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TRABALHOS ACEITOS

A 019- 04 Coexistence of Antiferromagnetic Order and Unconventional Superconductivity in Heavy-Fermion $CeRh_{1-x}Ir_xIn_5$ Compounds: Nuclear Quadrupole Resonance Studies.

A 020- 04 Nonequilibrium Ensemble Formalism.

A 021-04 A Raman Scattering-based Method to Probe the Carrier Drift Velocity in Seminconductors: Application to Gallium Nitride.

A 022- 04 Two Superconducting Phases in $CeRh_{1-x}Ir_xIn_5$.

A 023- 04 Random Spin Freezing in Ce_2MIn_8 (M=Co,Rh,Ir) Heavy-fermion Materials.

TRABALHOS PUBLICADOS

P 097 - 04 à P 143- 04

TRABALHOS ACEITOS PARA PUBLICAÇÃO EM PERIÓDICOS

A 019-04 Coexistence of Antiferromagnetic Order and Unconventional Superconductivity in Heavy-Fermion $CeRh_{1-x}Ir_xIn_5$ Compounds: Nuclear Quadrupole Resonance Studies.

Zheng G., Yamaguchi N., Kan H., Kitaoka Y., Sarrao J.L., Pagliuso P.G., Moreno N.O., and Thompson J.D.

We present a systematic In NQR study on the heavy-fermion compounds $CeRh_{1-x}Ir_xIn5$ (x=0.25, 0.35, 0.45, 0.5, 0.55, and 0.75). The results provide strong evidence for the microscopic coexistence of antiferromagnetic (AF) order and superconductivity (SC) in the range of 0.35=x=0.55. Specifically, for x=0.5, T_N is observed at 3 K with a subsequent onset of superconductivity at T_c=0.9 K. T_c reaches a maximum (0.94 K) at x=0.45 where T_N is found to be the highest (4.0 K). Detailed analysis of the measured spectra indicate that the same electrons participate in both SC and AF order. The nuclear spin-lattice relaxation rate $1/T_1$ shows a broad peak at T_N and follows a T^3 variation below T_c, the latter property indicating unconventional SC as in $CeIrIn_5$ (T_c=0.4 K). We further find that, in the coexistence region, the T^3 dependence of $1/T_1$ is replaced by a T-linear variation below T~0.4 K, with the value $(T_1)_{Tc}/(T_1)_{low\ T}$ increasing with decreasing x, likely due to low-lying magnetic excitations associated with the coexisting magnetism.

Physical Review B 70, accepted on August 2004.

A 020-04 Nonequilibrium Ensemble Formalism.

Roberto Luzzi, Áurea R. Vasconcellos, and J. Galvão Ramos

It is summarized what can be considered as the present situation in what regards to the construction of an ensemble formalism-Gibbs´style - for the case of far-from-equilibrium systems. The main questions involved are subsummed and the construction of a general nonequilibrium grand-canonical ensemble is presented. Very brief considerations on statistics differing from the conventional Boltzmann-Gibbs one are presented.

Physica A: Stat. Mech.and its Applic., accepted on August 2004.

A 021-04 A Raman Scattering-based Method to Probe the Carrier Drift Velocity in Seminconductors: Application to Gallium Nitride.

A. V. Andrade-neto, A. R. Vasconcellos, V. N. Freire, and R. Luzzi.

A simple expression relating the carrier drift velocity in semicnductors under an electric field to Raman scattering data is derived resorting to a full nonequilibrium picture for electrons and holes. It allows to probe with high optical precision both the ultrafast transient as well as the steady state carriers´drift velocity in semiconductor systems. This is achieved by simply modifying the experimental geometry, thus changing the angle between the transferred wave vector Q and the applied electric field E, and measuring the frequency shift promoted by the presence of the field to be observed in the single-particle and plasmon scattering spectra. An application to zincblende gallium nitride is presented to highlight to power of the method.

Applied Physics Letters, accepted on August 2004

A 022-04 Two Superconducting Phases in $CeRh_{1-x}Ir_xIn_5$.

Nicklas M., Sidorov V.A., Borges H.A., Pagliuso P.G., Sarrao J.L., and Thompson J.D.

Pressure studies of $CeRh_{1-x}Ir_xIn_5$ indicate two superconducting phases as a function of x, one with T_c = 2 K for x < 0.9 and the other with T_c < 1.2 K for x > 0.9. The higher T_c phase, phase-1, emerges in proximity to an antiferromagnetic quantum-critical point; whereas, Cooper pairing in the lower T_c phase-2 is inferred to arise from fluctuations of a yet to be found magnetic state. The T-x-P phase diagram of $CeRh_{1-x}Ir_xIn_5$, though qualitatively similar, is distinctly different from that of $CeCu_2(Si_{1-x}Ge_x)_2$.

Physical Review B (Rapid), accepted on June 2004.

A 023-04 Random Spin Freezing in Ce_2MIn_8 (M=Co,Rh,Ir) Heavy-fermion Materials.

Morris G.D., Heffner R.H., Moreno N.O., Pagliuso P.G., Sarrao J.L., Dunsiger S.R., Nieuwenhuys G.J., MacLaughlin D.E. and Bernal O.O.

Previous specific heat and resistivity measurements have established a preliminary phase diagram for the evolution of magnetic order in heavy-fermion materials $Ce_2M_xIr_{1-x}In_8$, M=Co, Rh; a possible quantum critical point (QCP) was postulated for Ce_2IrIn_8. Zero-field muon spin relaxation studies in Ce_2RhIn_8 find very rapidly damped oscillations below the Néel temperature T_N=2.8K, indicating a broad field distribution consistent with the presence on an incommensurate magnetic structure. In Ce_2IrIn_8, and in samples in which several percent of Ir is substituted by Co or Rh, muon spin relaxation spectra reveal the onset of a Lorentzian field distribution, with zero mean, characteristic of disordered spin freezing. The onset temperature for this freezing depends on composition; it is smallest, but still nonzero, in Ce_2IrIn_8, ruling out a QCP. The evolution of magnetism in the temperature-composition phase diagram indicates that the type of magnetic ordering depends systematically on the degree of Ce-M hybridization and the local Ce environment.

Physical Review B 69 [214415] , accepted on July 2004.

ERRATA

CAPÍTULO EM LIVRO NO PRELO

L 001-04 Ensemble formalisms for nonequilibrium systems and an associated irreversible statistical thermodynamics.

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

"Trends in Statistical Physics`` (Review Series Research Trends) accepted on May 2004.

