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A 005 - 06
A 006 - 06

Nonlinear Transport in n-III-Nitrides: Selective Amplification and Emission of Coherent LO Phonons
Survival probability of large rapidity gaps in a QCD model with a dynamical infrared mass scale

TRABALHOS PUBLICADOS

Julho à Agosto 2006

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TRABALHO ACEITO PARA PUBLICAÇÃO

A 005 - 06 Nonlinear Transport in n-III-Nitrides: Selective Amplification and Emission of Coherent LO Phonons

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

The nonequilibrium macrostate of the LO phonon system in strongly-polar n-doped III-Nitrides, in the presence of electric fields of intermediate to high intensities, is characterized. The emergence of a kind of resonance consisting in the selective amplification of LO vibrations in a privileged and localized off-center region of the Brillouin zone is demonstrated. It has associated a phenomenon akin to a Cherenkov-like effect involving a preferential emission of LO phonons in a selected cone with its axis along the direction of the electric field. Moreover, it is predicted the onset of emission (stimulated amplification) of weakly decaying coherent LO phonons generated by the drifting electrons.

Solid State Communications, accepted on August 2006.

A 006 - 06 Survival probability of large rapidity gaps in a QCD model with a dynamical infrared mass scale

We compute the survival probability $\langle |S|^2 \rangle$ of large rapidity gaps (LRG) in a QCD based eikonal model with a dynamical gluon mass, where this dynamical infrared mass scale represents the onset of nonperturbative contributions to the diffractive hadron-hadron scattering. Since rapidity gaps can occur in the case of Higgs boson production via fusion of electroweak bosons, we focus on $WW \rightarrow H$ fusion processes and show that the resulting $\langle |S|^2 \rangle$ decreases with the increase of the energy of the incoming hadrons, in line with the available experimental data for LRG. We obtain $\langle |S|^2 \rangle = 27.6 \pm 7.8\%$ ($18.2 \pm 7.0\%$) at Tevatron (CERN-LHC) energy for a dynamical gluon mass $m_g = 400$ MeV.

Physics Letters B, accepted on August 2006

TRABALHOS PUBLICADOS

P 137 - 06 "AdS geometry, projective embedded coordinates and associated isometry groups"

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

This work is intended to investigate the geometry of anti-de Sitter spacetime (AdS), from the point of view of the Laplacian Comparison Theorem (LCT), and to give another description of the hyperbolic embedding standard formalism of the de Sitter and anti-de Sitter spacetimes in a pseudoeuclidean spacetime. After Witten proved that general relativity is a renormalizable quantum system in (1+2) dimensions, it is possible to point out few interesting motivations to investigate AdS spacetime. A lot of attempts were made to generalize the gauge theory of gravity in (1+2) dimensions to higher ones. The first one was to enlarge the Poincare group of symmetries, supposing an AdS group symmetry, which contains the Poincare group. Also, the AdS/CFT correspondence asserts that a maximal supersymmetric Yang-Mills theory in four-dimensional Minkowski spacetime is equivalent to a type IIB closed superstring theory. The 10-dimensional arena for the type IIB superstring theory is described by the product manifold $S^5 \times AdS$, an impressive consequence that motivates the investigations about the AdS spacetime in this paper, together with the de Sitter spacetime. Classical results in this mathematical formulation are reviewed in a more general setting together with the isometry group associated to the de Sitter spacetime. It is known that, out of the Friedmann models that describe our universe, the Minkowski, de Sitter, and anti-de Sitter spacetimes are the unique maximally isotro-

pic ones, so they admit a maximal number of conservation laws and also a maximal number of Killing vectors. In this paper it is shown how to reproduce some geometrical properties of AdS, from the LCT in AdS, choosing suitable functions that satisfy basic properties of Riemannian geometry. We also introduce and discuss the well-known embedding of a four-sphere and a four-hyperboloid in a five-dimensional pseudoeuclidean spacetime, reviewing the usual formalism of spherical embedding and the way how it can retrieve the Robertson-Walker metric. With the choice of the de Sitter metric static frame, we write the so-called reduced model in suitable coordinates. We assume the existence of projective coordinates, since de Sitter spacetime is orientable. From these coordinates, obtained when stereographic projection of the de Sitter four-hemisphere is done, we consider the Beltrami geodesic representation, which gives a more general formulation of the seminal full model described by Schrodinger, concerning the geometry and the topology of de Sitter spacetime. Our formalism retrieves the classical one if we consider the metric terms over the de Sitter splitting on Minkowski spacetime. From the covariant derivatives we find the acceleration of moving particles, Killing vectors and the isometry group generators associated to de the Sitter spacetime.

International Journal of Theoretical Physics 45[3], 575-588. 2006.

P 138 - 06 "Advances and challenges in electron-molecule scattering physics - A report of the 14th International Symposium on Electron-Molecule Collisions and Swarms"

Khakoo, M. A., Lima, M. A. P., and Tennyson, J.

A report is presented of the 13th International Symposium on Electron - Molecule Collisions Physics (Instituto de Física, Unicamp, Campinas, Brazil, 27 - 30 July 2005). This workshop covered low-energy electron interactions with atoms, molecules and condensed matter systems. Several important aspects of this symposium were to bring together theory and experimental advances in this field for gaseous targets as well as showcasing the increasing diversity of electron - molecule collision applications in condensed matter and biological applications. A summary session was held wherein were discussed aspects of the future of the field, including the development of new theoretical and experimental capabilities.

Physica Scripta 74[1], C7-C14. 2006.

P 139 - 06 "Amorphous silicon deposited by xenon ion beam assisted deposition"

Barbieri, P. F., de Oliveira, M. H., Champi, A., and Marques, F. C

In this work, we present some properties of amorphous silicon deposited by ion beam assisted deposition (IBAD). The films were prepared using a Kauffman ion gun using xenon (Xe) gas to sputter a silicon target. Another ion gun was adopted to simultaneously bombard the film with Xe during the growth of the film with xenon in the 0-300 eV energy range. Rutherford backscattering (RBS) was used to determine the concentration of the implanted Xe atoms and the density of the films. It was observed that the implantation of Xe do not affect much the stress of the films, which is compressive and about -0.6 GPa for all samples. The concentration of implantation Xe reach a maximum at energy of about 50 eV decreasing as the ion energy increases. The density of the films follows the concentration of Xe, suggesting that the densification of the film is not due to a compactation process supplied by the Xe bombardment of the films, but rather due to the incorporation of a heavy atom into the matrix.

Journal of Non-Crystalline Solids 352[9-20], 1016-1019. 2006.

P 140 - 06 "Analytical results for a Bessel function times Legendre polynomials clasP 187 - 06 "Surface composition and structure of palladium ultra-thin films deposited on Ni(111)"

Carazzolle, M. F., Maluf, S. S., de Siervo, A., Nascente, P. A. P., Landers, R., and Kleiman, G. G.

Ultra-thin palladium films deposited on the Ni(111) surface were characterized by X-ray photoelectron spectroscopy (XPS), lowenergy electron diffraction (LEED) and X-ray photoelectron diffraction (XPD). For low coverage, LEED shows a (1 x 1) pattern similar to that of the substrate. For intermediate coverage, the LEED pattern displays extra spots around the main (1 x 1) spots, resembling a Moire coincidence pattern, probably associated with the formation of Pd bi-dimensional islands oriented in different directions on the Ni(111) surface. The results obtained by XPS and XPD corroborate this finding. The LEED pattern displays this structure up to 500 degrees C. Annealing at 650 degrees C brings back the (1 x 1) pattern, which is associated with a Pd island coalescence and alloy formation by Pd diffusion in the first atomic layers of the Ni(111). In this paper we present a detailed study of this surface structure via a comparison between XPD experiment and theory.

Surface Science 600[11], 2268-2274. 2006.

P 141 - 06 "Anomalous Hall effect in graphite"

Kopelevich, Y., Pantoja, J. C. M., da Silva, R. R., Mrowka, F., and Esquinazi, P.

We report on the experimental observation of an anomalous Hall effect (AHE) in highly oriented pyrolytic graphite samples. The overall data indicate that the AHE in graphite can be self-consistently understood within the frameworks of the magnetic-field-driven excitonic pairing models.

Physics Letters A 355[3], 233-236. 2006.

