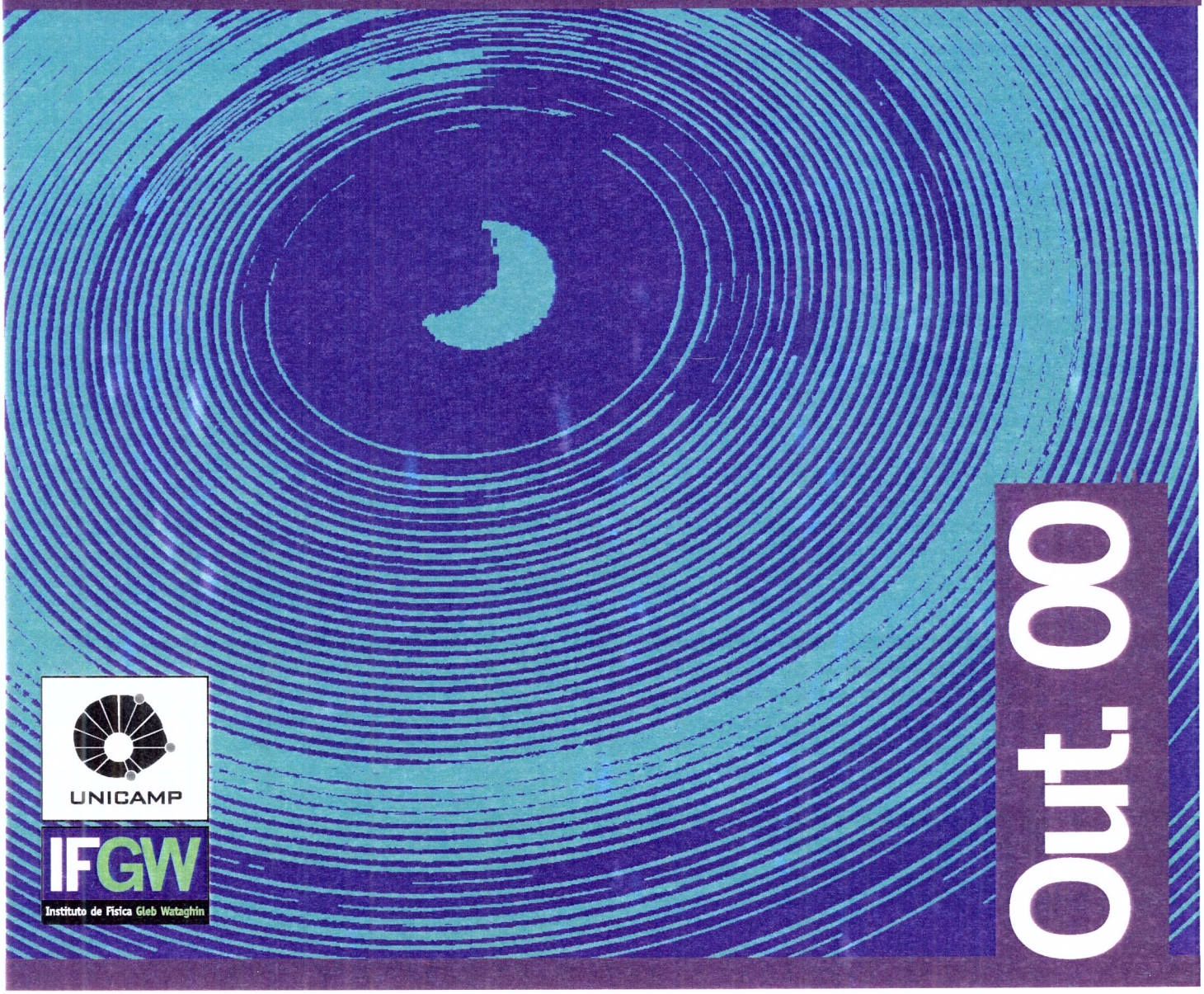
Abstracta

Ano II - N.10



Trabalhos Aceitos para Publicação em Periódicos

A 051-00 Photoemission from Pt(111)-Rb and Pt(111)-(4x1)-RbO Using Polarized Synchrotron Radiation.

A 052- 00 Influence of the stress on the core electron level energies of noble gases implanted in hard amorphous carbon films.

A 053-00 The role of finite hole mass in the negatively charged exciton in two dimensions.

A 054- 00 ELECTRICAL ISOLATION AND TRANSPARENCY IN ION-IRRADIATED p-InGaP/GaAs/InGaAs STRUCTURES.