TRABALHOS PUBLICADOS

P 97- 04 "A simple model for solidification of undercooled metallic samples"

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

A simple model for reproducing temperature recalescence behaviour in spherical undercooled liquid metallic samples, undergoing crystallization transformations, is presented. The model is applied to constant heat extraction rate, uniform but time dependent temperature distribution inside the sample (even after the start of crystallization), a classical temperature dependent rate of nucleation (including contributions from different specific heats for different phases and also a catalytic factor to model the possibility of heterogeneous distributed impurities) and the solidified grain interface velocity is taken proportional to the temperature undercooling. Different assumptions are considered for the sample transformed fraction as function of the extended volume of nuclei, like the classical Kolmogoroff, Johnson-Mehl, Avrami one (corresponding to random distribution of nuclei), the Austin-Rickett one (corresponding to some kind of clusterized distribution) and also an empirical one corresponding to some ordering in the distribution of nuclei. As an example of application, a published experimental temperature curve for a zirconium sample in the electromagnetic containerless facility TEMPUS, during the 2nd International Microgravity Laboratory Mission in 1994, is modeled. Some thermo-physical parameters of interest for Zr are discussed.

Japanese Journal of Applied Physics Part 1-Regular Papers ShortNotes & Review Papers 43[6A], 3624-3628. 2004.

P 98- 04"Abrupt field-induced transition triggered by magnetocaloric effect in phase-separated manganites"

Ghivelder, L., Freitas, R. S., das Virgens, M. G., Continentino, M.
A., Martinho, H., Granja, L.,Quintero, M., Leyva, G., Levy, P., and Parisi, F

The occurrence at low temperatures of an ultrasharp field-induced transition in phase-separated manganites is analyzed. Experimental results show that magnetization and specific-heat steplike transitions below 5 K are correlated with an abrupt change of the sample temperature, which happens at a certain critical field. This temperature rise, a magnetocaloric effect, is interpreted as produced by the released energy at the transition point and is the key to understand the existence of the abrupt field-induced transition. A qualitative analysis of the results suggests the existence of a critical growing rate of the ferromagnetic phase, beyond which an avalanche effect is triggered.

Physical Review B 69[21]. 2004.

P 099- 04 "Anomalous slow dynamics in quantum spin chains"

Carvalho, J. G., Medeiros, D., and Cabrera, G. G

We solve the dynamics of quantum spin chains when the initial condition is prepared as a spatially inhomogeneous state of the magnetization. Particularly long-lived states are found for which the relaxation time diverges and the whole relaxation process slows down as a consequence of constructive interference at degenerate stationary points. These states may be of interest for performing quantum computation. (C) 2004 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 272-76, 886 887. 2004.

P 100- 04 "Antiatom-atom scattering with the close coupling model"

Chakraborty, S., Basu, A., Chaudhuri, P., Sinha, P. K., and Ghosh, A. S.

Collisions involving atoms and antiatoms have been investigated at low incident energies using close-coupling approximation (CCA). We investigate ortho-positronium-ortho-positronium (o-Ps-o-Ps) scattering up to incident energy 3.4 eV. Antihydrogen-hydrogen elastic scattering has been studied in the energy range 10(-10) to 10(-2) a.u., whereas antihydrogen-helium system has been investigated in the range 10(-16) to 10(-2) a.u. The s-wave elastic scattering parameters, viz., scattering length, effective range, phase shift, cross section etc., have been reported. The present predictions have been compared with the other corresponding theoretical predictions wherever available. Usefulness of CCA model to investigate these systems at thermal energies has been emphasized. (C) 2004 Elsevier B.V. All rights reserved

***Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms* 221, 12-20. 2004.**

P 101- 04 "Apparent split between magnetic and structural phase transitions in epitaxial MnAs films"

Iikawa, F., Knobel, M., Santos, P. V., Adriano, C., Couto, O. D. D., Brasil, M. J. S. P., Giles, C., Magalhaes-Paniago, R., and Daweritz, L.

We investigate the magnetic field dependence of the magnetic and structural phase transition of an epitaxial MnAs layer grown on GaAs (100) by using SQUID magnetometry and X-ray diffraction. The phase transition temperatures obtained from magnetic and structural results revealed an apparent splitting for magnetic field less than similar to 1 kOe, while for higher magnetic fields a behavior similar to that reported for bulk MnAs is observed. (C) 2004 Elsevier B.V. All rights reserved

***Journal of Magnetism and Magnetic Materials* 272-76, 1154-1156. 2004.**

P 102- 04 "Domain-wall profile in the presence of anisotropic exchange interactions: Effective on-site anisotropy"

Rodriguez, A. O. G., Ferrer, A. V., and Caldeira, A. O.

Starting from a D-dimensional XXZ ferromagnetic Heisenberg model in an hypercubic lattice, it is demonstrated that the anisotropy in the exchange coupling constant leads to a D-dependent effective on-site anisotropy interaction often ignored for D>1. As a result the effective width of the wall depends on the dimensionality of the system. It is shown that the effective one-dimensional Hamiltonian is not the one-dimensional XXZ version as assumed in previous theoretical work. We derive a new expression for the wall profile that generalizes the standard Landau-Lifshitz form. Our results are found to be in very good agreement with earlier numerical work using the Monte Carlo method. Preceding theories concerning the domain wall contribution to magnetoresistance have considered the role of D only through the modification of the density of states in the electronic band structure. This Brief Report reveals that the wall profile itself contains an additional D dependence for the case of anisotropic exchange interactions

***Physical Review B* 69[21]. 2004.**

P 103- 04 "Effects of non-standard neutrino interactions on MSW-LMA solution to the solar neutrino problem"

Guzzo, M. M., de Holanda, P. C., and Peres, O. L. G.

We show that the non-standard neutrino interactions can play a role as subleading effect on the solar neutrino oscillations. We observe that very small flavor universality violations of order of 0.1-0.2 G(F) is sufficient to induce two phenomena: suppression of the v(e)-Earth regeneration and a shift of the resonance layer in the Sun. We obtain these phenomena even in the absence of any flavor changing interactions. We discuss their consequences and confront with a global analysis of solar + KamLAND results. We conclude that a new compatibility region in the Deltam(2) x tan(2)thetacircle dot, which we call very low large mixing angle region is found for Deltam(2) similar to 10(-5) eV(2) and tan(2)thetacircle dot = 0.45. (C) 2004 Elsevier B.V. All rights reserved

Physics Letters B 591[1-2], 1-6. 2004.

P 104 - 04 "Experimental and theoretical study of demagnetization fields in superconducting samples of orthorhombic shape"

Navau, C., Cardoso, C. A., de Lima, O. F., and Araujo-Moreira, F. M.

