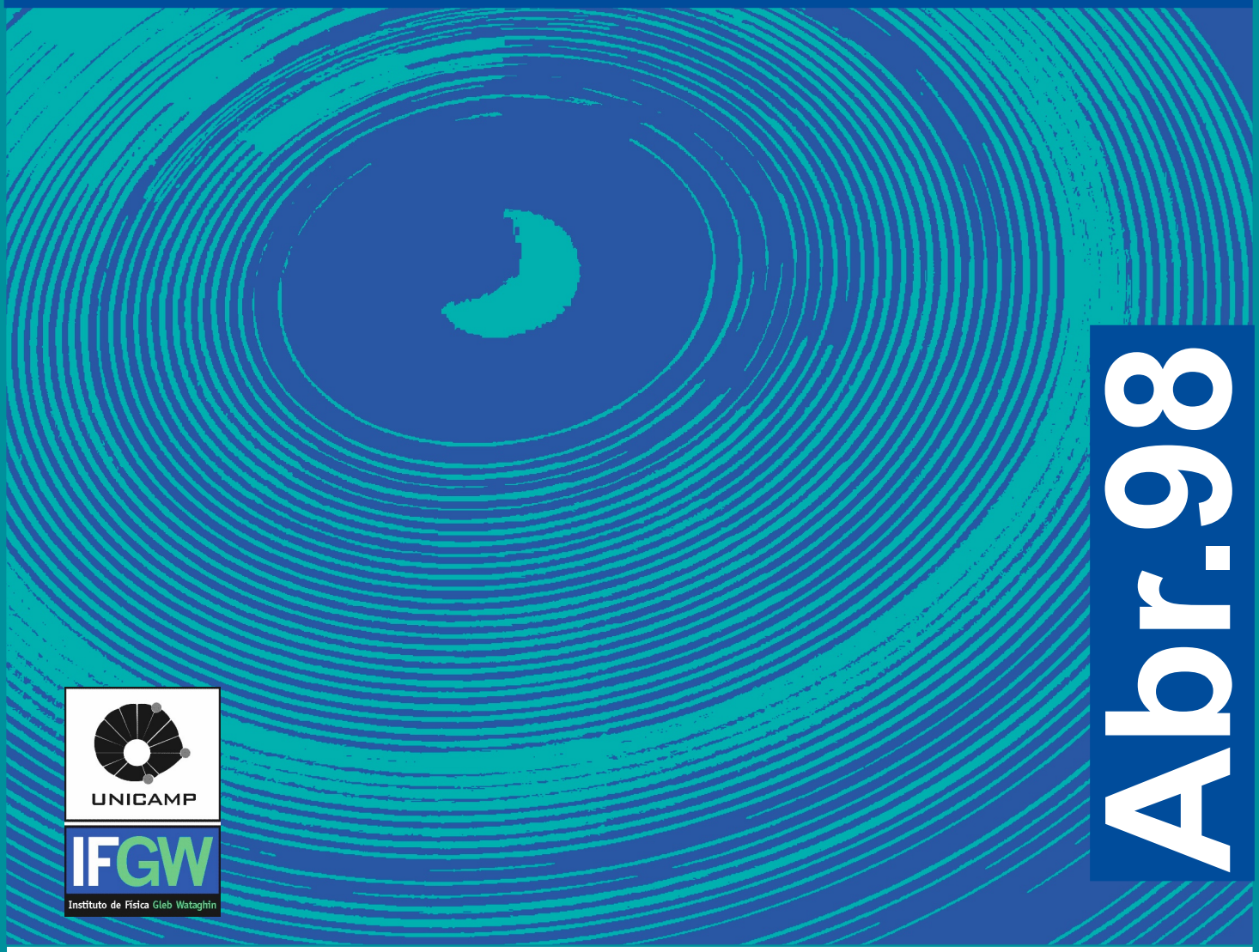
Abstracta

Ano II - N. 03



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Trabalhos Aceitos para Publicação

A009-98 à A022-98

Trabalho Aceito em Congresso

C001-98 à C002-98

ACCEPTED PAPERS FOR JOURNAL PUBLICATION

A 009-98 Optoelectronic and Structural Properties of a-Ge1-xCx:H Prepared by rf-Reactive co-Sputtering.

Vilcarromero, J. , Marques, F. C. and Freire Jr., F. L.

