



# Abstracta

Ano VII - N. 02

**ABR.05**

## TRABALHOS PUBLICADOS

Fevereiro 2005 à Março 2005

P 052 à P 082/ 2005

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## TRABALHOS PUBLICADOS

### P 052- 05 "A kinetic model for two step crystallization"

Clemente, R. A. and Saleh, A. A.

A simple phenomenological model for the crystallization kinetic of two step phase transformations is proposed. The treatment assumes that an amorphous or undercooled liquid material begins to transform into a transient metastable phase which starts to grow, at the same time the final phase starts to grow inside the metastable one, consuming it but without exceeding it. The starting material and the different phases are all assumed of the same chemical composition and the transformation processes are assumed interface controlled. As a result the starting material completely transforms to the final phase and no trace of the transient one will remain. The model properly take into account the impingement of growing grains and can be applied to a number of transformations like solidification of undercooled liquid metallic alloys and devitrification of glasses and amorphous solids

*Journal of the Physical Society of Japan* 74[2], 773-775. 2005.

### P 053- 05 "The Casimir operator of SO(1,2) and the Poschl Teller potential: an AdS approach"

da Rocha, R. and de Oliveira, E. C.

We present and discuss some features of the anti-de Sitter spacetime, that is jointly with de Sitter and Minkowski is only, the unique maximal isotropic manifold. Among all possible lorentzian manifolds, we restrict our attention to the anti-de Sitter (AdS) spacetime, with metric  $diag(1, -1, -1)$ . We start by presenting the conformal time metric of AdS and we then show how we can obtain the Schrodinger formalism [1]. The Lie algebra  $so(1,2)$  is introduced and used to construct spin and ladder operators. After presenting the unitary representations, the AdS(1,2) spacetime is suitably parametrized and a representation of SO(1,2) is obtained, from which the Schrodinger equation with Poschl-Teller potential is immediately deduced. Finally, we discuss some relations between the relativistic harmonic oscillator and the Klein-Gordon equation, using the AdS(1,2) static frame. Possible applications of the presented formalism are provided

*Revista Mexicana de Fisica* 51[1], 1-4. 2005.

### P 054- 05 "Concentration effects of volatile anesthetics on the properties of model membranes: A coarse-grain approach"

Pickholz, M., Saiz, L., and Klein, M. L.

To gain insights into the molecular level mechanism of drug action at the membrane site, we have carried out extensive molecular dynamics simulations of a model membrane in the presence of a volatile anesthetic using a coarse-grain model. Six different anesthetic (halothane)/lipid (dimyristoylphosphatidylcholine) ratios have been investigated, going beyond the low doses typical of medical applications. The volatile anesthetics were introduced into a preassembled fully hydrated 512-molecule lipid bilayer and each of the molecular dynamics simulations were carried out at ambient conditions, using the NPT ensemble. The area per lipid increases monotonically with the halothane concentration and the lamellar spacing decreases, whereas the lipid bilayer thickness shows no appreciable differences and only a slight increase upon addition of halothane. The density profiles of the anesthetic molecules display a bimodal distribution along the membrane normal with maxima located close to the lipid-water interface region. We have studied how halothane molecules interact between the two maxima of the bimodal distribution and we observed a different mechanism at low and high anesthetic concentrations. Through the investigation of the reorientational motions of the lipid tails, we found that the anesthetic molecules increase the segmental order of the lipids close to the membrane surface.

*Biophysical Journal* 88[3], 1524-1534. 2005.

### P 055- 05 "Eikonal representation in the momentum-transfer space"

Carvalho, P. A. S., Martini, A. F., and Menon, M. J.