In this work we present a model for the calculation of the magnetic properties of superconductors of orthorhombic shape in the perfect shielding state when an external uniform magnetic field is applied in the direction of one of the principal axes of the sample. Our model accounts for demagnetization effects and it is free of fitting parameters and boundary value conditions. We consider planar linear circuits that lie perpendicular to the direction of the applied field. Calculation of the value of the currents is based on magnetic energy minimization. The model is proved to be accurate enough to reproduce experimental results as long as the dimension along the applied field is not much lower than the other dimensions. Calculations of surface currents, as well as measurements and calculations of magnetization and initial susceptibility, are reported. We also present an empirical formula that provides a good fit to the initial susceptibility of a general sample of orthorhombic shape. Demagnetization effects observed on the experimental results are explained in terms of the induced currents in the superconductor. (C) 2004 American Institute of Physics

Journal of Applied Physics 96[1], 486-493. 2004.

P 105- 04 "Experimental study of the magnetocaloric effect in Gd5Sn2Si2 compound"

Campoy, J. C. P., Plaza, E. J. R., Carvalho, A. M. G., Coelho, A. A.,
Gama, S., and von Ranke, P J.

We report an experimental study of the magnetocaloric effect (MCE) in the Gd5Sn2Si2 compound. The MCE DeltaS(mag)(T) as a function of temperature is obtained from magnetization M(H,T) measurements up to 5T. A second order magnetic transition is observed at T-C similar to 220 K with DeltaS(mag) = 4.5 J/mol K. T-C and transition width DeltaT(C) depends on thermal treatments for homogeneity and crystallographic ordering. At low temperatures, T similar to 87 K, we also observed a second peak in DeltaS(mag) which is associated with the presence of antiferromagnetic Gd5Sn4-xSix. (C) 2004 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 272-76, 2375 2376. 2004.

P 106- 04 "Homestake result, sterile neutrinos, and low energy solar neutrino experiments"

de Holanda, P. C. and Smirnov, A. Y.

The Homestake result is about similar to2sigma lower than the Ar-production rate, Q(Ar), predicted by the large mixing angle (LMA) Mikheyev-Smirnov-Wolfenstein solution of the solar neutrino problem. Also there is no apparent upturn of the energy spectrum (Requivalent toN(obs)/N-SSM) at low energies in SNO and Super-Kamiokande. Both these facts can be explained if a light, Deltam(01)(2)similar to(0.2-2)x10(-5) eV(2), sterile neutrino exists which mixes very weakly with active neutrinos: sin(2) 2alphasimilar to(10(-5)-10(-3)). We perform both the analytical and numerical study of the conversion effects in the system of two active neutrinos with the LMA parameters and one weakly mixed sterile neutrino. The presence of sterile neutrino leads to a dip in the survival probability in the intermediate energy range E=(0.5-5) MeV thus suppressing the Be, or/and pep, CNO, as well as B electron neutrino fluxes. Apart from diminishing Q(Ar) it leads to decrease of the Ge-production rate and may lead to the decrease of the BOREXINO signal as well as the CC/NC ratio at SNO. Future studies of the solar neutrinos by SNO, SK, BOREXINO, and KamLAND as well as by the new low energy experiments will allow us to check this possibility

Physical Review D 69[11]. 2004.

P 107- 04 "Influence of hydrogen on the magnetic behaviour of Gd5Ge2Si2Hx, 0.1 <= x <= 2.5"

Alves, C. S., Colucci, C. C., Gama, S., Carvalho, A. M. C., and Coelho, A. A.

The influence of hydrogen absorption on T-C and M-S of the Gd5Ge2SiHx alloys, with 0.1 less than or equal to x less than or equal to 2.5 was studied by thermomagnetic analysis from 2 to 370 K. The M (T) curves show the first order magnetic transition at 260 K only for the sample with x = 0.1. All the samples presented the second-order magnetic transition between 296 (x = 0.1) and 212 K (x = 2.5). For the sample with X greater than or equal to 1.2 is also observed a new antiferromagnetic transition at approximate to 45 K. The M (H) curves revealed that the M-S tends to increase with the hydrogen amount into the alloy. (C) 2004 Published by Elsevier B.V

Journal of Magnetism and Magnetic Materials 272-76, 2391 2392. 2004.

P 108- 04"IonRock: software for solving strain gradients of ion-implanted semiconductors by X-ray
diffraction measurements and evolutionary programming"

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

We present a program that uses an optimization algorithm to fit rocking curves of ion-implanted semiconductors. This is an inverse problem that cannot be solved by simple methods. However, using recursion formulae for rocking curve calculations and a model of ion distribution after implantation, it is possible to fit experimental data with a general-purpose optimization method. In our case, we use a modified version of the genetic algorithm, which has been shown to be a good technique for this problem. The program also calculates rocking curves for a given ion profile, such as those generated by ion implantation simulation programs. (C) 2004 Elsevier B.V. All rights reserved

Computer Physics Communications 160[2], 158-165. 2004.

P 109- 04 "Local order structure and surface acidity properties of a Nb2O5/SiO2 mixed oxide prepared by the sol-gel processing method"

Francisco, M. S. P., Landers, R., and Gushikem, Y.

The sol-gel processing method was used as an alternative route to obtain Nb2O5 phase homogenously dispersed in the SiO2 matrix, improving the thermal stability of the Bronsted acid sites, Nb-OH and Nb-OH-Si groups. The local niobium structure and the influence of the amount of niobia, on the surface of the Nb2O5/SiO2 system were studied by XAS and XPS, respectively. For the samples calcined at 423 and 873 K, the 3d(5/2) BE values are at ca. 208.2 eV, indicating an ionic character for Nb(V) species in the SiO2 matrix, probably associated to Si-O-Nb linkages. The features of Nb K-edge XANES spectra of samples show the absence of Nb=O species. The Nb K-edge EXAFS oscillations exhibit a shoulder at ca. 5.6 Angstrom(-1), which probably arises from Nb-O-Si. This fact corroborates the EXAFS simulation data of the second coordination shell, whose best fitting is achieved with three distances, two Nb-Nb lengths and one Nb-Si.
Journal of Solid State Chemistry 177[7], 2432-2439. 2004.

P 110 -04 "Magnetic and magnetocaloric properties of Nd monopnictides"

Plaza, E. J. R., Alves, C. S., Coelho, A. A., Gama, S., and von Ranke, P. J.