P 142 - 06 "Ballistic transport in open quantum dots: Scar wavefunctions and resonance line shapes"

Mendoza, M. and Schulz, P. A.

We present simulations of transport through highly transmitting open cavities within a lattice Green's function formalism. The qualitative relation between the line shape of the conductance and the symmetries of the corresponding scar wavefunctions is discussed. This system presents similar scar wavefunctions at different conductance plateaus. At the high plateau index limit the scars associated with bouncing ball classic orbits suffer a transition from accessible to quasi-unaccessible from outside the square billiard.

Brazilian Journal of Physics 36[2A], 423-426. 2006.

P 143 - 06 "Band gap of hexagonal 2D photonic crystals with elliptical holes recorded by interference lithography"

Quinonez, F., Menezes, J. W., Cescato, L., Rodriguez-Esquerre, V. F., Hernandez-Figueroa, H., and Mansano, R. D.

Two-dimensional hexagonal photonic crystals can be recorded using the simple superimposition of two interference patterns rotated by 60 degrees. Such process generates high contrast masks, however, it generates elliptical cross section structures instead of cylinders. We study the PBG properties of the experimentally feasible geometries, using this technique and we demonstrate that the effect of this asymmetric shape is a reduction in the PBG map area, for TE polarization, in comparison with cylindrical structures. On the other hand, it appears a PBG for TM polarization.

Optics Express 14[11], 4873-4879. 2006.

P 144 - 06 "Carbon nano-structures containing nitrogen and hydrogen prepared by ion beam assisted deposition"

Paredez, P., Marchi, M. C., da Costa, M. E. H. M., Figueroa, C. A., Kleinke, M. U., Ribeiro, C. T. M., Sanchez-Lopez, J. C., Rojas, T. C., and Alvarez, F.

In this paper, we report the synthesis and some properties of nano-structured carbon films grown on nanometric nickel particles at 700 degrees C by ion beam assisted deposition (IBAD). In situ photoelectron emission spectroscopy (XPS) reveals the presence of nitrogen in the carbon layer coating the nickel particles. Atomic force microscopy (AFM) displays regular dome-like structures with a mean width, height, and density of similar to 170 nm, similar to 22 nm, and similar to 1.4×10^9 domes/cm², respectively. Raman spectroscopy shows the characteristic frequencies associated with graphite and disordered structures. Disorder increases on increasing nitrogen content. High-resolution transmission electron microscopy (HRTEM) confirms the presence of multiwall well-organized graphite layers covering the nickel particles. The field emission properties of the structures are reported.

Journal of Non-Crystalline Solids 352[9-20], 1303-1306. 2006.

P 145 - 06 "Chirality dynamics for a fermionic particle non-minimally coupling with an external magnetic field"

Bernardini, A. E.

We proceed with the construction of normalizable Dirac wave packets for treating chiral oscillations in the presence of an external magnetic field. Both chirality and helicity quantum numbers correspond to variables of fundamental importance in the study of chiral interactions, in particular, in the context of neutrino physics. In order to clarify a subtle aspect in the confront of such concepts which, for massive particles, represent different physical quantities, we are specifically interested in quantifying chiral oscillations for a fermionic Dirac-type particle (neutrino) non-minimally coupling with an external magnetic field B by solving the corresponding interacting Hamiltonian (Dirac) equation. The viability of the intermediate wave-packet treatment becomes clear when we assume B orthogonal/parallel to the direction of the propagating particle.

Journal of Physics A-Mathematical and General 39[22], 7089-7097. 2006.

P 146 - 06 "Clifford algebra-parametrized octonions and generalizations"

da Rocha, R. and Vaz, J.

Introducing products between multivectors of Cl-0,Cl-7 (the Clifford algebra over the metric vector space R-0,R-7) and octonions, resulting in an octonion, and leading to the non-associative standard octonionic product in a particular case, we generalize the octonionic X-product, associated with the transformation rules for bosonic and fermionic fields on the tangent bundle over the 7-sphere S-7, and the XY-product. This generalization is accomplished in the u- and (u, v)-products, where u, v is an element of Cl-0,Cl-7 are fixed, but arbitrary. Moreover, we extend these original products in order to encompass the most general-non-associative-products (R circle plus R-0,R-7) x Cl-0,Cl-7 -> R circle plus R-0,R-7, Cl-0,Cl-7 x (R circle plus R-0,R-7) -> R circle plus R-0,R-7 and Cl-0,Cl-7 x Cl-0,Cl-7 -> R circle plus R-0,R-7. We also present the formalism necessary to construct Clifford algebra-parametrized octonions, which provides the structure to present the O-1,O-u algebra. Finally we introduce a method to construct O-algebras endowed with the (u, v)-product from O-algebras endowed with the u-product. These algebras are called O-like algebras and their octonionic units are parametrized by arbitrary Clifford multivectors. When

u is restricted to the underlying paravector space $R \oplus R \cdot 0, R \cdot 7 \rightarrow Cl_0, Cl_7$ of the octonion algebra O , these algebras are shown to be isomorphic. The products between Clifford multivectors and octonions, leading to an octonion, are shown to share graded-associative, super-symmetric properties. We also investigate the generalization of Moufang identities, for each one of the products introduced. (c) 2006 Published by Elsevier Inc

Journal of Algebra 301[2], 459-473. 2006.

P 147 - 06 "Coherent properties and Rabi oscillations in two-level donor systems"

Latge, A., Ribeiro, F. J., Bruno-Alfonso, A., Oliveira, L. E., and Brandi, H. S.

Coherent properties and Rabi oscillations in two-level donor systems, under terahertz excitation, are theoretically investigated. Here we are concerned with donor states in bulk GaAs and GaAs-(Ga,Al)As quantum dots. We study confinement effects, in the presence of an applied magnetic field, on the electronic and on-center donor states in GaAs-(Ga,Al)As dots, as compared to the situation in bulk GaAs, and estimate some of the associated decay rate parameters. Using the optical Bloch equations with damping, we study the time evolution of the $1s$ and $2p(+)$ states in the presence of an applied magnetic field and of a terahertz laser. We also discuss the role played by the distinct dephasing rates on the photocurrent and calculate the electric dipole transition moment. Results indicate that the Rabi oscillations are more robust as the total dephasing rate diminishes, corresponding to a favorable coherence time.

Brazilian Journal of Physics 36[2A], 419-422. 2006. P

148 - 06 "Comment on: "Low temperature Phanerozoic history of the Northern Yilgarn Craton, Western Australia" by U. D. Weber et al. [Tectonophysics 400 (2005) 127-151]"

Guedes, S., Hadler, J. C., Lunes, P. J., and Tello, C. A.

Tectonophysics 419[1-4], 103-105. 2006.

P 149 - 06 "Continuous variable quantum key distribution using polarized coherent states"

Vidiella-Barranco, A. and Borelli, L. F. M.

We discuss a continuous variables method of quantum key distribution employing strongly polarized coherent states of light. The key encoding is performed using the variables known as Stokes parameters, rather than the field quadratures. Their quantum counterpart, the Stokes operators S_i ($i=1,2,3$), constitute a set of non-commuting operators, being the precision of simultaneous measurements of a pair of them limited by an uncertainty-like relation. Alice transmits a conveniently modulated two-mode coherent state, and Bob randomly measures one of the Stokes parameters of the incoming beam. After performing reconciliation and privacy amplification procedures, it is possible to distill a secret common key. We also consider a non-ideal situation, in which coherent states with thermal noise, instead of pure coherent states, are used for encoding.

International Journal of Modern Physics B 20[11-13], 1287-1296. 2006.

P 150 - 06 "Cyclotron effective mass and Lande g factor in GaAs-Ga_{1-x}Al_xAs quantum wells under growth-direction applied magnetic fields"

Dios-Leyva, M., Porras-Montenegro, N., Brandi, H. S., and Oliveira, L. E.

We have performed a theoretical study of the cyclotron effective mass and electron effective Lande g (parallel to) factor in semiconductor GaAs-Ga_{1-x}Al_xAs quantum wells under an applied magnetic field parallel to the growth direction of the quantum well. The theoretical approach is within the nonparabolic and effective-mass approximation and via an Ogg-McCombe effective Hamiltonian [Proc. Phys. Soc. London 89, 431 (1969); Phys. Rev. 181, 1206 (1969)] for the electron in the conduction band of the GaAs-Ga_{1-x}Al_xAs heterostructure, which allows a unified treatment of both the cyclotron mass and g (parallel to) factor. Calculations are performed for different widths of the GaAs-Ga_{1-x}Al_xAs quantum wells and as functions of the applied magnetic field, with results in very good agreement with reported experimental measurements of the electron cyclotron effective mass and g (parallel to) factor.

