Of r2PA for symmetrical polymethines and fluorenes can be explained by symmetry breaking leading to the deviation of the orientation of the participating transition dipole moments from their "classical" orientations.

Chemical Physics 321[3], 257-268. 2006.

P 080- 06 "Where are ELKO spinor fields in Lounesto spinor field classification?"

Da Rocha, R. and Rodrigues, W. A.

This paper proves that from the algebraic point of view ELKO spinor fields belong together with Majorana spinor fields to a wider class, the so-called flagpole spinor fields, corresponding to the class 5, according to Lounesto spinor field classification. We show moreover that algebraic constraints imply that any class 5 spinor field is such that the 2-component spinor fields entering its structure have opposite helicities. The proof of our statement is based on Lounesto general classification of all spinor fields, according to the relations and values taken by their associated bilinear covariants, and can eventually shed some new light on the algebraic investigations concerning dark matter

Modern Physics Letters A 21[1], 65-74. 2006.

Abstracta

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