The behavior of Nd monopnictides in the paramagnetic regime is studied with a Hamiltonian that includes crystalline field interactions, molecular and quadrupolar fields. Experimental results have been obtained from polycrystalline samples, and from analysis of low field curves we deduced molecular and quadrupolar field parameters. From the magnetization data, the NdP and NdAs magnetocaloric potentials -DeltaS(mag) are well reproduced, and their experimental isofields are in agreement with the one calculated from the model and the proposed parameters.
Journal of Magnetism and Magnetic Materials 272-76, 2373-2374. 2004.

P 111- 04 "Magnetic properties of the RuSr(2)Ln(1.5)Ce(0.5)Cu(2)O(10-delta) (Ln = Y, Ho and Dy) and RuSr2YCu2O8-delta rutheno-cuprate families: a comparative study"

Cardoso, C. A., Araujo-Moreira, F. M., Awana, V. P. S., Kishan, H., Takayama-Muromachi, E., and de Lima, O. F.

The magnetic behavior of polycrystalline samples of the magneto-superconductors RuSn(2)Ln(1.5)Ce(0.5)Cu(2)O(10-delta) (LnRu-1222, Ln = Y, Ho and Dy) and RuSr2YCu2O8-delta (YRu-1212) is analyzed, and compared. Clear evidences for the occurrence of a spin glass phase on all LnRu-1222 samples are provided by ac susceptibility (chi(ac)) and do magnetization measurements. A frequency-dependent peak in chi(ac) vs. T measurements, at low magnetic field, is observed. The strong suppression of this peak in the presence of magnetic fields as low as 500 Oe, as well as the results of thermoremanent magnetization (TRM) and isothermal remanent magnetization (IRM) measurements, suggest a spin glass behavior. Interestingly, the same measurements on the YRu-1212 sample show no indication of glassy behavior, contrasting with the results for LnRu-1222. We suggest that frustration of the Ru magnetic moments due to the presence of oxygen vacancies would be favored only in the LnRu-1222 compounds, thus causing the glassy behavior. This idea is supported by the observation of large oxygen deficiency that affects the RuO2 planes in Ru-1222, but does not occur in Ru-1212.
Physica C-Superconductivity and Its Applications 405[3-4], 212

P 112- 04 "Magnetotransport and electric properties of CO-SiO2-Si structure"

de Carvalho, H. B., Brasil, N. P., Knobel, M., and Denardin, J. C.

We present an investigation on the transport and magnetotransport properties of thin Co films deposited onto Si substrates with a thin native oxide layer. We observed a marked transition on the transport properties of our films at similar to250 K. Around this temperature the conduction changes from electronic to hole-like and the resistance undergoes a clear drop. This effect can be explained by a conduction channel switching from the upper metallic film to the Si hole inversion layer as we increase the sample temperature. We show that this channel switching may be controlled by applying an external bias to the structure.
Journal of Magnetism and Magnetic Materials 272-76, 1157-1159. 2004.

P 113- 04 "New far-infrared laser lines from CH3OD methanol deuterated isotope"

Costa, L. F. L., Cruz, F. C., Moraes, J. C. S., and Pereira, D.

We report on a study of the CH3OD molecule in a search for new far-infrared (FIR) laser lines. For optical pumping of large offset vibrational absorption transitions, a continuous-wave waveguide CO2 laser with 300 MHz tunability around each line was used for the first time. As a consequence, 17. new far-infrared laser emissions were observed. For these lines, we also present data on wavelength, intensity, offset, relative polarization, and optimum operation pressure
Ieee Journal of Quantum Electronics 40[7], 946-948. 2004.

P 114 - 04 "On the determination of the phase composition of the Gd5Ge2Si2 alloy"

Gama, S., Alves, C. S., Coelho, A. A., Ribeiro, C. A., Persiano, A. I. C., and Silva, D.

Samples of the compound Gd5Ge2Si2 were prepared by arc-melting and heat-treated at high temperatures. They were characterized by metallographic analysis and magnetization measurements. The observed phases were characterized using energy dispersive spectroscopy and subsequently using wavelength dispersive spectroscopy. The results indicate an imbalance in the proportion of Si and Ge for both observed phases, and good magnetocaloric properties for the heat-treated samples.

Journal of Magnetism and Magnetic Materials 272-76, 848-849. 2004.

P 115- 04 "Origin of the A(1g) and B-1g electronic Raman scattering peaks in the superconducting state of YBa2Cu3O7-delta"

Martinho, H., Martin, A. A., Rettori, C., and Lin, C. T.

The electronic Raman scattering was investigated in optimally oxygen-doped YBa2Cu3O7-delta single crystals as well in crystals doped with nonmagnetic, Zn2+ and magnetic Ni2+ impurities. We found that the intensity of the A(1g) peak is impurity independent and its energy to T-c ratio is nearly constant (2Delta/k(B)T(c)similar to5). Moreover, the signal at the B-1g channel is completely smeared out when nonmagnetic Zn2+ impurities are present. These results are discussed in terms of the current models of Devereaux , Venturini , and Zeyher and Greco

Physical Review B 69[18]. 2004.

P 116- 04 "Pd growth on Cu(111): stress relaxation through surface alloying?"

Paniago, R., de Siervo, A., Soares, E. A., Pfannes, H. D., and Landers, R.

On the basis of a high-precision reflection high-energy electron diffraction (RHEED) investigation details of the growth of Pd on a Cu(1 1 1) single crystal substrate at room temperature are reported. Because of the +7.6% misfit of the Pd lattice spacing as compared to Cu, perfect pseudomorphous growth would result in highly stressed ultra-thin films. RHEED analysis shows that as a function of Pd coverage initially the film starts to grow with the in-plane Cu(1 1 1) lattice parameter. With increasing coverage the lattice parameter rapidly changes to the "natural" lateral lattice parameter of Pd(1 1 1). We propose that a progressive increase of the equilibrium lateral lattice parameter by alloying (Vegards law) releases the stress in the Pd/Cu(1 1 1) system. With a coverage of n > 2 ML (n = number of monolayers, ML) pure Pd layers are formed, since the in-plane lattice parameter equals the expected value for Pd at n = 2 ML. Our conclusion that Pd-Cu surface alloying acts as a relaxation mechanism in this quasi-pseudomorphous growth system, corroborates scanning tunneling microscopy [Surf. Sci. 408 (1998) 43] which also suggests formation of a random surface alloy in the earlier stages of Pd growth on Cu(1 1 1). (C) 2004 Elsevier B.V. All rights reserved

Surface Science 560[1-3], 27-34. 2004.