By means of empirical fits to the differential cross section data on pp and (p) over bar elastic scattering, above 10 GeV (center-of-mass energy), we determine the eikonal in the momentum-transfer space ( $q(2)$ -space). We make use of a numerical method and a novel semi-analytical method, through which the uncertainties from the fit parameters can be propagated up to the eikonal in the  $q(2)$ -space. A systematic study of the effect of the experimental information at large values of the momentum transfer is developed and discussed in detail. We present statistical evidence that the imaginary part of the eikonal changes sign in the  $q(2)$ -space and that the position of the zero decreases as the energy increases; after the position of the zero, the eikonal presents a minimum and then goes to zero through negative values. We discuss the applicability of our results in the phenomenological context, outlining some connections with nonperturbative QCD. A short review and a critical discussion on the main results concerning "model-independent" analyses are also presented

*European Physical Journal C* 39[3], 359-376. 2005.

### P 056- 05 "Electronic structure information of metals and alloys from Auger and photoemission"

Kleiman, G. G.

We report some of the results of extensive experimental and theoretical studies by our group of the XPS and Auger spectra of the transition and noble metals and some of their alloys: we concentrate on those aspects of the spectra which regard the determination of electronic structure. Consideration of the Auger kinetic energies yields insight into screening mechanisms and suggests methods for extracting electronic structure changes in alloys from XPS and XAES shifts. We demonstrate that the charge transfer in a number of alloys (AuPd, CuPd, AgPd, AuCu, AgAu and CuNi) appears to be negligible (i.e., on the order of hundredths of electrons/atom). Examples (i.e., AuZn, AuMg, AuPd, AgPd and CuNi) of the results for the d- and sp-electron occupations are given.

*Journal of Molecular Catalysis A-Chemical* 228[1-2], 137-143. 2005.

### P 057- 05 "Evidences for intermediate valence behavior in CeNi5In"

Rojas, D. P., Pereira, L. C. J., Salamakha, P., Lopes, E. B., Waerenborgh, J. C., da Silva, L. M., and Gandra, F. G.

We report results on transport, magnetic and specific heat measurements of the CeNi5In compound. It was found to crystallize in the hexagonal CeNi5Sn type of structure, space group P6(3)/mmm with parameters  $a = 4.891(1)$  angstrom and  $c = 19.878(1)$  angstrom. The magnetic susceptibility curve shows an absolute small value of order of  $10(-3)$  emu/mol and deviation from Curie-Weiss behavior for  $T < 100$  K. The low temperature ( $T < 10$  K) specific heat and resistivity data is consistent with Fermi liquid properties. The results suggest a probable intermediate valence or spin fluctuation behavior for the title intermetallic compound.

*Journal of Alloys and Compounds* 391[1-2], L5-L7. 2005.

### P 058- 05 "Fabrication and characterization of a PbTe quantum dots multilayer structure"

Rodriguez, E., Jimenez, E., Jacob, G. J., Neves, A. A. R., Cesar, C. L., and Barbosa, L. C.

Multilayer PbTe quantum dots (QDs) and SiO2 were grown by pulsed laser deposition (PLD) and Plasma enhanced chemical vapor deposition (PECVD) techniques. The crystalline structure, QD size and size dispersion were observed by high-resolution transmission electron microscopy (HRTEM) measurements. This technique allows one to grow PbTe QDs as small as 1.8 nm diameter and 0.6 nm size dispersion. The whole structure can be used in a Fabry-Perot cavity for an optical device operating at the mid-infrared region. (C) 2004 Elsevier B.V. All rights reserved

*Physica E-Low-Dimensional Systems & Nanostructures* 26[1-4], 361-365. 2005.

**P 059- 05** "Ferromagnetic nanoclusters formed by Mn implantation in GaAs"

Couto, O. D. D., Brasil, M. J. S. P., Iikawa, F., Giles, C., Adriano, C., Bortoleto, J. R. R., Pudenzi, M. A. A., Gutierrez, H. R., and Danilov, I.

Ferromagnetic clusters were incorporated into GaAs samples by Mn implantation and subsequent annealing. The composition and structural properties of the Mn-based nanoclusters formed at the surface and buried into the GaAs sample were analyzed by x-ray and microscopic techniques. Our measurements indicate the presence of buried MnAs nanoclusters with a structural phase transition around 40degreesC, in accord with the first-order magneto-structural phase transition of bulk MnAs. We discuss the structural behavior of these nanoclusters during their formation and phase transition, which is an important point for technological applications.