Journal of Applied Physics 99[10]. 2006.

P 151 - 06 "Delocalized states in damaged DNA"

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

Recent studies suggest that base pairing is an efficient electronic delocalization mechanism. However, defects may break down such effect. In the present work we show how a simple model of defects suppresses the delocalization, which survives only for low defect concentrations.

Brazilian Journal of Physics 36[2A], 459-461. 2006.

P 152 - 06 "Dynamical localization of the Hofstadter spectra"

Rivera, P. H. and Schulz, P. A.

Recent results on magnetoresistance in a two dimensional electron gas (2DEG) under crossed magnetic and microwave fields show a new class of oscillations, suggesting a new kind of zero-resistance states. We consider the problem from the point of view of the electronic structure dressed by photons due to an in-plane linearly polarized ac field. In the strong modulation limit predictions on dressed Hofstadter spectra are discussed, which could be of interest since the bare spectra have been observed in the past few years.

Brazilian Journal of Physics 36[2A], 357-360. 2006.

P 153 - 06 "Effect of processing parameters on control of defect centers associated with second-order harmonic generation and photosensitivity in SiO₂:GeO₂ glass preforms"

Cuevas, R. F., Sekiya, E. H., Garcia-Quiroz, A., Da Silva, E. C., and Suzuki, C. K.

In this research, the effect of the H-2/O-2 ratio and the processing temperature parameters on the inducing and enhancement of the defect centers associated to the second-order optical non-linearity in SiO₂:GeO₂ glass preforms, prepared by vapor-phase axial deposition method, have been investigated. The formation of germanium oxygen deficient centers and the development of paramagnetic structures induced in the glass preforms after X-ray irradiation were investigated using UV-Vis absorption spectroscopy and electronic spin resonance. The results indicate that the concentration of germanium oxygen deficient centers increases exponentially when the H-2/O-2 ratio decreases, while the processing temperature increases, simultaneously. The electronic spin resonance spectra profiles, shows that defects of the electron trapped centers type [Ge(1), Ge(2)] are induced by the effect of X-ray irradiation. An efficient generation of defect centers associated to the second-order optical non-linearity in SiO₂:GeO₂ glass preforms, occurring in samples prepared with low H-2/O-2 ratios and high processing temperatures, have been observed.

Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms 247[2], 285-289. 2006.

P 154 - 06 "Efficient 1 GHz Ti : sapphire laser with improved broadband continuum in the infrared"

Nogueira, G. T. and Cruz, F. C.

We demonstrate a 1 GHz prisinless femtosecond Ti:sapphire ring laser that emits 890 MW for 7.6 W of pump power over a continuum extending from 585 to 1200 nm at -20 dB below the maximum. A broadband continuum is obtained with the net cavity group delay dispersion having -50 to 100 fs(2) oscillations from 700 to 900 nm. Further broadening is obtained by use of a slightly convex cavity mirror that increases self-phase modulation. Approximately 17% (75%) of the intracavity (output) power is generated in single pass through the crystal, outside the cavity bandwidth, and concentrated in the low-gain IR from 960 to 1200 nm.

Optics Letters 31[13], 2069-2071. 2006.

P 155 - 06 "Electrical properties of individual and small ensembles of InAs/InP nanostructures"

Vicaro, K. O., Gutierrez, H. R., Bortoleto, J. R. R., Nieto, L., von Zuben, A. A. G., Seabra, A. C., Schulz, P. A., and Cotta, M. A.

We investigate electrical properties of InAs/InP semiconductor nanostructures by conductive atomic force microscopy (C-AFM) and current measurements at low temperatures in processed devices. Different conductances and threshold voltages for current onset were observed for each type of nanostructure. In particular, the extremity of the wire could be compared to a dot with similar dimensions. The processed devices were used in order to access the in-plane conductance of an assembly of a reduced number of nanostructures. Here, fluctuations on I-V curves at low temperatures (< 40 K) were observed. At these low temperatures and for a suitable range of applied voltages, random telegraph noise (RTN) in the current was observed for devices with dots. These fluctuations can be associated to electrons trapped in dots, as suggested by numerical simulations. A crossover from a semiconductor-like to a metallic transport behavior is also observed for similar parameters.

Physica Status Solidi A-Applications and Materials Science 203[6], 1353-1358. 2006.

P 156 - 06 "Electronic transport through a quantum wire with a side-coupled quantum dot"

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

We describe the Kondo resonance in quantum dots employing the atomic model. We calculate approximate Green's functions of the impurity Anderson model employing the exact solution of the system with a conduction band with zero width, and we use the completeness condition to choose the position of that band. At low temperatures, there are two solutions close to the chemical potential μ , satisfying this condition, and we choose the one with minimum Helmholtz free energy, considering that this corresponds to the Kondo solution. At high temperatures, this solution no longer exist, corresponding to the disappearance of the Kondo peak. We present curves of density of states that characterize the Kondo peak structure problem. As a simple application we calculate the conductance of a side-coupled quantum dot and we obtain good agreement with recent experimental results.

Brazilian Journal of Physics 36[2A], 397-400. 2006.

P 157 - 06 "Enhanced nitrogen diffusion induced by atomic attrition"

Ochoa, E. A., Figueroa, C. A., Czerwicz, T., and Alvarez, F.

The nitrogen diffusion in steel is enhanced by previous atomic

attrition with low energy xenon ions. The noble gas bombardment generates nanoscale texture surfaces and stress in the material. The atomic attrition increases nitrogen diffusion at lower temperatures than the ones normally used in standard processes. The stress causes binding energy shifts of the Xe 3d(5/2) electron core level. The heavy ion bombardment control of the texture and stress of the material surfaces may be applied to several plasma processes where diffusing species are involved.

Applied Physics Letters 88[25]. 2006.

P 158 - 06 "Evaluation of diamond-like carbon coatings produced by plasma immersion for orthopaedic applications"

Uzumaki, E. T., Lambert, C. S., Belangero, W. D., Freire, C. M. A., and Zavaglia, C. A. C.

The purpose of the present study was to evaluate the properties of diamond-like carbon (DLC) coating on Ti alloy (Ti-13Nb-13Zr) produced by plasma immersion. Measurements of mechanical properties and corrosion behaviour were investigated. The corrosion studies (polarization test and electrochemical impedance spectroscopy) indicated that DLC coating could improve corrosion resistance in the simulated body fluid environment. In vivo tests were carried out by inserting 5 x 1 mm diameter DLC-coated Ti-13Nb-13Zr cylinders into both muscular tissue and femoral condyles of rats for intervals of 4 and 12 weeks post-operatively. Histological analyses showed that the DLC coatings were well tolerated in both types of implantation, demonstrating the in vivo biocompatibility of the DLC coatings produced by plasma immersion.

Diamond and Related Materials 15[4-8], 982-988. 2006.

P 159 - 06 "Gd³⁺ and Eu²⁺ local environment in Ca_{1-x}Eu_xB₆ (0.0001 ≤ x ≤ 0.30) and Ca_{1-x}Gd_xB₆ (0.0001 ≤ x ≤ 0.01)"

Urbano, R. R., Pagliuso, P. G., Rettori, C., Schlottmann, P., Fisk, Z., Chapler, B., and Oseroff, S. B.