P 117 -04 "Phase diagrams and universality classes of random antiferromagnetic spin ladders"

Hoyos, J. A. and Miranda, E.

The random antiferromagnetic two-leg and zigzag spin- 1/2 ladders are investigated using the real space renormalization group scheme and their complete phase diagrams are determined. We demonstrate that the first system belongs to the same universality class of the dimerized random spin- 1/2 chain. The zigzag ladder, on the other hand, is in a random singlet phase at weak frustration and disorder. Otherwise, we give additional evidence that it belongs to the universality class of the random antiferromagnetic and ferromagnetic quantum spin chains, although the universal fixed point found in the latter system is never realized. We find, however, a new universal fixed point at intermediate disorder

Physical Review B 69[21]. 2004.

P 118- 04 "Phonons in the bilayered magnetic manganite La2-2xSr1+2xMn2O7 (x=0.30,0.50)"

Martinho, H., Rettori, C., Huber, D. L., Mitchell, J. F., and Oseroff, S. B.

We have studied the ab-plane Raman-active phonons of the bilayered magnetic manganite La2-2xSr1+2xMn2O7 for x = 0.30 and 0.50. The Raman response was deconvoluted to seven modes in both cases and their symmetries and T-dependence analyzed. We found that the T-dependence of the linewidth and frequency of almost phonons follows the two-phonon anharmonic decay and the usual Gruneisen behavior, respectively, with exception of the 1000 cm(-1) mode for x = 0.30 that softens similar to 150 cm(-1) below T-C due to their strong spin-phonon coupling. We also notice that some modes for x = 0.50 before associated to two- and three-phonons Raman process appeared to us as being one-phonon Raman peaks. (C) 2003 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 272-76, 1736-1737. 2004.

P 119- 04 "Polarization effects in the calculation of N1s binding energies of carbon-nitrogen molecules"

Carvalho, A. C. M. and dos Santos, M. C.

Core ionization N1s energies have been calculated for model molecules containing nitrogen atoms binding to sp(3), sp(2), and sp carbon atoms. These systems are representative of the chemical bonds in carbon nitride materials. The embedding of the molecules in a polarizable medium was considered. The polarization effects were accounted for by means of the self-consistent reaction field method. The dielectric constant of the surrounding medium was taken from experimental data for CNx samples as a function of nitrogen concentration. Binding energies were obtained from delta self-consistent field calculations that explicitly consider electronic relaxation. Results are consistent with larger molecules being less affected by the polarization effects than smaller species. The interpretation of the measured N1s binding energy features of carbon nitride alloys has been reviewed.

Journal of Non-Crystalline Solids 338-40, 254-257. 2004.

P 120- 04 "Positron impact electronic excitation of N-2"

Chaudhuri, P., Varella, M. T. D., de Carvalho, C. R. C., and Lima, M. A. P.

We present the results of scattering cross sections for positron impact excitation of electronic states of nitrogen molecule (N-2) using the Schwinger multichannel method (SMC). All calculated cross sections took three collision channels into account (X(1)Sigma(g) and degenerate a(1)Pi(g), states). Present theoretical results for excitation to the a(1)Pi(g). states failed to reproduce the near-threshold structure observed in the recent and the only available experimental data [Sullivan et al., Phys. Rev. Lett. 87 (2001) 073201-1]. Scattering calculations from the a(1)Pi(g), states (elastic and superelastic) are also reported. A spurious resonant structure found in the excitation to the a(1)Pi(g) states was detected in a square integrable basis set calculation designed to reproduce the first Born approximation (FBA). Such spurious structure was removed by taking out the trial configuration state functions in which the positron was weakly coupled to the target. This may be a promising technique to separate unphysical resonances from the physical ones. We also observe that a combination between SMC scattering amplitudes (l less than or equal to, 2) with FBA ones (1 greater than or equal to 3) significantly improved the cross sections at higher energies. (C) 2004 Elsevier B.V. All rights reserved

Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials

P 121- 04 "Quantum linear mutual information and classical correlations in globally pure bipartite systems"

Angelo, R. M., Vitiello, S. A., de Aguiar, M. A. M., and Furuya, K.

We investigate the correlations of initially separable probability distributions in a globally pure bipartite system with two degrees of freedom for classical and quantum systems. A classical version of the quantum linear mutual information is introduced and the two quantities are compared for a system of oscillators coupled with both linear and non-linear interactions. The classical correlations help to understand how much of the quantum loss of purity are due to intrinsic quantum effects and how much is related to the probabilistic character of the initial states, a characteristic shared by both the classical and quantum pictures. Our examples show that, for initially localized Gaussian states, the classical statistical mutual linear entropy follows its quantum counterpart for short times. For non-Gaussian states the behavior of the classical and quantum measures of information are still qualitatively similar, although the fingerprints of the non-classical nature of the initial state can be observed in their different amplitudes of oscillation. (C) 2004 Elsevier B.V. All rights reserved.

Physica A-Statistical Mechanics and Its Applications 338[3 4], 458-470. 2004.

P 122- 04 "Single-frequency blue light source based on optically injected diode lasers"

Manoel, D. D., Figueira, D. S. L., Pereira, D., and Cruz, F. C.

We describe a diode-laser-based system capable of generating >50 mW of single-frequency radiation near 425 nm. An alternative extended cavity diode laser injection seeds a semiconductor amplifier, whose output is frequency doubled by a nonlinear crystal placed in a power enhancement cavity. This system is particularly well suited for high-resolution spectroscopy in the blue region, and for laser cooling and trapping of calcium atoms. (C) 2004 Society of Photo-Optical Instrumentation Engineers

Optical Engineering 43[6], 1311-1313. 2004.

P 123- 04 "Semiclassical approximations based on complex trajectories"

Ribeiro, A. D., de Aguiar, M. A. M., and Baranger, M.

The semiclassical limit of the coherent state propagator <z"\e(-i (H) over capT/h)\z'> involves complex classical trajectories of the Hamiltonian (H) over tilde (u,v)=<v\(H) over cap \u> satisfying u(0)=z' and v(T)=z"*. In this work we study mostly the case z'=z". The propagator is then the return probability amplitude of a wave packet. We show that a plot of the exact return probability brings out the quantal images of the classical periodic orbits. Then we compare the exact return probability with its semiclassical approximation for a soft chaotic system with two degrees of freedom. We find two situations where classical trajectories satisfying the correct boundary conditions must be excluded from the semiclassical formula. The first occurs when the contribution of the trajectory to the propagator becomes exponentially large as (h) over bar goes to zero. The second occurs when the contributing trajectories undergo bifurcations. Close to the bifurcation the semiclassical formula diverges. More interestingly, in the example studied, after the bifurcation, where more than one trajectory satisfying the boundary conditions exist, only one of them in fact contributes to the semiclassical formula, a phenomenon closely related to Stokes lines. When the contributions of these trajectories are filtered out, the semiclassical results show excellent agreement with the exact calculations
Physical Review e 69[6]. 2004.