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*Applied Physics Letters* 86[7]. 2005.

**P 060- 05** "Frustration effects on small-world networks"

Campos, P. R. A., De Oliveira, V. M., and Moreira, F. G. B.

We investigate the frustration effects on small-world networks by studying antiferromagnetic Ising model in two dimensions. When the rewiring is constrained to those sites such that the interaction still occurs between spins in distinct sublattices and frustration does not take place, we observe that the system behaves as in previous investigations of ferromagnetic Ising model. However, when the rewiring procedure does not only produce interactions between spins in distinct sublattices, small-world configurations can effectively produce geometrical frustration and we attain a different critical behavior. In the frustrated case, the critical temperature decreases with the augment of the rewiring probability and the magnetic ordering presents two different regimes for low and high p

*International Journal of Modern Physics C* 15[9], 1269-1277. 2004.

**P 061- 05** "General relativistic model for the gravitational field of active galactic nuclei surrounded by a disk"

Vogt, D. and Letelier, P. S.

An exact but simple general relativistic model for the gravitational field of active galactic nuclei is constructed, based on the superposition in Weyl coordinates of a black hole, a Chazy-Curzon disk and two rods, which represent matter jets. The influence of the rods on the matter properties of the disk and on its stability is examined. We find that in general they contribute to destabilize the disk. Also the oscillation frequencies for perturbed circular geodesics on the disk are computed, and some geodesic orbits for the superposed metric are numerically calculated

*Physical Review D* 71[4]. 2005.

**P 062- 05** "High resolution, large spectral range, in variable-included-angle soft X-ray monochromators using a plane VLS grating"

Reininger, R. and de Castro, A. R. B.

We give a unified discussion of two different approaches to the design of grazing incidence monochromators with a variable line spacing (VLS) grating for soft X-ray undulator sources. Neither one uses an entrance slit and both work with a fixed position exit slit. In one approach, being constructed at LNLS and designed for the energy range  $100 < E < 1000$  eV, the choice of the VLS parameters allows for the operation at a variable c-value with a single plane grating and little sacrifice in the maximum resolving power. In this case source size limited resolving power of circa 40 000 is expected at 100 eV. In the second approach, for the storage ring in Wisconsin, two gratings covering the energy range  $40 < E < 1500$  eV are used, one capable of delivering a resolving power larger than 20 000 at 860 eV and the other lower resolving power but much higher flux.

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*Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment* 538[1-3], 760-770. 2005.

**P 063- 05** "Linear and circularly polarized light to study anisotropy and resonant scattering in magnetic thin films"

Tolentino, H. C. N., Cezar, J. C., Souza-Neto, N. M., and Ramos, A. Y.

The remarkable polarization properties of synchrotron light have lead to the advent of modern synchrotron-related spectroscopic studies with angular and/or magnetic selectivity. Here an overview is given of the prominent aspects of the polarization of the light delivered by a bending magnet, and some dichroic properties in X-ray absorption spectroscopy (XAS). Two studies developed at the Brazilian Synchrotron Light Laboratory are then reported, exemplifying the profit gained using linear and circular polarization of X-rays for the study of magnetic thin films and multilayers. Angle-resolved XAS was used in strained manganite thin films to certify a model of local distortion limited within the MnO6 polyhedron. A pioneering experience of X-ray magnetic scattering at grazing incidence associated with dispersive XAS in a Co/Gd multilayer draws new perspectives for magnetic studies in thin films and multilayers under atmospheric conditions in the hard X-ray range

*Journal of Synchrotron Radiation* 12, 168-176. 2005.

**P 064- 05** "Mapping contacts between regulatory domains of skeletal muscle TnC and TnI by analyses of single-chain chimeras"

Tirolì, A. O., Tasic, L., Oliveira, C. L. P., Bloch, C., Torriani, I., Farah, C. S., and Ramos, C. H. I.