Local environment of Gd³⁺ and Eu²⁺ 4f(7) ions, $S = 7/2$, in Ca_{1-x}Eu_xB₆ (0.0001 ≤ x ≤ 0.30) and Ca_xGd_xB₆ (0.0001 ≤ x ≤ 0.01) is investigated by means of electron spin resonance (ESR). For x ≤ 0.001 the spectra show resolved fine structures due to the cubic crystal electric field and, in the case of Eu, the hyperfine structure due to the nuclear hyperfine field is also observed. The resonances have Lorentzian line shape, indicating insulating host for the Gd³⁺ and Eu²⁺ ions. As x increases, the ESR lines broaden due to local distortions caused by the Ca/Gd, Eu ions substitution. For Gd (x approximate to 0.001) and Eu (x approximate to 0.02), the spectra present superposition of Lorentzian and Dysonian resonances, suggesting a coexistence of insulating and metallic hosts for the Gd³⁺ and Eu²⁺ ions. The Gd³⁺ and Eu²⁺ fine structures are still observable up to x approximate to 0.003 for Gd and x approximate to 0.15 for Eu. For larger values of x the fine and hyperfine structures are no longer observed, the line width increases, and the line shape becomes pure Dysonian anticipating the metallic and semimetallic character of GdB₆ and EuB₆, respectively. These results clearly show that in the low concentration regime the Ca_{1-x}R_xB₆ (R = Gd, Eu) systems are intrinsically inhomogeneous. No evidence of weak ferromagnetism (WF) was found in the ESR spectra of either metallic or insulating phases of these compounds, suggesting that, if WF is present in these materials, the Gd³⁺ and Eu²⁺ 4f(7)-electrons are shielded from the WF field.

Physica Status Solidi A-Applications and Materials Science 203[7], 1550-1555. 2006.

P 160 - 06 "Generalized quantum-state sharing"

Gordon, G. and Rigolin, G.

We present two quantum-state sharing protocols where the channels are not maximally entangled states. By properly

choosing the measurement basis it is possible to achieve unity fidelity transfer of the state if the parties collaborate. We also show that contrary to the protocols where we have maximally entangled channels these protocols are probabilistic. We then compare the efficiency of both protocols and sketch the generalization of the protocols to N parties.

Physical Review A 73[6]. 2006.

P 161 - 06 "Influence of hydrogen on the thermomechanical properties of a-CN_x : H and a-CN_x films deposited by glow discharge and ion beam assisted deposition"

Champi, A., Barbieri, P. F., and Marques, F. C.

The coefficient of thermal expansion (CTE), Young's modulus, Poisson's ratio, stress and hardness of a-CN_x and a-CN_x:H were investigated as a function of nitrogen concentration. Hydrogenated films were prepared by glow discharge, GD, and unhydrogenated films were prepared by ion beam assisted deposition, IBAD. Using nanoindentation measurements and the thermally induced bending technique, it was possible to extract separately, Young's modulus and Poisson's ratio. A strong influence of hydrogen, in a-CN_x:H films, was observed on the CTE, which reaches about similar to 9×10^{-6} C⁻¹, close to that of graphite (similar to 8×10^{-6} C⁻¹) for nitrogen concentration as low as 5 at.%. On the other hand, the CTE of unhydrogenated films increases with nitrogen concentration, at a much lower rate, reaching 5.5×10^{-6} C⁻¹ for 33 at.% nitrogen.

Journal of Non-Crystalline Solids 352[21-22], 2264-2266. 2006.

P 162 - 06 "Liquidus projection of the Nb-Cr-Al system near the Al-3(Nb,Cr)+Cr(Al,Nb) eutectic region"

Souza, S. A., Ferrandini, P. L., Nunes, C. A., Coelho, A. A., and Caram, R.

The system Nb-Cr-Al was investigated in the region near the Al-3(Nb,Cr) + Cr(Al,Nb) eutectic and the liquidus projection of that region was determined based on the microstructural characterization of arc melted alloys. The characterization utilized scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), differential thermal analysis (DTA) and X-ray diffraction (XRD). The results allowed one to determine three primary solidification liquidus surfaces ((Cr,Al)(2)Nb, Cr(Al,Nb) and Al-3(Nb,Cr)), that are originated from the binary systems Cr-Nb, Cr-Al and Al-Nb. It is proposed the occurrence of the invariant reaction $L + (Cr,Al)(2)Nb \rightleftharpoons Al-3(Nb,Cr) + Cr(Al,Nb)$ and of a point of minimum, which involves a three phase reaction, $L \rightleftharpoons Al-3(Nb,Cr) + Cr(Al,Nb)$. All alloys studied showed formation of the Al-3(Nb,Cr) + Cr(Al,Nb) eutectic as the last solidification step with Al(Nb)Cr, precipitating from Cr(Al,Nb).

Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing 424[1-2], 77-82. 2006.

P 163 - 06 "Low resolution structure of the human alpha 4 protein (IgBP1) and studies on the stability of alpha 4 and of its yeast ortholog Tap42"

Smetana, J. H. C., Oliveira, C. L. P., Jablonka, W., Pertinhez, T. A., Carneiro, F. R. G., Montero-Lomeli, M., Torriani, I., and Zanchin, N. I. T.

The yeast Tap42 and mammalian alpha 4 proteins belong to a highly conserved family of regulators of the type 2A phosphatases, which participate in the rapamycin-sensitive signaling pathway, connecting nutrient availability to cell growth. The mechanism of regulation involves binding of Tap42 to Sit4 and PPH21/22 in yeast and binding of a4 to the catalytic subunits

of type 2A-related phosphatases PP2A, PP4 and PP6 in mammals. Both recombinant proteins undergo partial proteolysis, generating stable N-terminal fragments. The full-length proteins and a4 C-terminal deletion mutants at amino acids 222 (alpha 4 Delta 222), 236 (alpha 4 Delta 236) and 254 (alpha 4 Delta 254) were expressed in *E. coli*. alpha 4 Delta 254 undergoes proteolysis, producing a fragment similar to the one generated by full-length a4, whereas alpha 4 Delta 222 and alpha 4 Delta 236 are highly stable proteins. alpha 4 and Tap42 show alpha-helical circular dichroism spectra, as do their respective N-terminal proteolysis resistant products. The cloned truncated proteins alpha 4 Delta 222 and alpha 4 Delta 236, however, possess a higher content of a-helix, indicating that the C-terminal region is less structured, which is consistent with its higher sensitivity to proteolysis. In spite of their higher secondary structure content, alpha 4 Delta 222 and alpha 4 Delta 236 showed thermal unfolding kinetics similar to the full-length alpha 4. Based on small angle X-ray scattering (SAXS), the calculated radius of gyration for alpha 4 and Tap42 were 41.2 ± 0.8 angstrom and 42.8 ± 0.7 angstrom and their maximum dimension similar to 142 angstrom and similar to 147 angstrom, respectively. The radii of gyration for alpha 4 Delta 222 and alpha 4 Delta 236 were 21.6 ± 0.3 angstrom and 25.7 ± 0.2 angstrom, respectively. Kratky plots show that all studied proteins show variable degree of compactness. Calculation of model structures based on SAXS data showed that alpha 4 Delta 222 and alpha 4 Delta 236 proteins have globular conformation, whereas alpha 4 and Tap42 exhibit elongated shapes.

Biochimica et Biophysica Acta-Proteins and Proteomics 1764[4], 724-734. 2006.

P 164 - 06 "Magnetic-field-driven quantum critical behavior in graphite and bismuth"

Kopelevich, Y., Pantoja, J. C. M., da Silva, R. R., and Moehlecke, S.

We study magnetotransport properties of graphite and rhombohedral bismuth samples and found that in both materials applied magnetic field induces the metal-insulator- (MIT) and reentrant insulator-metal-type (IMT) transformations. The corresponding transition boundaries plotted on the magnetic field-temperature (B-T) plane nearly coincide for these semimetals and can be best described by power laws $T \sim (B-B_c)^k$, where B_c is a critical field at $T = 0$ and $k = 0.45 \pm 0.05$. We show that insulator-metal-insulator (IMI) transformations take place in the Landau level quantization regime and illustrate how the IMT in quasi-3D graphite transforms into a cascade of IMI transitions, related to the quantum Hall effect in quasi-2D graphite samples. We discuss the possible coupling of superconducting and excitonic correlations with the observed phenomena, as well as signatures of quantum phase transitions associated with the M-I and I-M transformations.

Annals of Physics 321[7], 1575-1587. 2006.

P 165 - 06 "Magnetic properties of GaN/MnxGa1-xN digital heterostructures: First-principles and Monte Carlo calculations"

Marques, M., Ferreira, L. G., Teles, L. K., Scolfaro, L. M. R., Furthmuller, J., and Bechstedt, F.