Optoelectronic, structural and mechanical properties of hydrogenated amorphous germanium carbon (a-Ge1-xCx:H) alloys are presented. The films were prepared by the rf-co-sputtering technique using graphite-germanium composite targets. Films with carbon contents in the 0 < x < 1 range were prepared under the same conditions used to obtain a-Ge:H films with good optoelectronic properties. The trends of the optical gap, infrared absorption, dark conductivity and mechanical stress as a function of the carbon content suggest that the properties of films with low carbon concentration are mainly controlled by the incorporation of sp3- hybridized carbon. These films have good optoelectronic and structural properties. As the carbon content increases, the properties of the films are determined by the concentration of sp2 carbon sites.

Journal of Applied Physics 84 (1), 61-68, Mar 1998

A 010-98 SISTEMA PARA DETERMINAÇÃO SIMULTÂNEA DO STRESS, BIAXIAL MODULUS E COEFICIENTE DE DILATAÇÃO TÉRMICA DE FILMES FINOS.

Lima Jr., M. M. de, Lacerda , R. G. , e Marques, F. C.

Apresentamos um sistema que permite a determinação do stress de filmes finos em função da temperatura. Descrevemos também um procedimento para a obtenção do coeficiente de dilatação térmica e do biaxial modulus, utilizando a variação do stress em função da temperatura de diversos substratos. As propriedades termomecânicas de filmes finos de prata depositados por evaporação térmica foram também obtidas.

Revista de Física Aplicada e Instrumentação 12 (1), 1997

A 011-98 Nitrogen in Germanium .

Chambouleyron, I. and Zanatta, A. R.

The known properties of nitrogen as an impurity in, and as an alloy element of, the germanium network are reviewed in this contribution. Amorphous and crystalline germanium-nitrogen alloys are interesting materials with potential applications for protective coatings and window layers for solar conversion devices. They may also act as effective diffusion masks for III-V electronic devices. The existing data are compared with similar properties of other group IV nitrides, in particular with silicon nitride. To a certain extent, the general picture mirrors the one found in Si-N systems, as expected from the similar valence structure of both elemental semiconductors. However, important differences appear in the deposition methods and alloy composition, the optical properties of as grown films, and the electrical behavior of nitrogen-doped amorphous layers. Structural studies are reviwed, including band structure calculations and the energies of nitrogen-related defects, which are compared wiht experimental data. Many important aspects of the electronic structure of Ge-N alloys are not yet completely understood and deserve a more careful investigation, in particular the structure of defects associated to N- inclusion. The N-doping of the a-Ge:H network appears to be very effective, the activation energy of the most effectively doped samples becoming around 120meV. This is not the case with N-doped a-Si:H, the reasons for the difference being still an open question. The lack of data on stoichiometric b - Ge3N4 prevents any reasonable assessment on the possible uses of the alloy in electronic and ceramic applications.

Journal of Applied Physics 84 (1), 1-30, 1998

A 012-98 Static-Exchange Cross Sections for Electron-Eollisions with B2H6, C2H6, Si2H6, and Ge2H6.

Bettega, M. H. F. , Oliveira, A. J. S. , Natalense, A. P. P. , Lima, M. A. P. and Ferreira, L. G.

We report integral and differential cross sections from 5-30 eV for elastic scattering of electrons by X2H6 (X=B, C, Si, Ge) obtained using the Schwinger Multichannel Method with Pseudopotentials [M.H.F. Bettega, L.G.Ferreira and M.A.P. Lima, Phys. Rev. A {\bf 47}, 1111 (1993)]. We compare our results with available experimental data and other theoretical results, and also with previous results for XH4 (X=C, Si, Ge) [M.H.F. Bettega, A.P.P. Natalense, M.A.P. Lima, and L.G. Ferreira, J. Chem. Phys. 103, 10566 (1995)]. To our knowledge this is the first ab initio calculation of the B2H6 and Ge2H6 electron scattering cross sections.

The European Physical Journal D 1 (3), 291-296, 1998

A 013-98 Electronic Excitation of XH4 (X = C, Si, Ge, Sn, Pb) by Electron Impact.

Bettega, M. H. F , Ferreira, L. G. and Lima, M. A. P.