The troponin (Tn) complex is formed by TnC, TnI and TnT and is responsible for the calcium-dependent inhibition of muscle contraction. TnC and TnI interact in an antiparallel fashion in which the N domain of TnC binds in a calcium-dependent manner to the C domain of TnI, releasing the inhibitory effect of the latter on the actomyosin interaction. While the crystal structure of the core cardiac muscle troponin complex has been determined, very little high resolution information is available regarding the skeletal muscle TnI-TnC complex. With the aim of obtaining structural information regarding specific contacts between skeletal muscle TnC and TnI regulatory domains, we have constructed two recombinant chimeric. proteins composed of the residues 1-91 of TnC linked to residues 98-182 or 98-147 of TnI. The polypeptides were capable of binding to the thin filament in a calcium-dependent manner and to regulate the ATPase reaction of actomyosin. Small angle X-ray scattering results showed that these chimeras fold into compact structures in which the inhibitory plus the C domain of TnI, with the exception of residues 148-182, were in close contact with the N-terminal domain of TnC. CD and fluorescence analysis were consistent with the view that the last residues of TnI (148-182) are not well folded in the complex. MS analysis of fragments produced by limited trypsinolysis showed that the whole TnC N domain was resistant to proteolysis, both in the presence and in the absence of calcium. On the other hand the TnI inhibitory and C-terminal domains were completely digested by trypsin in the absence of calcium while the addition of calcium results in the protection of only residues 114-137

*Febs Journal* 272[3], 779-790. 2005.

**P 065- 05** "Morphological and magnetic properties of carbon-nickel nanocomposite thin films"

Fonseca, F. C., Ferlauto, A. S., Alvarez, F., Goya, G. F., and Jardim, R. F.

Carbon-nickel nanocomposite thin films were prepared by ion beam cosputtering a graphite target having a nickel chip attached to its surface. The amount of Ni incorporated in the films was controlled by the size of the Ni chip (from 5 to 22 wt %), and measured by in situ x-ray photoelectron spectroscopy (XPS). High-resolution transmission electron microscopy images indicated that the films have a granular structure with nanosize Ni particles embedded in an amorphous carbon matrix. The Ni particles have an average radius of similar to 2 nm, with a rather narrow size distribution. Magnetization measurements revealed that films are superparamagnetic and present blocking temperatures  $T_B < 13$  K. The combined results of XPS and magnetic measurements indicate that Ni particles are free from oxide layers. In addition, the estimated value of their anisotropy constant was found to be higher than the expected value for bulk Ni. The origin of this discrepancy is associated with both shape and interaction anisotropies.

*Journal of Applied Physics* 97[4]. 2005.

**P 066- 05** "Multiposition multipass Thomson scattering diagnostic for tokamak NOVA-UNICAMP"

Monteiro, M. J. R. and Machida, M.

In this article, the use of an 8 x 8-matrix independent 10-stage dynode multichannel photomultiplier for multipass Thomson scattering is described. Light from a pulsed ruby laser is irradiated 12 times in the central region of plasma using the resonator cavity of a multipass system, and integrated scattered light is detected for the first time using the multichannel photomultiplier XP1752 from Philips. The simultaneous measurements of electron temperature and density at four spatial positions, which can be extended by increasing the numbers of Analog-to-Digital Converter (ADC) channels and signal output windows, have been performed throughout full discharge by a shot-to-shot procedure. An electron temperature  $T_e$  of 50 eV and a density  $n(e)$  of  $5 \times 10^{12} \text{ cm}^{-3}$  were measured for the tokamak, NOVA-UNICAMP. Because of the use of a low-power ruby laser (typically 1 J) and scattered light amplification using a multipass system, the level of stray light was kept low and absolute density measurements were made possible by nitrogen Rayleigh scattering

*Japanese Journal of Applied Physics Part 1-Regular Papers Short Notes & Review Papers* 44[1A], 383-388. 2005.