The energetic and magnetic properties of wurtzite GaN/MnxGa1-xN digital heterostructures are investigated by first-principles total energy calculations, within the spin density-functional theory, and Monte Carlo simulations. In a wurtzite GaN model sample, periodic in the c axis, we replace a GaN monolayer (a plane) by a plane with composition MnxGa1-xN, and study its properties for varying the GaN spacer layer thickness and Mn concentration x . The 100% MnN monolayer possesses an antiferromagnetic (AFM) ground state when, in the periodic sample, it is isolated from the other MnN monolayers by more than four GaN spacer layers. The case of submonolayers ($x < 1$) is studied by Monte Carlo simulations based on an Ising Hamiltonian, whose parameters are obtained from ab initio calculations on five configurations. At 700 degrees C, up to the concentration of 8% Mn, the two-dimensional (2D) alloy is stable. However, above this concentration, there is a strong tendency to the formation of MnN clusters with an AFM ground state defined

by ferromagnetic Mn rows coupled antiferromagnetically with other Mn rows. The behavior of the magnetization with the temperature is completely different in these two concentration regimes, with the 2D MnN cluster being very stable, whereas the 2D alloy presents low magnetic transition temperatures.

Physical Review B 73[22]. 2006.

P 166 - 06 "Mechanical and vibrational properties of carbon nitride alloys"

Champi, A. and Marques, F. C.

A study of ultraviolet and visible Raman spectroscopy was made in amorphous carbon nitride (a-C:N-x) and amorphous hydrogenated carbon nitride (a-C:N-x:H) thin films. Two growth techniques were used: 1) glow discharge was used for depositing hydrogenated films with diamond-like (at -200V of bias) and graphite-like (-800V of bias) structure and 2) ion beam assisted deposition (IBAD) to deposit non-hydrogenated films and to obtain high nitrogen concentrations (similar to 30%). The difference in energy between the visible and UV Raman, the so called G dispersion parameter, was investigated for both series of films. This parameter brings additional information concerning the structure of the films regarding size and concentration of graphitic clusters, and qualitative information on the sp(2)/Sp(3) concentration. The characterization of the structural properties in these films indicates an increase of graphite clusters with the incorporation of nitrogen.

Brazilian Journal of Physics 36[2A], 462-465. 2006.

P 167 - 06 "Non-linear electron mobility in n-doped III-Nitrides"

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

A theoretical study of the mobility of n-doped III-Nitrides in wurtzite phase is reported. We have determined the non-equilibrium thermodynamic state of the bulk n-InN, n-GaN, and n-AlN systems - driven far away from equilibrium by a strong electric field - in the steady state, which follows after a very fast transient. For this we solve the set of coupled nonlinear integro-differential equations of evolution of the nonequilibrium thermodynamic variables, for the three materials, to obtain their steady state values. The dependence of the mobility (which depends on the nonequilibrium then-nodynamic state of the sample) on the electric field strength and the concentration (of electrons and impurities) is derived, which decreases with the increase of the electric field strength and the concentration of carriers, evidencing the influence of the nonlinear transport involved.

Brazilian Journal of Physics 36[2A], 255-257. 2006.

P 168 - 06 "Noncubic symmetry in Ca_{1-x}Eu_xB₆ (0.15 less than or similar to x <= 1.00): An electron-spin-resonance study"

Urbano, R. R., Pagliuso, P. G., Rettori, C., Schlottmann, P., Fisk, Z., and Oseroff, S. B.

The Eu²⁺ (4f⁷, S=7/2) g value in Ca_{1-x}Eu_xB₆ (0.15 less than or similar to x <= 1.00) was measured by means of electron spin resonance at two frequencies (fields), 9.4 (approximate to 3.4 kOe) and 34.4 GHz (approximate to 12.1 kOe). The g value was found to be anisotropic and magnetic-field dependent. The amplitude of the anisotropy increases at low temperatures. The observed angular and temperature dependences of the g value suggest tetragonal symmetry caused, presumably, by a distortion along a direction perpendicular to the largest crystal face, the [001] direction. Due to the platelet shape of the samples, part of the anisotropy of the g value can also be attributed to demagnetization effects. The g values decrease at higher fields, which is interpreted

in terms of a two-band model involving an exchange interaction between the localized Eu²⁺ 4f(7) electrons with conduction Eu²⁺ 5d-like electrons and B 2p-like holes.

Journal of Applied Physics 99[8]. 2006.

P 169 - 06 "Observation of field-induced single impurity behavior in the heavy fermion compound Ce₃Co₄Sn₁₃"

Cornelius, A. L., Christianson, A. D., Lawrence, J. L., Fritsch, V., Bauer, E. D., Sarrao, J. L., Thompson, J. D., Pagliuso, P. G.

We have performed heat capacity measurements in magnetic fields to 90 kOe on single crystals of the cubic heavy fermion compound Ce₃Co₄Sn₁₃. In zero field, there are no signs of long-range magnetic order down to 0.35 K. However, C/T increases rapidly below 2 K, reaching a very large maximum value of similar to 4 J/mol Ce-K around 0.8 K in zero field, and the high-field magnetic entropy approaches Rln 2 at 20 K. Above 25 kOe, the data are consistent with a Kondo impurity with T-K = 1.2 K. Short-range magnetic correlations are suppressed by magnetic fields giving way to single impurity behavior above 25 kOe.

Physica B-Condensed Matter 378-80, 113-114. 2006.

P 170 - 06 "Optical emission spectroscopy of benzyl radicals produced in a radio-frequency plasma"

Pereira, R. V., Miyao, Y., and Pessine, F. B. T.

The benzyl radical was studied by optical emission spectroscopy in gas phase. This radical was produced in a radio-frequency (RF, 13.56 MHz) discharge, using benzyl alcohol (OCH₂OH) as a precursor. The fluorescence from the first excited electronic state 1(2)A(2) to ground state 1(2)B(2) (450 nm) was studied as a function of several external parameters (pressure, RF power, electrodes and mixtures of the inert gases Ar, Ne, He, N₂, with the precursor). We also used a DC discharge to produce this radical but, in this case, the decomposition was fast. We observed changes in the electronic transitions of this radical, and found the best conditions to study it by optogalvanic spectroscopy.

Spectrochimica Acta Part A-Molecular and Biomolecular Spectroscopy 64[4], 901-905. 2006.

P 171 - 06 "Oxygen plasma etching of carbon nano-structures containing nitrogen"

Acuna, J. J. S., Figueroa, C. A., da Costa, M. E. H. M., Paredes, P., Ribeiro, C. T. M., and Alvarez, F.

In this paper we report a study of the oxygen plasma etching effect on CN_x nano-structures grown on tiny nickel islands (similar to 1-5 nm) previously deposited onto oxidized silicon wafers. In order to eliminate the ill-formed structures, broad oxygen ion beam plasma was used to irradiate the nano-structured CN_x material (similar to 3.4 at.% N). The structures were prepared by ion beam assisted deposition (IBAD) and etched in situ by an oxygen ion beam at room temperature. In situ characterization by XPS and ex situ Raman, FEG-SEM, AFM, and field emission measurements were employed to study the evolution of the nano-structures. Raman spectra show two narrow and well defined D and G bands (disorder and graphitic bands) in the formed nano-structure.

Journal of Non-Crystalline Solids 352[9-20], 1314-1318. 2006.

P 172 - 06 "Photoluminescence and optical absorption of Cs₂NaScF₆ : Cr³⁺"

Sosman, L. P., da Fonseca, R. J. M., Tavares, A. D., Nakaema, M. K. K., and Bordallo, H. N.

The main objective of this paper is the characterization of the spectroscopic properties of new materials that are prospective laser media. This approach allows for the comparison of the properties of the Cr³⁺ in different environments. Here, we have studied the photoluminescence and optical absorption of Cs₂NaScF₆:Cr³⁺ single crystals. On the basis of near-infrared luminescence measurements at 2, 77, and 300 K the observed lines originated from the Cr³⁺-centres were associated with the T-4(2)(F-4) → 4A(2)(F-4) transition and the lifetimes were obtained. In spite of the quenching observed as a function of temperature at least 10% of the 2 K emission intensity for Cs₂NaScF₆ doped with 1% of Cr³⁺ remains at room temperature. Besides, the 2 K emission broad band could be well described in terms of normal modes of the octahedral complex [CrF₆](3-), and the Racah and crystal-field parameters calculated.

Journal of Fluorescence 16[3], 317-323. 2006.

P 173 - 06 "Photoluminescence measurements on cubic InGaN layers deposited on a SiC substrate"

Pacheco-Salazar, D. G., Leite, J. R., Cerdeira, F., Meneses, E. A., Li, S. F., As, D. J., and Lischka, K.