P 124- 04 "SixGe1-x films and heterojunctions produced by epitaxial crystallization of a-SixGe1-x alloys on GaAs"

Dondeo, F., Santos, P. V., Kostial, H., Krispin, P., Pudenzi, M. A. A., and Chambouleyron, I.

We studied the structural and electrical properties of crystallized a-SixGe1-x alloys with 0 less than or equal to x less than or equal to 1 on (100) GaAs substrates. Raman spectroscopy on laser crystallized films shows the Si-Si, Ge-Ge, and Si-Ge vibrations characteristic of crystalline SixGe1-x alloys. The Raman polarization selection rules indicate that, while SixGe1-x films with x up to 25% are epitaxial, those with higher Si concentrations are polycrystalline with oriented grains. Heterojunctions formed by crystallizing a-Ge films on p-type GaAs exhibit Ohmic behavior. Ge/n-GaAs heterojunctions, in contrast, show rectification with current versus voltage characteristics compatible with the behavior of n-n structures. These heterojunctions are sensitive to light with wavelengths up to 1600 nm, thus demonstrating that they can be used as detectors in the spectral range for optical communications (1300-1550 nm). (C) 2004 Elsevier B.V. All rights reserved

Journal of Non-Crystalline Solids 338-40, 197-200. 2004.

P 125- 04 "Solar neutrinos: the SNO salt phase results and physics of conversion"

de Holanda, P. C. and Smirnov, A. Y.

We have performed analysis of the solar neutrino data including results from the SNO salt phase as well as the combined analysis of the solar and the KamLAND results. The best-fit values of neutrino parameters are Deltam(2) = 7.1 x 10(-5) eV(2), tan(2)theta = 0.40 with the boron flux f(B) = 1.04. New SNO results strongly disfavor maximal mixing and the h-LMA region (Deltam(2) > 10(-4) eV(2)) which is accepted now at the 36 level. We find the 3(7 upper bounds: Deltam(2) < 1.7 x 10(-4) eV(2) and tan(2)theta < 0.64, and the lower bound Deltam(2) > 4.8 x 10(-5) eV(-1). Non-zero 13-mixing does not change these results significantly. The present data determine quantitatively the physical picture of the solar neutrino conversion. At high energies relevant for SNO and Super-Kamiokande the deviation of the effective survival probability from the nonoscillatory value is about 10-14%. The oscillation effect contribution to this difference is about 10'% and the earth regeneration about 3-4%. At low energies (E < 1 MeV) the matter corrections to vacuum oscillation effect are below 5%. The predictions for the forthcoming measurements are given which include the spectral distortion and CC/NC ratio at SNO, the day night asymmetry, the KamLAND spectrum and rate. (C) 2004 Elsevier B.V. All rights reserved

Astroparticle Physics 21[3], 287-301. 2004.

P 126- 04 "Static and dynamic conductivity for a model of Tl2Mn2O7"

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

The compound Tl2Mn2O7 exhibits colossal magneto resistance, which is not adequately explained by the double exchange mechanism. We use Hubbard operators to reformulate a previous model of Ventura and Alascio (Phys. Rev. B 56 (1997) 14533), and we obtain approximate one-electron Green's functions (GF) for this model, using a method introduced by Foglio and Figueira (Phys. Rev. B 60 (1999) 11361). With these GF we calculate the static and dynamic conductivity, both with and without applied magnetic fields. (C) 2003 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 272-76, 280-281. 2004.

P 127- 04 "Strong spatial beryllium doping selectivity on InGaP layers grown on pre-patterned GaAs substrates by chemical beam epitaxy"

de Castro, M. P. P., von Zuben, A. A., Frateschi, N. C., Santo, L. L. E., Galvao, D. S., Bettini, J., and de Carvalho, M. M. G.

We present an investigation of beryllium doping selectivity in InGaP layers grown by chemical beam epitaxy on pre-patterned substrates. We observed a resistivity of 3.1 X 10(-2) and 4.5 x 10(-2) Omega cm for (1 1 1)A planes with the growth at 500degreesC and 540degreesC, respectively. The layers on (0 0 1) planes show a resistivity of 8.9 x 10(-1) Omega cm with the growth at 500degreesC, being essentially undoped with the growth at 540degreesC (.) We show how this strong doping selectivity can be explained by Be3P2 cluster formation growth, which depends on growth temperature and planar crystalline structure. (C) 2004 Elsevier B.V. All rights reserved

Journal of Crystal Growth 266[4], 429-434. 2004.

P 128 -04 "Structural and magnetic properties of NiFe2O4-SnO2 nanocomposite"

Albuquerque, A. S., Ardisson, J. D., Macedo, W. A. A., Plivelic, T. S., Torriani, I. L., Larrea, J. J.and Saitovitch, E. B.

The structural and magnetic properties of the NiFe2O4-SnO2 composite, obtained by ball-milling during different times. were investigated by X-ray diffraction, small-angle X-ray scattering, Mossbauer spectroscopy and vibrating sample magnetometry. The results showed the reduction of the crystalline particle size and modification in the nature of the system interfaces as a consequence of the mechanical treatment. Specimens with smaller particles displayed strong superparamagnetism. Large variation of the hysteresis loops for the different milling times was observed. (C) 2003 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials **272-76, 2211-2213. 2004.**

P 129- 04 "Structural properties of amorphous carbon nitride films prepared by ion beam assisted deposition"

Ferlauto, A. S., Champi, A., Figueroa, C. A., Ribeiro, C. T. M., Marques, F. C., and Alvarez, F.

Amorphous carbon nitride films (a-CNx) with nitrogen concentration ranging from 0 to 30 at.% were prepared by ion beam assisted deposition at different substrate temperatures, T = 150, 350 and 550 degreesC. In situ X-ray photoelectron spectroscopy, infrared spectroscopy, hardness and intrinsic stress measurements were applied to investigate the effects of the nitrogen incorporation and temperature in the structural properties of the films. For all T, N incorporation up to 20 at.% leads to increases in hardness and stress of the films. These changes are attributed to modifications of the bonding configurations of the disordered matrix that surrounds the small graphitic clusters in the films. On the other hand, increases in substrate temperature lead to increases in the size of ordered graphitic clusters in the films but have little effect in their overall mechanical properties. (C) 2004 Elsevier B.V. All rights reserved

Journal of Non-Crystalline Solids **338-40, 486-489. 2004.**

P 130- 04 "Study of anhysteretic magnetization loops of Co-0.35(SiO2)(0.65) granular film"

Brandl, A. L., Denardin, J. C., Socolovsky, L. M., Knobel, M., and Allia, P.