**P 067- 05** "Nearly 100% diffraction efficiency fixed holograms in oxidized iron-doped LiNbO<sub>3</sub> crystals using self-stabilized recording technique"

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

We analyse the advantages and limitations of self-stabilized holographic recording for fixing in photorefractive iron-doped LiNbO<sub>3</sub> crystals. We study the effect of the degree of oxidation on the development of the fixed grating, confirm the importance of highly oxidized crystals to obtain fixed holograms with high diffraction efficiency and put it on a quantitative basis. We also discuss the effect of iron-concentration and the way oxidation may introduce dopant-saturation effects in the recording. Accounting on the different parameters here considered we propose a very simple and well performing procedure to produce nearly 100% diffraction efficiency fixed gratings.

*Optics Communications* 247[1-3], 39-48. 2005.

**P 068- 05** "Observation of asymmetric transverse voltage in granular high-T<sub>c</sub> superconductors"

da Luz, M. S., de Carvalho, F. J. H., dos Santos, C. A. M., Shigue, C. Y., Machado, A. J. S., and da Silva, R. R.

This work reports the influence of the granularity on the transverse voltage as a function of the temperature,  $V_{XY}(T)$ , in polycrystalline samples of  $\text{Bi}_2\text{Sr}_2\text{Ca}_0.8\text{Pr}_0.2\text{Cu}_2\text{O}_{8+\delta}$  composition. It is observed nonzero transverse voltage at zero external magnetic field in the vicinity of the superconducting transition while far away from it, both above and below, no such voltage was detected. Measurements of  $V_{XY}(T)$  in both directions of magnetic field allowed to calculate the symmetric and asymmetric transverse voltages in the full range of the applied magnetic field studied (zero up to 9 T). The symmetric transverse voltage as a function of the temperature presents sign reversal of the Hall resistance and positive Hall voltage at normal state such as expected for hole-doped high critical temperature superconductors. On the other hand, the asymmetric component of  $V_{XY}(T)$  shows a peak near the superconducting transition which has been recently reported in literature.  $V_{XY}(T)$  curves measured in a sample with double superconducting transition, which was confirmed by ac-susceptibility measurements and hysteresis loops of the magneto-resistance, present two peaks in the asymmetric component. These peaks are related to the intergranular and intragranular transitions and can be explained within the framework of Josephson and Abrikosov vortices and anti-vortices motion. By comparing the temperature dependence of the asymmetric transverse voltage and the derivative of longitudinal voltage is possible to observe a specific relation between both transport properties, which is noted to be valid not only at zero applied magnetic field but also under applied field. (c) 2004 Elsevier B.V. All rights reserved

*Physica C-Superconductivity and Its Applications* 419[3-4], 71-78. 2005.

**P 069- 05** "Optimization techniques for the estimation of the thickness and the optical parameters of thin films using reflectance data"

Ventura, S. D., Birgin, E. G., Martinez, J. M., and Chambouleyron, I.

The present work considers the problem of estimating the thickness and the optical constants (extinction coefficient and refractive index) of thin films from the spectrum of normal reflectance  $R$ . This is an ill-conditioned highly underdetermined inverse problem. The estimation is done in the spectral range where the film is not opaque. The idea behind the choice of this particular spectral range is to compare the film characteristics retrieved from transmittance  $T$  and from reflectance data. In the first part of the paper a compact formula for  $R$  is deduced. The approach to deconvolute the  $R$  data is to use well-known information on the dependence of the optical constants on photon energy of semiconductors and dielectrics and to formulate the estimation as a nonlinear optimization problem. Previous publications of the group on the subject provide the guidelines for designing the new procedures. The consistency of the approach is tested with computer-generated thin films and also with measured  $R$  and  $T$  spectral data of an a-Si:H film deposited onto glass. The algorithms can handle satisfactorily the problem of a poor photometric accuracy in reflectance data, as well as a partial linearity of the detector response. The results on gedanken films and on a-Si:H indicate a very good agreement between expected and retrieved values. (C) 2005 American Institute of Physics

*Journal of Applied Physics* 97[4]. 2005.

**P 070- 05** "Oriented carbon nanostructures containing nitrogen obtained by ion beam assisted deposition"

Paredes, P., Figueroa, C. A., Zagonel, L. F., Reichert, F. R., Ribeiro, C. R. M., Point, S., Godon, C., Minea, T. M., and Alvarez, F.