A 055-00 Contrast enhancement in the detection of defects in transparent layered structures: The use of optothermal interference technique in solar cell investigation.

A056-00 Near equilibrium dynamics of non-homogeneous Kirchhoff filaments in viscous media.

A 057-00 Equilibrium and Stability of Ellipsoidal Liquid Metal Drops in TEMPUS Like Experiments.

Trabalhos Publicados

P 014-00 Silica-zirconia-phosphate composites: a study of their synthesis, proton exchange capacity and ammonia gas adsorption.

P 015-00 Identifying carcinogenic activity of methylated and non- methylated polycyclic aromatic hydrocarbons (PAHs) through electronic and topological indices.

P 016-00 The biomechanics of rapid maxillary sutural expansion.

P 017-00 Electron energy-loss spectroscopy of strongly correlated systems in infinite dimensions.

Livro Publicado

L 002-00 STATISTICAL FOUNDATIONS OF IRREVERSIBLE THERMODYNAMICS.

Trabalhos aceitos para publicação em periódicos

A 051- 00 Photoemission from Pt(111)-Rb and Pt(111)-(4x1)-RbO Using Polarized Synchrotron Radiation.

Jonder Morais, Andreas Oelsner,Gerd Schönhense, Gerhard H. Fecher, Richard Landers, Abner de Siervo, George G. Kleiman.

In various experiments it has been demonstrated that the circular dichroism in the angular distribution of photoelectrons (CDAD) is not only observed from oriented initial states (aligned adsorbed molecules or magnetized samples),but also arises as a consequence of the scattering of photoelectrons from the surrounding atoms in a solid or an adsorbate.In this work we will show first measurements performed at the SGM beamline of the Brazilian Synchrotron Light Source (LNLS) on a (4x1) superstructure of the 1ML RbO adsorbed on Pt(111).Measurements from the 4s core levels of Rb adsorbed at Pt(111) were also performed at the PM-III beamline at BESSY.The measured variations of the intensity and the CDAD with respect to the photon energy are interpreted in terms of photoelectron diffraction.The results will be used to discuss the possibility of photoelectron holography using circularly polarized light.

Journal Electron Spectroscopy and Related Phenomena, accepted on September 2000

A 052-00 Influence of the stress on the core electron level energies of noble gases implanted in hard amorphous carbon films.

R. G. Lacerda*, P. Hammer, F. Alvarez and F. C. Marques

In this work, we report the influence of the structural properties of the amorphous carbon matrix on the core level electrons of implanted noble gases(Ar, Ne and Kr) used in the sputtering deposition process. The films were prepared in an ion-beam-assisted deposition chamber (IBAD) including two Kauffman ion sources. Some fractional noble gas is trapped in the film during the assisted deposition and is subjected to the highly strained environment of the carbon matrix. X-ray photoelectron spectroscopy shows that the noble gas core level energies shift linearly to lower binding energies on increasing compressive stress. It is suggested that these shifts are caused by the compression of the outer valence wave function of the implanted gas and by extra-screening effect from valence electrons of the host atoms. It is proposed the use of noble gas core level energy as a probe to determine the film stress.

Diamond and Related Materials, accepted on September 2000.

A 053-00 The role of finite hole mass in the negatively charged exciton in two dimensions.

Gustavo A. Narvaez, Pawel Hawrylak and Jose' A. Brum

The role of finite hole mass on the ground and excited states of the negatively charged exciton in two dimensions is discussed. We present results of configuration-interaction calculation using exact excitonic states and results of a variational calculation of the ground-state energy to elucidate the interplay of finite hole mass and electron-electron interactions.

Physica E, accepted on September 2000.

A 054-00 ELECTRICAL ISOLATION AND TRANSPARENCY IN ION-IRRADIATED p-InGaP/GaAs/ InGaAs STRUCTURES.

I.Danilov, L.L.Pataro, M.P.P.de Castro and N.C.Frateschi.

He^+ion irradiation was applied for the electrical isolation of p-$In_{0.49}Ga_{0.51}P$ in InGaP/GaAs/InGaAs structures. Sheet resistance of approximately $1x10^6$ Ω/ was achieved with doses above $1x10^{13}$ cm^{-2} at 100 keV. Thermal stability of isolation was maintained for annealing temperatures up to 500°C. Photoluminescence results show that InGaP transparency to InGaAs/GaAs quantum well emission is closely related to sheet resistance changes in irradiated structure.