In this work we report optical experiments on pseudomorphic cubic In_xGa_{1-x}N epilayers grown on cubic GaN/3C-SiC templates. We make a detailed study of photoluminescence (PL) and photoluminescence excitation spectroscopy on these samples, with spectra taken at various temperatures (between 2 K and 300 K) and using variable wavelength sources to excite the PL spectra. The combined use of these techniques suggests the existence of indium-rich clusters, constituting a negligibly small fraction of the volume of the total layer. Our results reinforce the notion that the large Stokes-like shift (a difference of approximately 300 meV between emission and absorption) observed in these samples is due to the fact that light absorption occurs in the bulk alloy of average composition while recombination occurs within the indium-rich clusters.

Semiconductor Science and Technology 21[7], 846-851. 2006.

P 174 - 06 "Plasma dynamics studies during deposition of thin film PbTe on a glass substrate"

Rodriguez, E., Jimenez, E., Moya, L., Cesar, C. L., Cardoso, L. P., and Barbosa, L. C.

PbTe thin films were prepared by pulsed laser deposition using a Nd:YAG laser (532 nm) in an argon atmosphere. Dynamic processes in the gas phase induced by Nd:YAG laser ablation of PbTe are investigated by analyzing the light emitted by the plume. Pressure in the chamber varied from 1.0 x 10⁻⁵ to 1.0 mbar. Space and time-resolved optical spectroscopy measurements indicate the presence of both neutral, Pb(I) and Te(I) and ionized, Pb(II) and Te(II), species. The velocities of the species remain unchanged for argon pressures up to 10⁻¹ mbar, which suggests that expansion of the plume occurs without further collision with the foreign gas in this pressure range. It is found that an addition of 5 x 10⁻¹ mbar Ar enhances the emission line intensity and leads to a decrease in species velocity observed at large distances from the target surface. Furthermore, a region of maximum emission intensity at distance of 5-10 mm from the target is found when a gas environment is present.

Vacuum 80[8], 841-849. 2006.

P 175 - 06 "Pressure-temperature-composition phase diagram of Ce₂MIn₈ (M = Rh, Ir)"

Hering, E. N., Borges, H. A., Ramos, S. M., Fontes, M. B., Saitovitch, E. B., Bittar, E. M., Pagliuso, P. G., Moreno, N. O., Thompson, J. D., and Sarrao, J. L.

In this work a preliminary pressure-temperature-composition phase diagram for the Ce₂Rh(1-x)IrxIn₈ heavy-fermions (HF) materials is reported, built from pressure-dependent electrical resistivity (ρ(T)) measurements on single-crystalline samples. Although neither of the two end members is an ambient-pressure SC, a transition to a zero-resistance (ZR) state was found at ambient pressure (T-C approximate to 600mK) in a narrow Ir concentration range (around x = 0.5). Pressures not higher than 10 kbar are sufficient to suppress this ZR state for all measured concentrations, in contrast to the 115 materials.

Physica B-Condensed Matter 378-80, 423-425. 2006.

P 176 - 06 "Propagation of ultrashort pulses in multilevel systems under electromagnetically induced transparency"

de Araujo, L. E. E.

In this paper, I numerically investigate the propagation of ultrashort pulses through an extended collection of multilevel systems under the condition of electromagnetically induced transparency. The transparency of a weak probe pulse is induced by a much stronger coupling pulse. In the limit of a weak probe excitation and a large number of excited states, I show that the free-induction decay signal that would naturally follow the excitation pulse is strongly suppressed, and the envelope of the probe pulse suffers a distortion in its temporal profile as the pulse propagates into the medium. This distortion is characterized by a stronger absorption of the leading edge of the pulse than that of its trailing edge. The temporal phase of the pulse, however, remains constant throughout propagation.

Physical Review A 73[5]. 2006.

P 177 - 06 "Raman scattering studies in dilute magnetic semiconductor Zn_{1-x}Co_xO"

Samanta, K., Bhattacharya, P., Katiyar, R. S., Iwamoto, W., Pagliuso, P. G., and Rettori, C.

Raman spectra of ZnO and Co substituted Zn_{1-x}Co_xO (ZCO) were carried out using the Raman microprobe system with an Ar⁺ ion laser source of 514.5 nm wavelength. The shift towards the lower frequency side of the nonpolar E-2(low) mode and the broadening due to Co substitution in ZnO were analyzed using the phonon confinement model. The magnetic measurements showed ferromagnetic behavior with the maximum saturation magnetization (1.2 μ_B/Co) for 10% Co substitution, which decreased with further increase in Co concentrations. The intensities of E-1(LO) at 584 cm⁻¹ and multiphonon modes at 540 cm⁻¹ were increased with an increase in Co substitution. The additional Raman modes in ceramic targets of ZCO spectra for higher concentration of Co substitution (x=15%-20%) were identified to be due to the spinel ZnCo₂O₄ secondary phase.

Physical Review B 73[24]. 2006.

P 178 - 06 "Resonant Raman scattering of electrons in quantum wells: Identification of elementary excitations"

Silva, A. A. P., Vasconcellos, A. R., and Luzzi, R.

Inelastic scattering of light by electrons in a quantum well was studied. We considered the resonant Raman scattering associated with intersubband electronic excitations. Evidence is provided that when the two lowest subbands are considered four types of excitations are present. They give rise to two scattering lines

associated with single-particle excitations and another two associated with collective charge-density excitations, while spin-density excitations are not considered. The shape of the Raman spectrum strongly depends on several characteristics in the experiment, namely, the quantum well width, the concentration of the carriers, many-body effects, the temperature, and, mainly, the momentum-transfer dependent on the laser-photon frequency and the experimental geometry. Particular experimental results are satisfactorily described.

Physical Review B 73[23]. 2006.

P 179 - 06 "Role of electronic energy loss on the magnetic properties Of Mg_{0.95}Mn_{0.05}Fe₂O₄ nanoparticles"

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

Effects of 100 MeV Si⁷⁺ and Ni⁸⁺ ion irradiation on Mg-Mn ferrite nanoparticles have been studied. The bulk sample was synthesized using the solid-state reaction technique. For obtaining nanoparticles, the bulk sample was milled using high-energy ball mill for 12 h. The well-characterized nanoparticles having an average particle size of similar to 6 nm were irradiated with 100 MeV Si and Ni ions at various fluences in the range 5×10^{12} - 5×10^{13} ions/cm² to see the effects of increasing electronic energy loss on their magnetic properties. The magnetization measurements performed on the 100 MeV Si ion irradiated nanoparticles sample revealed that the values of coercivity and the saturation magnetization have been enhanced about two times as compared to the unirradiated sample. It is explained on the basis that after irradiation by 100 MeV Si ions, the surface states pinning of domains is released which causes enhancement in the saturation magnetization and coercivity. On the other hand, the saturation magnetization decreases slightly after irradiation by Ni ions. The results have been explained on the basis of electronic energy loss dependence in the nanoparticles.

Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms 248[1], 37-41. 2006.

P 180 - 06 "Role of oxygen vacancies in the magnetic and dielectric properties of the high-dielectric-constant system CaCu₃Ti₄O₁₂: An electron-spin resonance study"

Pires, M. A., Israel, C., Iwamoto, W., Urbano, R. R., Aguero, O., Torriani, I., Rettori, C., Pagliuso, P. G., Walmsley, L., Le, Z., Cohn, J. L., and Oseroff, S. B.

We report experiments of electron spin resonance (ESR) of Cu²⁺ in polycrystalline samples of CaCu₃Ti₄O₁₂ post-annealed in different atmospheres. After being synthesized by solid state reaction, pellets of CaCu₃Ti₄O₁₂ were annealed for 24 h at 1000 degrees C under air, Ar or O₂. Our temperature dependent ESR data revealed for all samples nearly temperature independent g value (2.15(1)) and linewidth for T > T_N approximate to 25 K. However, the values of ESR linewidth are strongly affected by the oxygen content in the sample. For instance, argon post-annealed samples show a much larger linewidth than the O₂ or air post-annealed samples. We attribute this broadening to an increase of the dipolar homogeneous broadening of the Cu²⁺ ESR lines due to the presence of oxygen vacancies which induce an S=1/2 spin inside the TiO₆ octahedra. Correlation between a systematic dependence of the ESR linewidth on the oxygen content and the high dielectric constant of these materials is addressed. Also, ESR, magnetic susceptibility, and specific heat data for a single crystal of CaCu₃Ti₄O₁₂ and for polycrystals of CdCu₃Ti₄O₁₂ are reported.