In this paper, we report the deposition of graphite multilayers containing nitrogen covering nanometric nickel particles. In-situ photoelectron emission spectroscopy (XPS) reveals the presence of nitrogen in the carbon layer covering the nickel particles. The field emission properties of the structures are reported. Atomic force microscopy displays regular domelike structures. Raman spectroscopy shows the characteristic frequencies associated with graphite and disordered structures. High-resolution transmission electron microscopy confirms the presence of multiwall well-organized graphite layers covering the nickel particles. Disorder increases on increasing nitrogen content. The samples were prepared in-situ by depositing first a few atomic layers of nickel and subsequent islands formation by thermal annealing. Then, an argon ion beam bombards an ultrapure carbon target and simultaneously the growing film is assisted with a second low-energy nitrogen ion beam (ion beam assisted deposition)

*Journal of Nanoscience and Nanotechnology* 5[2], 188-191. 2005.

**P 071- 05** "Photoluminescence and the Raman scattering in porous GaSb produced by ion implantation"

Danilov, Y. A., Biryukov, A. A., Goncalves, J. L., Swart, J. W., Iikawa, F., and Teschke, O.

Atomic-force microscopy, photoluminescence, and Raman scattering are used to study the formation of the porous layer in ion-implanted GaSb. As the ion dose increases, first a system of hillocks is formed at the GaSb surface and then a porous layer is produced. The height of the step at the boundary between the porous layer and the unirradiated region can be as large as 1  $\mu\text{m}$ . A broad band is observed in the photoluminescence spectrum in the range from 1.1 to 1.65 eV for ion-implanted GaSb; the intensity of this band increases with the ion dose. Additional lines peaked at 111 and 145  $\text{cm}^{-1}$  are observed in the Raman spectra of porous GaSb. These lines are characteristic of an oxidized semiconductor. The data obtained indicate that the porous layer that formed as a result of ion implantation into GaSb exhibits properties that are characteristic of nanocrystalline systems. (C) 2005 Pleiades Publishing, Inc

*Semiconductors* 39[1], 132-135. 2005.

**P 072- 05 "Prediction of ordered phases of encapsulated C-60, C-70, and C-78 inside carbon nanotubes"**

Troche, K. S., Coluci, V. R., Braga, S. F., Chinellato, D. D., Sato, F., Legoas, S. B., Rurali, R., and Galvao, D. S.

We report the first detailed fully atomistic molecular dynamics study of the encapsulation of symmetric (C-60) and asymmetric fullerenes (C-70 and C-78) inside single-walled carbon nanotubes of different diameters. Different ordered phases have been found and shown to be tube diameter dependent. Rotational structural disorder significantly affecting the volume fraction of the packing was observed for the molecular arrangements of asymmetric fullerenes. Although these effects make more difficult the existence of ordered phases, our results showed that complex packing arrangements (very similar to the ones obtained for C-60) are also possible for C-70 and C-78. Comparisons with results from continuum and hard-sphere models, ab initio electronic structure calculations, and simulations of the high-resolution transmission electron microscopy images of the obtained fullerene packing phases are also presented

*Nano Letters* 5[2], 349-355. 2005.

**P 073- 05 "Quantum dots, efficient fluorescent markers for red cells"**

Castro, V., Farias, P. M. A., Santos, B. S., Menezes, F. D., Ferreira, R. C., Lima, P. R. M., Fontes, A., Barias-Castro, M. L., and Cesar, C. L.

*Blood* 104[11], 741A-741A. 2004.

**P 074- 05 "Real-time observation of ground state proton transfer: a model study"**

Arasaki, Y., Yamazaki, K., Varella, M. T. D., and Takatsuka, K.

We propose a femtosecond dump-probe photoelectron spectroscopy scheme for the real-time observation of ground state proton transfer. Feasibility of such a scheme is investigated with quantum wavepacket dynamics on a model potential. Formation of a proton transfer wavepacket by dumping from an eigenstate or from a delocalized mixture of eigenstates is discussed. Characteristic features of proton transfer observed in the time-dependent ion signal and photoelectron kinetic energy spectra are shown, along with a method of extracting the signals from a background unrelated to proton transfer. (c) 2004 Elsevier B.V. All rights reserved

*Chemical Physics* 311[3], 255-268. 2005.