Journal of Applied Physics, accepted on October 2000.

A 055-00 Contrast enhancement in the detection of defects in transparent layered structures: The use of optothermal interference technique in solar cell investigation.

J. A. Batista, A. M. Mansanares and. E. C. da Silva, C. C. Vaz, L. C. M. Miranda.

This article shows the enhanced sensitivity of the optothermal interference technique in the detection of local differences (nonhomogeneity in thickness and optothermal parameters), compared to the conventional optical interference, when investigating layered transparent structures. The measured signal is sensitive to the reflectance variation at the distinct interfaces, function of temperature, as well as to the optical phase lag between the reflected beams. Measurements made on solar cells show contrast of the order of 100% in the optothermal interference, while the conventional optical interference presents a contrast of only 15% .A model based on the reflectance variation at each interface describes the signal behavior as a function of modulation frequency. Theoretical calculation based on this model evidences the influence of the optothermal parameters in the signal contrast.

Journal of Applied physics, accepted on August 2000.

A 056-00 Near equilibrium dynamics of non-homogeneous Kirchhoff filaments in viscous media.

A.F. Fonseca and M.A.M. de Aguiar

We study the near equilibrium dynamics of non-homogeneous elastic filaments in viscous media using the Kirchhoff model of rods. Viscosity is incorporated in the model as an external force, that we approximate by the resistance felt by an infinite cylinder immersed in a slowly moving fluid. We use the recently developed method of Goriely and Tabor to study the dynamics in the vicinity of the simplest equilibrium solution for a closed rod with non-homogeneous distribution of mass, namely, the planar ring configuration. We show that small variations of the mass density along the rod is sufficient to couple the symmetric modes of the homogeneous rod problem, producing asymmetric deformations that modify substantially the dynamical coiling, even at quite low Reynolds number. The higher density segments of the rod tend to become more rigid and less coiled. We comment possible applications to DNA.

Physical Review E, accepted on October 2000.

A 057-00 Equilibrium and Stability of Ellipsoidal Liquid Metal Drops in TEMPUS Like Experiments.

Abdala Mohamed Saleh, Roberto Antonio Clemente.

The equilibrium problem of a liquid metallic drop in the external field produced by two sets of coils (for heating and positioning), carrying currents at different frequencies, in ambient of microgravity has been analytically considered. The free boundary problem resulting from considering infinite conductivity for the drop and its surface tension has been solved almost exactly. The stability of such equilibria with respect to rigid displacements has also been explicitly calculated. Axial and lateral shifts are stable and for rigid rotational displacements restoring torques are also obtained. However, the positioning coils can give unstable contribution if the elongation of the drop is smaller than about two. This can offer an explanation to the some time destroying motion of the drop in TEMPUS experiments when the heating coil was switched off.

Journal of Physics Society of Japan, accepted on October 2000.

Trabalhos Publicados

P 014-00 Silica-zirconia-phosphate composites: a study of their synthesis, proton exchange capacity and ammonia gas adsorption.

Alfaya, A. A. S., Gushikem, Y., and de Castro, S. C.

Phosphoric acid was adsorbed on SiO2/ZrO2 mixed oxides prepared by a sol-gel processing method. The obtained composites, SiO2/ZrO2/phosphate with variable compositions, are very porous, having specific surface areas between 400 and 650 m(2)g(-1) and average pore volumes between 0.29 and 0.38 cm(3) g(-1). The binding energy P-2p = 134.5 eV and the atomic ratio P/Zr similar to 2, both determined by the X-ray photoelectron spectroscopy technique, and corroborated by the P-31 high power decoupling magic angle spinning and NMR techniques indicated that H2PO4- is the species present in the composites. The materials are all thermally very stable, and the phosphate entities show little thermal mobility. Under heat treatment up to 1273 K, the SiO2/ZrO2/phosphate samples did not show any phase transition corresponding to the transformation of phosphate to the pyrophosphate species. Large proton exchange capacities, between 1.22 and 2.90 mmol g(-1), were obtained. Ammonia gas was rapidly adsorbed by the materials with the formation of NH4+ on the solid surface; thermodesorption occurred above 949 K.

Microporous and Mesoporous Materials 39[1-2], 57-65. 2000.

P 015-00 Identifying carcinogenic activity of methylated and non- methylated polycyclic aromatic hydrocarbons (PAHs) through electronic and topological indices.

Braga, R. S., Barone, P. M. V. B. , and Galvão, D. S.