Magnetization curves of Co-0.35(SiO2)(0.65) granular film were measured from 70 up to 390 K. Although the anhysteretic magnetization loops could be well described using an integral of Langevin functions weighted by a distribution function of moments, the fitting parameters show an anomalous behavior. The median magnetic moments exhibit a low-temperature limit close to zero, and all have values well below the value expected from TEM analyses, with observed differences up to 82%. (C) 2003 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials **272-76, 1526-1527. 2004.**

P 131- 04 "Synchrotron radiation multiple diffraction in the characterization of the PrAl2 magnetocaloric compound"

dos Santos, A. O., Campoy, J. C. P., Coelho, A. A., Gama, S., and Cardoso, L. P.

X-ray multiple diffraction technique using synchrotron radiation is applied to characterize the PrAl2 magnetocaloric compound. Renninger scans (phi-scans) of the (0 0 2) primary reflection were measured in the Brazilian Synchrotron Laboratory (LNLS). The (53 (3) over bar) (535) four-beam case provided a = 8.0277(5) Angstrom and the sample surface polishing effect was clearly observed through the measurement of Bragg-surface diffraction (BSD) peak and the mapping (MBSD) of its multiple diffraction condition. (C) 2003 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 272-76, 2154-2156. 2004.

P 132- 04 "The bundles of algebraic and Dirac-Hestenes spinor fields"

Mosna, R. A. and Rodrigues, W. A.

Our main objective in this paper is to clarify the ontology of Dirac-Hestenes spinor fields (DHSF) and its relationship with even multivector fields, on a Riemann-Cartan spacetime (RCST) M=(M,g,del,tau(g),up arrow) admitting a spin structure, and to give a mathematically rigorous derivation of the so-called Dirac-Hestenes equation (DHE) in the case where M is a Lorentzian spacetime (the general case when M is a RCST will be discussed in another publication). To this aim we introduce the Clifford bundle of multivector fields (Cl(M,g)) and the left (Cl-Spin1,3(el)(M)) and right (Cl-Spin1,3(er)(M)) spin-Clifford bundles on the spin manifold (M,g). The relation between left ideal algebraic spinor fields (LIASF) and Dirac-Hestenes spinor fields (both fields are sections of Cl-Spin1,3(el)(M)) is clarified. We study in detail the theory of covariant derivatives of Clifford fields as well as that of left and right spin-Clifford fields. A consistent Dirac equation for a DHSF Psiis an element ofsec Cl-Spin1,3(el)(M) (denoted DECll) on a Lorentzian spacetime is found. We also obtain a representation of the DECll in the Clifford bundle Cl(M,g). It is such equation that we call the DHE and it is satisfied by Clifford fields psi(Xi)is an element ofsec Cl(M,g). This means that to each DHSF Psiis an element ofsec Cl-Spin1,3(el)(M) and spin frame Xiis an element ofsec P-Spin1,3(e)(M), there is a well-defined sum of even multivector fields psi(Xi)is an element ofsec Cl(M,g) (EMFS) associated with Psi. Such an EMFS is called a representative of the DHSF on the given spin frame. And, of course, such a EMFS (the representative of the DHSF) is not a spinor field. With this crucial distinction between a DHSF and its representatives on the Clifford bundle, we provide a consistent theory for the covariant derivatives of Clifford and spinor fields of all kinds. We emphasize that the DECll and the DHE, although related, are equations of different mathematical natures. We study also the local Lorentz invariance and the electromagnetic gauge invariance and show that only for the DHE such transformations are of the same mathematical nature, thus suggesting a possible link between them.

P 133- 04 "The change in magnetic properties of Fe3Al compound due to substitution of Fe by Co"

Coelho, A. A., Imaizumi, M., Laks, B., Araujo, A. A., Mota, M. A.,Gama, S., Jafelicci, M., and Varanda, L. C.

The magnetic moment using self-consistent spin-polarized energy band calculations of Fe3Al and Fe2CoAl Heusler phases are presented. These results are compared with the experimental values obtained from the magnetization curves of these materials.

Journal of Magnetism and Magnetic Materials 272-76, 769-770. 2004.

P 134- 04 "The electronic structure of oligothiophenes"

dos Santos, M. C. and Pickholz, M.

In the present work we report on quantum chemical calculations of oligothiophenes. The conformation and the electronic structure associated to single molecules and molecular pairs in the ground and first excited states, as well as intermolecular polaron pairs were obtained and their binding energies were calculated as a function of oligomer size. Calculations at the Hartree-Fock level using 3-21G* basis set were carried out to obtain molecular conformations. Correlation effects at the second order Moller Plesset perturbation theory were accounted for in the calculation of ground state energies, whereas a full singles configuration interaction using 6-31G* basis was performed to calculate excited states energies. Polaron pairs were shown to be stable species even in small oligomers, supporting the polaron model of elementary excitations. The results will be analyzed in the light of new experimental findings on polaron pairs.

Journal of Non-Crystalline Solids 338-40, 586-589. 2004.

P 135- 04 "The periodical ordering of the asphericity of 4f charge density at holinium single crystal"

Yokaichiya, F., Franco, M. K. K. D., Yokaichiya, D. K., and Giles, C.

This work presents X-ray scattering studies of the 2tau satellite peaks related to the periodical ordering of the asphericity of the 4f charge density of the metalic pure holmium single crystal. The thermal evolution of these satellite peaks demonstrates that the aspherical helical ordering has the same behavior as the magnetic helical ordering in the antiferromagnetic and ferromagnetic phases. (C) 2003 Elsevier B.V. All rights reserved

Journal of Magnetism and Magnetic Materials 272-76, 603-604. 2004.

P 136- 04 "The Staebler-Wronski effect in amorphous germanium"

Whitaker, J., de Lima, M. M., Marques, F. C., and Taylor, P. C.

We report the observation of a metastable Staebler-Wronski effect in hydrogenated amorphous germanium (a-Ge:H) at room temperature. Both metastable and stable (irreversible) increases in the spin density were observed by electron spin resonance (ESR) after irradiation with 1.17 eV light. The inducing and annealing kinetics are compared to the well-studied behavior in hydrogenated amorphous silicon (a-Si:H).