**P 075- 05 "Resonant magnetic tunnel junction at 0 degrees K: I-V characteristics and magnetoresistance"**

Dartora, C. A. and Cabrera, G. G.

In this paper we analyze the main transport properties of a simple resonant magnetic tunnel junction (FM-IS-METAL-IS-FM structure) taking into account both elastic and magnon-assisted tunneling processes at low voltages and temperatures near 0 degrees K. We show the possibility of magnetoresistance inversion as a consequence of inelastic processes and spin-dependent transmission coefficients. Resonant tunneling can also explain the effect of scattering by impurities located inside an insulating barrier. (C) 2005 American Institute of Physics

*Journal of Applied Physics* 97[3]. 2005.

**P 076- 05 "Semiclassical Husimi functions for spin systems"**

Novaes, M. and de Aguiar, M. A. M.

We derive a semiclassical approximation to the Husimi functions of stationary states of spin systems. We rederive the Bohr-Sommerfeld quantization for spin by locating the poles of the corresponding local Green function. The residues correspond to the Husimi functions, which are seen to agree very well with exact calculations

*Physical Review A* 71[1]. 2005.

**P 077- 05 "Short-range charge order in RNiO3 perovskites (R=Pr, Nd, Eu, Y) probed by x-ray-absorption spectroscopy"**

Piamonteze, C., Tolentino, H. C. N., Ramos, A. Y., Massa, N. E., Alonso, J. A., Martinez-Lope, M. J., and Casais, M. T.

The short-range organization around Ni atoms in orthorhombic RNiO3 (R=Pr, Nd, Eu) perovskites has been studied over a wide temperature range by Ni K-edge x-ray-absorption spectroscopy. Our results demonstrate that two different Ni sites, with different average Ni-O bond lengths, coexist in those orthorhombic compounds and that important modifications in the Ni nearest-neighbors environment take place across the metal-insulator transition. We report evidences for the existence of short-range charge order in the insulating state, as found in the monoclinic compounds. Moreover, our results suggest that the two different Ni sites coexist even in the metallic state. The coexistence of two different Ni sites, independently on the R ion, provides a common ground to describe these compounds and sheds interesting light in the understanding of the phonon-assisted conduction mechanism and unusual antiferromagnetism present in all RNiO3 compounds

*Physical Review B* 71[1]. 2005.

**P 078- 05 "Spectral analysis and the dynamic response of complex networks"**

de Aguiar, M. A. M. and Bar-Yam, Y.

The eigenvalues and eigenvectors of the connectivity matrix of complex networks contain information about its topology and its collective behavior. In particular, the spectral density  $\rho(\lambda)$  of this matrix reveals important network characteristics: random networks follow Wigner's semicircular law whereas scale-free networks exhibit a triangular distribution. In this paper we show that the spectral density of hierarchical networks follows a very different pattern, which can be used as a fingerprint of modularity. Of particular importance is the value  $\rho(0)$ , related to the homeostatic response of the network: it is maximum for random and scale-free networks but very small for hierarchical modular networks. It is also large for an actual biological protein-protein interaction network, demonstrating that the current leading model for such networks is not adequate

*Physical Review e* 71[1]. 2005.

**P 079- 05 "Thermal entanglement in the two-qubit Heisenberg XYZ model"**

Rigolin, G.

We study the entanglement of a two-qubit one-dimensional XYZ Heisenberg chain in thermal equilibrium at temperature T. We obtain an analytical expression for the concurrence of this system in terms of the parameters of the Hamiltonian and T. We show that depending on the relation among the coupling constants, it is possible to increase the amount of entanglement of the system by increasing its anisotropy. We also show numerically that for all sets of the coupling constants entanglement is a monotonically decreasing function of the temperature T, proving that we must have at least an external magnetic field in the z-direction to obtain a behavior where entanglement increases with T

*International Journal of Quantum Information* 2[3], 393-405. 2004.