Physical Review B 73[22]. 2006.

P 181 - 06 "Similarities and differences in e(+/-)-molecule scattering: Applications of the Schwinger multichannel method"

Arretche, F., da Costa, R. F., Sanchez, S. D., Hisi, A. N. S., De Oliveira, E. M., Varela, M. T. D. N., and Lima, M. A. P.

In this paper, we present a comparative study of low energy electron and positron scattering by H₂ and N₂ molecules, using the Schwinger multichannel (SMC) method. We briefly discuss the elastic collision of electrons and positrons-by H, below positronium formation threshold. The electronic excitation of N₂ by electron impact is then compared with available data in the literature and with previously published results by positron impact. Strategies to treat the nuclear dynamics in the collision process, specifically adiabatic approximation for direct scattering and boomerang model for resonant scattering, are introduced within the SMC context. Partial results for H₂ are shown.

Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms 247[1], 13-19. 2006.

P 182 - 06 "SnO₂ extended gate field-effect transistor as pH sensor"

Batista, P. D., Mulato, M., Graeff, C. F. D., Fernandez, F. J. R., and Marques, F. D.

Extended gate field-effect transistor (EGFET) is a device composed of a conventional ion-sensitive electrode and a MOSFET device, which can be applied to the measurement of ion content in a solution. This structure has a lot of advantages as compared to the Ion-Sensitive Field Effect Transistor (ISFET). In this work, we constructed an EGFET by connecting the sensing structure fabricated with SnO₂ to a commercial MOSFET (CD4007UB). From the numerical simulation of site binding model it is possible to determine some of the desirable characteristics of the films. We investigate and compare SnO₂ films prepared using both the Sol-gel and the Pechini methods. The aim is an amorphous material for the EGFET. The SnO₂ powder was obtained at different calcinating temperatures (200-500(0)C) and they were investigated by X-ray diffraction (XRD), infrared spectroscopy (IR), thermogravimetric analysis (TGA) and differential thermal analysis (DTA). The films were investigated as pH sensors (range 2-11)

Brazilian Journal of Physics 36[2A], 478-481. 2006.

P 183 - 06 "Statistical model applied to A(x)B(y)C(1-x-y)D quaternary alloys: Bond lengths and energy gaps of Al_xGa_yIn_{1-x-y}X (X=As, P, or N) systems"

Marques, M., Teles, L. K., Ferreira, L. G., Scolfaro, L. M. R., Furthmuller, J., and Bechstedt, F

We extend the generalized quasichemical approach (GQCA) to describe the A(x)B(y)C(1-x-y)D quaternary alloys in the zinc-blende structure. Combining this model with ab initio ultrasoft pseudopotential calculations within density functional theory, the structural and electronic properties of Al_xGa_yIn_{1-x-y}X (X=As, P, or N) quaternary alloys are obtained, taking into account the disorder and composition effects. Results for the bond lengths show that the variation with the compositions is approximately linear and also does not deviate very much from the value of the corresponding binary compounds. The maximum variation observed amounts to 3.6% for the In-N bond length. For the variation of band gap, we obtain a bowing parameter b=0.26 eV for the (Ga_{0.47}In_{0.53}As)_z(Al_{0.48}In_{0.52}As)_(1-z) quaternary alloy lattice matched to InP, in very good agreement with experimental data. In the case of AlGaInN, we compare our results for the band gap to data for the wurtzite phase. We also obtained a good agreement despite all evidences for cluster formation in this alloy. Finally, a bowing parameter of 0.22 eV is obtained for zinc-blende AlGaInN lattice matched with GaN

Physical Review B 73[23]. 2006.

P 184 - 06 "Stimulated Brillouin scattering from multi-GHz-guided acoustic phonons in nanostructured photonic crystal fibres"

Dainese, P., Russell, P. S. J., Joly, N., Knight, J. C., Wiederhecker, G. S., Fragnito, H. L., Laude, V., and Khelif, A.

Wavelength-scale periodic microstructuring dramatically alters the optical properties of materials. An example is glass photonic crystal fibre(1) (PCF), which guides light by means of a lattice of hollow micro/nanochannels running axially along its length. In this letter, we explore stimulated Brillouin scattering in PCFs with subwavelength-scale solid silica glass cores. The large refractive-index difference between air and glass allows much tighter confinement of light than is possible in all-solid single-mode glass optical fibres made using conventional techniques. When the silica-air PCF has a core diameter of around 70% of the vacuum wavelength of the launched laser light, we find that the spontaneous Brillouin signal develops a highly unusual multi-peaked spectrum with Stokes frequency shifts in the 10-GHz range. We attribute these peaks to several families of guided acoustic modes each with different proportions of longitudinal and shear strain, strongly localized to the core(2,3). At the same time, the threshold power for stimulated Brillouin scattering(4) increases fivefold. The results show that Brillouin scattering is strongly affected by nanoscale microstructuring, opening new opportunities for controlling light-sound interactions in optical fibres

Nature Physics 2[6], 388-392. 2006.

P 185 - 06 "Structural analysis of N-acetylglucosamine-6-phosphate deacetylase apoenzyme from *Escherichia coli*"

Ferreira, F. M., Mendoza-Hernandez, G., Castaneda-Bueno, M., Aparicio, R., Fischer, H., Calcagno, M. L., and Oliva, G.

We report the crystal structure of the apoenzyme of N-acetylglucosamine-6-phosphate (GlcNAc6P) deacetylase from *Escherichia coli* (EcNAGPase) and the spectrometric evidence of the presence of Zn²⁺ in the native protein. The GlcNAc6P deacetylase is an enzyme of the amino sugar catabolic pathway that catalyzes the conversion of the GlcNAc6P into glucosamine 6-phosphate (GlcN6P). The crystal structure was phased by the single isomorphous replacement with anomalous scattering (SIRAS) method using low-resolution (2.9 angstrom) iodine anomalous scattering and it was refined against a native dataset up to 2.0 angstrom resolution. The structure is similar to two other NAGPases whose structures are known from *Thermotoga maritima* (TmNAGPase) and *Bacillus subtilis* (BsNAGPase); however, it shows a phosphate ion bound at the metal-binding site. Compared to these previous structures, the apoenzyme shows extensive conformational changes in two loops adjacent to the active site. The *E. coli* enzyme is a tetramer and its dimer-dimer interface was analyzed. The tetrameric structure was confirmed in solution by small-angle X-ray scattering data. Although no metal ions were detected in the present structure, experiments of photon-induced X-ray emission (PIXE) spectra and of inductively coupled plasma emission spectroscopy (ICP-AES) with enzyme that was neither exposed to chelating agents nor metal ions during purification, revealed the presence of 1.4 atoms of Zn per polypeptide chain. Enzyme inactivation by metal-sequestering agents and subsequent reactivation by the addition of several divalent cations, demonstrate the role of metal ions in EcNAGPase structure and catalysis.

Journal of Molecular Biology 359[2], 308-321. 2006.

P 186 - 06 "Structural organization of cetyltrimethylammonium sulfate in aqueous solution: The effect of Na₂SO₄"

Feitosa, E., Brazolin, M. R. S., Naal, R. M. Z. G., Del Lama, M. P. F. D., Lopes, J. R., Loh, W., and Vasilescu, M.