Polycyclic aromatic hydrocarbons (PAHs) are a class of planar molecules, abundant in urban environment, which can induce chemical carcinogenesis. Their carcinogenic power varies in a large range, from very strong carcinogens to inactive ones. In a previous study, we proposed a methodology to identify the PAHs carcinogenic activity exploring electronic and topological indices. In the present work, we show that it is possible to simplify that methodology and expand its applicability to include methylated PAHs compounds. Using very simple rules, we can predict their carcinogenic activity with high accuracy (approximate to 89%).

Brazilian Journal of Physics 30[3], 560-568. 2000.

Trabalhos Publicados

P 016-00 The biomechanics of rapid maxillary sutural expansion.

Braun, S., Bottrel, J. A., Lee, K. G., Lunazzi, J. J., and Legan, H. L.

Micro-displacements (fringe patterns) in the bones of the craniofacial complex as seen through laser holography during midpalatal sutural expansion with the Hyrax appliance are used to define the centers of rotation of the maxillary halves in both the frontal and occlusal views. Biomechanical analyses of the maxillary expansion force system are concomitant with the holographic findings and strongly suggest that the stainless steel wires joining the teeth to any expansion device be of the largest diameter possible. In addition, in the case of the Hyrax expansion device, it is recommended that the manufacturer increase the diameter of the activating screw as well as those of the 2 adjacent wire guides. And, importantly, the use of acrylic as a structural member to join the teeth to a sutural expansion device should be avoided if tipping of the maxillary halves is to be minimized, as the acrylic lacks sufficient rigidity.

American Journal of Orthodontics and Dentofacial Orthopedics **118[3], 257-261. 2000.**

P 017-00 Electron energy-loss spectroscopy of strongly correlated systems in infinite dimensions.

Craco, L. and Laad, M. S.

We study the electron energy-loss spectra of strongly correlated electronic systems doped away from half-filling using dynamical mean-field theory (d = infinity). The formalism can be used to study the loss spectra in the optical (q = 0) limit, where it is simply related to the optical response, and hence can be computed in an approximation-free way in d = oo dimensions. We apply the general formalism to the one-band Hubbard model away from n = 1, with inclusion of site-diagonal randomness to simulate effects of doping. The interplay between the coherence-induced plasmon feature and the incoherence- induced high-energy continuum is explained in terms of the evolution in the local spectral density upon hole doping. Inclusion of static disorder is shown to result in qualitative changes in the low-energy features, in particular to the overdamping of the plasmon feature, resulting in a completely incoherent response. The calculated lineshapes of electron energy-loss spectra are compared to the lineshapes of experimentally observed spectra for the normal state of the high-T-c materials near optimal doping and good qualitative agreement is found.

Journal of Physics-Condensed Matter **12[34], 7647-7654. 2000.**

Livro Publicado

L 002-00 STATISTICAL FOUNDATIONS OF IRREVERSIBLE THERMODYNAMICS.

Roberto Luzzi, Aurea R. Vasconcellos, J. Galvão Ramos.

In this book we deal with some aspects of the physics of many-body systems driven away from equilibrium, that is,the characterization and irreversible evolution of their macroscopic state.First we briefly, and partially, consider aspects of the present status of phenomenological irreversible thermodynamics and nonequilibrium statistical mechanics.Several aspects, concepts, and ideas in the statistical physics and thermodynamics of nonlinear nonequilibrium systems have been discussed partially touching upon the question of the statistical foundations of irreversible thermodynamics on the basis of a Gibbs-like ensemble approach for nonequilibrium (and then dissipative) systems. After short comments on Classical Irreversible Thermodynamics, its conceptual and practical shortcomings are pointed out, as well as the efforts undertaken to go beyond its limits, consisting of particular approaches to a more general theory of Irreversible Thermodynamics. In particular, a search for statistical-mechanical foundations of Irreversible Thermodynamics, consisting in building a statistical thermodynamics , is based on the Nonequilibrium Statistical Operator Method. This important theory for the treatment of phenomena at the macroscopic level is based on a microscopic molecular description in the context of a nonequilibrium ensemble formalism. We draw attention to the fact that this method may be considered to be encompassed within Jaynes´Predictive Statistical Mechanics and based on the principle of maximization of informational entropy. Finally, we describe how, in fact, the statistical method provides foundations to phenomenological irreversible thermodynamics, thus giving rise to what can be referred to as Informational Statistical Thermodynamics. It is included an Appendix with a chronology of relevant events in the history of Thermodynamics and Statistical Mechanics.

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Abstracta

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