**P 080- 05** "Time-resolved photoluminescence in a-SiN : H < Nd > planar waveguides: evidence for stimulated emission"

Biggemann, D. and Tessler, L. R.

We performed lifetime measurements on the 1128 nmNd(3+) emission from a neodymium-doped amorphous hydrogenated silicon sub-nitride (a SiNx:H < Nd >) planar waveguide. The 1.5  $\mu$ m thick sample was prepared by reactive rf-sputtering. Lifetime measurements were performed exciting with a multiline Ar+ laser. The sample temperature was varied between 25 and 300 K, and the excitation power between 0.2 and 8 kW/cm<sup>2</sup>. In all measurement conditions the luminescence decay can be expressed by two exponentials. The fast decay has a lifetime between 40 and 60  $\mu$ s and the slow decay has a lifetime between 1 and 3 ms. The excitation photon energy is not resonant with any of the Nd<sup>3+</sup> transitions, consequently the excitation energy must be transferred from the host nitride to the Nd<sup>3+</sup> ions. The fast lifetime is almost independent of the temperature, indicating that it is related to the excitation transfer process. As the temperature increases the probability of carrier recombination through processes that do not excite Nd<sup>3+</sup> ions increases. The slow lifetime is associated with the intrinsic Nd<sup>3+</sup> lifetime. It is shorter at low temperatures and high excitation rates. At 26 K, it decreases by a factor 2 when the excitation power goes from 2 to 8 kW/cm<sup>2</sup>. The lifetime decrease with the excitation power is associated with the onset of stimulated emission from the Nd<sup>3+</sup> ions. (c) 2004 Elsevier B.V. All rights reserved

*Optical Materials* 27[5], 773-775. 2005.

**P 081- 05** "X-ray method to study temperature-dependent stripe domains in MnAs/GaAs(001)"

Magalhaes-Paniago, R., Coelho, L. N., Neves, B. R. A., Westfahl, H., Likawa, F., Daweritz, L., Spezzani, C., and Sacchi, M.

MnAs films grown on GaAs (001) exhibit a progressive transition between hexagonal (ferromagnetic) and orthorhombic (paramagnetic) phases at wide temperature range instead of abrupt transition during the first-order phase transition. The coexistence of two phases is favored by the anisotropic strain arising from the constraint on the MnAs films imposed by the substrate. This phase coexistence occurs in ordered arrangement alternating periodic terrace steps. We present here a method to study the surface morphology throughout this transition by means of specular and diffuse scattering of soft x rays, tuning the photon energy at the Mn 2p resonance. The results show the long-range arrangement of the periodic stripe-like structure during the phase coexistence and its period remains constant, in agreement with previous results using other techniques. (C) 2005 American Institute of Physics

*Applied Physics Letters* 86[5]. 2005.

**P 082- 05** "X-ray multiple diffraction on the shallow junction of B in Si(001)"

Orloski, R. V., Pudenzi, M. A. A., Hayashi, M. A., Swart, J. W., and Cardoso, L. P.

We apply X-ray multiple diffraction (XRMD) as a high resolution probe for analyzing the amorphous-crystal line interface (Si interstitial rich region) for different implantation energies and thermal treatment conditions during the formation of a shallow junction of B implanted in Si(001) crystals. Renninger scans (RS) ( $\phi$ -scans) of the three sets of samples were measured using the (002) primary reflection, forbidden by the Si space group. Si(002) RS of as-implanted samples showed an extra peak coming from the Si interstitial atoms in the implanted region. This hybrid peak provides a very sensitive probe for analyzing the occurrence of interstitial Si atoms close to the amorphous-crystalline interface. We report its behavior as a function of the thermal treatment. The separation between the vacancy rich and the interstitial rich regions explains these results on the basis of the Si interstitial annihilation for shallow implantation. Samples with deep implantation are outside the detection range of the technique. in agreement with results for etched samples. (C) 2004 Elsevier B.V. All rights reserved

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## Abstracta

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