We used dynamic light scattering (DLS), a steady-state fluorescence, time resolved fluorescence quenching (TRFQ), tensiometry, conductimetry, and isothermal titration calorimetry (ITC) to investigate the self-assembly of the cationic surfactant cetyltrimethylammonium sulfate (CTAS) in aqueous solution, which has SO₄²⁻ as divalent counterion. We obtained the critical micelle concentration (cmc), aggregation number (N_{agg}), area per monomer (a(0)), hydrodynamic radius (R-H), and degree of counterion dissociation (alpha) of CTAS micelles in the absence and presence of up to 1 M Na₂SO₄ and at temperatures of 25 and 40 degrees C. Between 0.01 and 0.3 M salt the hydrodynamic radius of CTAS micelle R-H approximate to 16 angstrom is roughly independent on Na₂SO₄ concentration; below and above this concentration range R-H increases steeply with the salt concentration, indicating micelle structure transition, from spherical to rod-like structures. R-H increases only slightly as temperature increases from 25 to 40 degrees C, and the cmc decreases initially very steeply with Na₂SO₄ concentration up to about 10 mM, and thereafter it is constant. The area per surfactant at the water/air interface, a(0), initially increases steeply with Na₂SO₄ concentration, and then decreases above ca. 10 mM. Conductimetry gives alpha = 0.18 for the degree of counterion dissociation, and N_{agg} obtained by fluorescence methods increases with surfactant concentration but it is roughly independent of up to 80 mM salt. The ITC data yield cmc of 0.22 mM in water, and the calculated enthalpy change of micelle formation, Delta H_{mic} = 3.8 kJ mol⁻¹, Gibbs free energy of micellization of surfactant molecules, Delta G_{mic} = -38.0 kJ mol⁻¹ and entropy T Delta S_{mic} = 41.7 kJ mol⁻¹ indicate that the formation of CTAS micelles is entropy-driven.

Journal of Colloid and Interface Science 299[2], 883-889. 2006.

P 187 - 06 "Surface composition and structure of palladium ultra-thin films deposited on Ni(111)"

Carazzolle, M. F., Maluf, S. S., de Siervo, A., Nascente, P. A. P., Landers, R., and Kleiman, G. G.

Ultra-thin palladium films deposited on the Ni(111) surface were characterized by X-ray photoelectron spectroscopy (XPS), lowenergy electron diffraction (LEED) and X-ray photoelectron diffraction (XPD). For low coverage, LEED shows a (1 x 1) pattern similar to that of the substrate. For intermediate coverage, the LEED pattern displays extra spots around the main (1 x 1) spots, resembling a Moire coincidence pattern, probably associated with the formation of Pd bi-dimensional islands oriented in different directions on the Ni(111) surface. The results obtained by XPS and XPD corroborate this finding. The LEED pattern displays this structure up to 500 degrees C. Annealing at 650 degrees C brings back the (1 x 1) pattern, which is associated with a Pd island coalescence and alloy formation by Pd diffusion in the first atomic layers of the Ni(111). In this paper we present a detailed study of this surface structure via a comparison between XPD experiment and theory.

Surface Science 600[11], 2268-2274. 2006.

P 188 - 06 "Synthetic melanin films: Assembling mechanisms, scaling behavior, and structural properties"

Lorite, G. S., Coluci, V. R., da Silva, M. I. N., Deziderio, S. N., Graeff, C. F. O., Galvao, D. S., and Cotta, M. A.

In this work we report on the surface characterization of melanin thin films prepared using both water-based and organic solvent-based melanin syntheses. Atomic force microscopy (AFM) analysis of these films suggests that the organic solvent synthesis provides relatively planar basic melanin structures; these

basic structures generate surface steps with height in the range of 2-3 nm and small tendency to form larger aggregates. The scaling properties obtained from the AFM data were used to infer the assembling mechanisms of these thin films which depend on the solvent used for melanin synthesis. The behavior observed in organic solvent-based melanin suggests a diffusion-limited aggregation process. Thus films with good adhesion to the substrate and smoother morphologies than water-prepared melanin films are obtained. Electronic structure calculations using a conductorlike screening model were also performed in order to elucidate the microscopic processes of thin film formation. Our results suggest that the agglomerates observed in hydrated samples originate from reaction with water at specific locations on the surface most likely defects on the planar structure.

Journal of Applied Physics 99[11]. 2006.

P 189 - 06 "Temporal atomic beam-splitter and atomic homodyne detection on two-mode Bose-Einstein condensates"

Da Cunha, B. R. and De Oliveira, M. C.

The Rabi regime for a Bose-Einstein condensate (BEC) in double-well potential occurring for sufficiently strong cross-collision strengths is analyzed. It is shown that in this regime the potential barrier acts as a temporal atomic beam splitter. An ideal 50:50 atomic beam splitter reached at specific intervals of time is employed for a balanced homodyne detection of the condensate relative phase.

International Journal of Modern Physics B 20[11-13], 1671-1678. 2006.

P 190 - 06 "The Brazilian gravitational wave detector Mario Schenberg: status report"

Aguiar, O. D., Andrade, L. A., Barroso, J. J., Bortoli, F., Carneiro, L. A., Castro, P. J., Costa, C. A., Costa, K. M. F., de Araujo, J. C. N., de Lucena, A. U., de Paula, W., Neto, E. C. D., de Souza, S. T., Fauth, A. C., Frajuca, C., Frossati, G., Furtado, S. R., Magalhaes, N. S., Marinho, R. M., Melo, J. L., Miranda, O. D., Oliveira, N. F., Ribeiro, K. L., Stellati, C., Velloso, W. F., and Weber, J.

The Mario Schenberg gravitational wave detector has been constructed at its site in the Physics Institute of the University of Sao Paulo as programmed by the Brazilian Graviton Project, under the full support of FAPESP (the Sao Paulo State Foundation for Research Support). We are preparing it for a first commissioning run of the spherical antenna at 4.2 K with three parametric transducers and an initial target sensitivity of h similar to 2×10^{-21} Hz^(-1/2) in a 60 Hz bandwidth around 3.2 kHz. Here we present the status of this project.

Classical and Quantum Gravity 23[8], S239-S244. 2006.

P 191 - 06 "The vortex decoupling transition in Bi2212 crystals with columnar defects"

de Lima, O. F., de Almeida, R. L., and Kumar, R.

Two Bi₂Sr₂CaCu₂O_{8+δ} single crystals were characterized, before and after irradiation with 200 MeV Ag ions under fluence of 5×10^{10} ionS/cm². Columnar defects were produced along the c-axis direction in one crystal, and in a direction tilted by an angle of 30 degrees with respect to the c-axis for the other crystal. The 3D-2D vortex decoupling lines were significantly shifted to higher temperatures, after irradiation of the crystals, for magnetic fields smaller than the matching value B_{Φ} approximate to 1 T. For $B > 3$ T the decoupling lines for the irradiated crystals tend smoothly to the same behavior observed in the original crystals, up to the maximum probed field of 5 T. Interest-

ingly the vortex pinning by columnar defects was found to be almost independent of the applied magnetic field direction, as revealed by the width of magnetization loops.

Physica C-Superconductivity and Its Applications 437-38, 61-64. 2006.

P 192 - 06 "XAS of high pressure Xe clusters in amorphous carbon and computational simulation for the fcc and hcp xenon crystalline phases"

Oliveira, M. H. and Marques, F. C

We report the investigation of Xe clusters in amorphous carbon by x-ray absorption spectroscopy (XAS) to understand the properties of solid xenon. Measurements have been performed on xenon L-3 absorption edge at room temperature (300K). Using computational XANES calculation for fcc and hcp structures it was possible to study the XANES fine structure origin and a relation between the x-ray absorption near edge structure and the lattice constant. Comparing those results with our experimental data we determined that the XAS fine near edge structure has a specific behavior for solid xenon and does not have this behavior for gas Xe end Xe diluted in others chemical elements matrices.

Brazilian Journal of Physics 36[2A], 282-285. 2006.

ERRATA

P 134 "Universal magnetic-field-driven metal-insulator-metal transformations in graphite and bismuth"

Kopelevich, Y., Pantoja, J. C. M., da Silva, R. R., and Moeckle, S

Applied magnetic field induces metal-insulator and reentrant insulator-metal transitions in both graphite and rhombohedral bismuth. The corresponding transition boundaries plotted on the magnetic field-temperature (B-T) plane nearly coincide for these semimetals and can be best described by power laws T similar to $(B-B_c)(\kappa)$, where B_c is a critical field at $T=0$ and $\kappa=0.45 \pm 0.05$. We show that insulator-metal-insulator (I-M-I) transformations take place in the Landau level quantization regime and illustrate how the insulator-metal transformation in graphite samples with a moderate anisotropy transforms into a cascade of I-M-I transitions, related to the quantum Hall effect in strongly anisotropic, quasi-two-dimensional graphite samples. We discuss the possible coupling of superconducting and excitonic correlations with the observed phenomena, as well as the signatures of quantum phase transitions associated with the M-I and I-M transformations.

Physical Review B 73[16]. 2006.

Abstracta

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