Journal of Non-Crystalline Solids 338-40, 374-377. 2004.

P 137- 04 "Theoretical study of strain-induced ordering in cubic InxGa1-xN epitaxial layers"

Teles, L. K., Ferreira, L. G., Scolfaro, L. M. R., and Leite, J. R.

Chemical ordering in cubic epitaxial InxGa1-xN layers is investigated by combining first-principles pseudopotential plane-wave total-energy calculations, a local concentration-dependent cluster-based method, and Monte Carlo simulations. It is found that for the unstrained or fully relaxed layers there are no stable ordered structures, indicating the tendency of the alloy to undergo phase separation, in agreement with previous calculations and experiment. The energetics of the InxGa1-xN layers pseudomorphycally grown on fully relaxed GaN (001) buffers shows that biaxial strain acts as the driving force for chemical ordering in the alloys. It is found that strained InxGa1-xN alloy comprises stable ordered structures which are (210)-oriented superlattices with composition in the range [0.5,0.63], the [AABB] alternation of planes (configuration "chalcopyrite") being the most stable phase.

***Physical Review B* 69[24]. 2004.**

P 138- 04 "Thermal expansion dependence on the Sp(2) concentration of amorphous carbon and carbon nitride"

Champi, A., Lacerda, R. G., Viana, G. A., and Marques, F. C.

The coefficients of thermal expansion of hydrogenated amorphous carbon (a-C:H) and carbon nitride (a-CNx:H) were determined using the thermally induced bending technique. Amorphous carbon films were prepared with different sp(2) concentrations by varying the bias voltage in a glow discharge system in methane atmosphere. Carbon nitride films (a-CNx:H) were deposited by introducing nitrogen gas. It was observed that the thermal expansion of a-C:H depends on the concentration of sp(2) bonded carbon, increasing to the value of graphite as the sp(2) concentration approaches 100%. Similar effect was also observed in the carbon nitride films.

***Journal of Non-Crystalline Solids* 338-40, 499-502. 2004.**

P 139- 04 "Thin films of synthetic melanin"

Deziderio, S. N., Brunello, C. A., da Silva, M. I. N., Cotta, M. A., and Graeff, C. F. O.

We have developed a new synthetic route to melanin, using different organic solvents, namely dimethyl sulfoxide and N,N-dimethyl formamide. Contrary to conventional water based melanin thin films can be made with organic solvents. Thin films were made either by room temperature solvent evaporation (casting) or using spin coating. X-ray diffraction, thermogravimetry, infrared transmission spectroscopy, UV-VIS transmission spectroscopy, electron spin resonance, atomic force microscopy (AFM) and temperature dependent conductivity have been used to characterize the material obtained. The new synthetic material is found to be similar to melanin made in water, however with an increase in thermal stability. AFM results shows that the thin films are made of graphitic-like planar structures, with root mean square roughness of similar to0.3 nm, separated by steps ranging from 1 to 3 nm in height. These sheets have lateral extensions of several microns, which make this new material potentially interesting as a 2D organic polymer.
Journal of Non-Crystalline Solids 338-40, 634-638. 2004.

P 140- 04 "Transitions between disordered phases in supercooled liquid silicon"
Miranda, C. R. and Antonelli, A.

We have investigated the transitions between disordered phases in supercooled liquid silicon using computer simulations. The thermodynamic properties were directly obtained from the free energy, which was computed using the recently proposed reversible scaling method. The calculated free energies of the crystalline and liquid phases of silicon at zero pressure, obtained using the environment dependent interatomic potential, are in excellent agreement with the available experimental data. The results show that, at zero pressure, a weak first-order liquid-liquid transition occurs at 1135 K and a continuous liquid-amorphous transition takes place at 843 K. These results are consistent with the existence of a second critical point for the liquid-liquid transition at a negative pressure. (C) 2004 American Institute of Physics.

Journal of Chemical Physics 120[24], 11672-11677. 2004.

P 141- 04 "Understanding the influence of the first-order magnetic phase transition on the magnetocaloric effect: application to Gds(SixGe(1-x))(4)"

von Ranke, P. J., de Oliveira, N. A., and Gama, S.

In this article, we investigate the influence of the first-order ferromagnetic-paramagnetic phase transition, on the magnetocaloric effect, under the combined effect of external magnetic field, pressure and magnetoelastic deformation. An application is made to Gd-5(SixGe1-x)(4), for x = 0.43 and 0.5. The obtained result leads to a good theoretical adjustment of the experimental data for isothermal magnetic entropy change.
Journal of Magnetism and Magnetic Materials 277[1-2], 78-83. 2004.

P 142- 04 "Vacancy-like defects in a-Si: a first principles study"

Miranda, C. R., Antonelli, A., da Silva, A. J. R., and Fazzio, A.

The structural and electronic properties of vacancies in a fully tetrahedral model of amorphous silicon have been investigated by ab initio calculations. A very rich behavior was observed after the atomic relaxation, from the complete rearrangement of the atoms (self-healing) to the creation of stable vacancies. We have observed that the vacancy internal relaxation volume is negative. After relaxation, the vacancy formation energies were found to be smaller than that of the crystal, and the deep gap levels either disappear or move towards the band edges.

Journal of Non-Crystalline Solids 338-40, 400-402. 2004.

P 143- 04 "Virial theorem, scaling properties and magnetic-field effects on Coulomb-bound states in semiconductor quantum wells"
Reyes-Gomez, E., Oliveira, L. E., and Dios-Leyva, M.

We have used the variational and fractional-dimensional space approaches, in the effective-mass approximation, in order to investigate the effects of applied magnetic fields on Coulomb-bound states, i.e. donor and exciton states, confined in GaAs-(Ga, Al)As quantum wells. In the variational procedure, we have used a simple hydrogenic-like envelope wavefunction whereas the anisotropic Coulomb-bound state+quantum well+magnetic-field system is modelled through an effective isotropic medium in the fractional-dimensional scheme. The magnetic fields are applied along the heterostructure growth direction, and calculations were performed for the binding energies, virial-theorem values and scaling properties. A virial-theorem value equal to 2 and a hyperbolic scaling for binding energies of Coulomb-bound states versus quantum-confined Bohr radii are obtained if one assumes a ground-state envelope wavefunction as a D-dimensional hydrogenic wavefunction, in contrast with results using the variational approach. Moreover, theoretical results within the variational approach lead to exciton-energy diamagnetic shifts in good agreement with available experimental measurements

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Abstracta

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