We calculate integral cross sections for the electronic excitation to the 3T2 states of XH4 (X = C, Si, Ge, Sn, Pb) by electron impact.This is the lowest lying excited state of these molecules. Our results were obtained with the Schwinger Multichannel method with pseudopotentials at the 2-state level of approximation. In the case of CH4 we compare our results with previous results of an all-electron calculation obtained at the same level of approximation, in which case we found an excellent agreement between the two calculations. Though these molecules are very similar, after discarding the cores, as the pseudopotential technique does, the inelastic cross sections are very distinctive and do not have a monotonic behavior with increasing proton number Z of the central atom.

Physical Review A 57 (6), 4987-4990, 1998

A 014-98 Low-energy electron scattering by N2, P2, As2, and Sb2.

Bettega,M. H. F, Lima, M. A. P. and Ferreira, L. G.

We report elastic integral, momentum transfer and differential cross sections from 10-30 eV for electron scattering by X2 (X=N, P, As,Sb). These results were obtained at the static-exchange approximation with the Schwinger Multichannel Method with Pseudopotentials [M.H.F. Bettega, L.G. Ferreira and M.A.P. Lima, Phys. Rev. A 47, 1111 (1993)]. Our results for N2 are in good agreement with experimental data. We also compare our results with previous calculations on XH3 (X=P, As, Sb) [M.H.F. Bettega, M.A.P. Lima, and L.G. Ferreira J. Chem. Phys. 105, 1029 (1996)] and found, as expected, that the X2 cross sections are larger than the corresponding XH3 cross sections.

Journal of Physics B: Atomic Molecular and Optical Physics 31 (9), 2091-2099, 1998

A 015-98 Evolution of Dissipative Processes Via a Statistical Thermodynamic Approach. I. Generalized Mor-Heisenberg-Langevin Equations.

Madureira , J. R. , Vasconcellos, A. R. and Luzzi, R.

Whitin the scope of a nonequilibrium statistical ensemble formalism we derive a hierarchy of equations of evolution for a set of basic thermo-hydrodynamic variables, which describe the macroscopic nonequilibrium state of a fluid of bosons. This set is composed of the energy density and number density and their fluxes of all order. The resulting equations can be considered as far-reaching generalizations of those in Mori's approach. They involve nonlocality in scape and retro-effects (i. e. correlations in space and time respectively), are highly nonlinear, and account for irreversible behavior in the macroscopic evolution of the system. The different contributions to these kinetic equations are analyzed and the Markovian limit is obtained. In the follow up article we consider the nonequilibrium thermodynamic properties that the formalism provides.

Journal of Physics B: Atomic Molecular and Optical Physics 31 (9), 2091-2099, 1998

A 016-98 Evolution of Dissipative Processes Via a Statistical Thermodynamic Approach . II. Thermodynamic Properties of a Fluid of Bosons.

Madureira, J. R., Vasconcellos, A. R. and Luzzi, R.

On the basis of the generalized Mori-Heisenberg-Langevin equations presented in the preceding paper, we derive and analyze the informational-statistical thermodynamic properties of a fluid of bosons away from equilibrium. We derive the informational entropy and its production, proceeding to an analysis of the several contributions to these state functions arising out of the evolution of dissipative processes in the system.

Journal of Chemical Physics 108 (18), 7568-7579, 1998

A 017-98 Nonlocal in-plane Resistance Due to Vortex-antivortex Dynamics in High-Tc Superconducting Films.

Kopelevich, Y. , Ciovacco, F. , Esquinazi, P. and Lorenz, M.

In high-Tc superconducting YBa2Cu3O7-d films and at no applied magnetic field we found both positive and negative in-plane nonlocal resistance in the vicinity of a vortex-antivortex unbinding transition, as it was predicted recently. The sign of the nonlocal resistance is due to the motion of unboundede vortex-antivortex (V-A), whereas a positive sign is attributed to the motion of a 2D V-A ordered lattice.

Journal of Chemical Physics 108 (18), 7580-7586, 1998

A- 018-98 Optical Characterization of Dielectric and Semiconductor Thin Tilms Using Transmission Data

Cisneros, J. I.

A method to calculate the optical fucntions n(l) and k(l) using the transmission spectrum of a dielectric or semiconducting thin film measured at normal incidence is described in this paper. The spectrum should include the low absorption region and the absorption edge in order to obtain the relevant optical characteristics of the material. The formulas are derived from electromagnetic theory with no simplifying assumptions. Transparent films are considered as a particular case for which a simple method of calculation is proposed. In the general case of absorbing films the method takes advantage of some properties of the trnsmittance T(l) in order to calculate the parameters separately in the teo regions mentioned above. The interference fringes and the optical path at the extrema of T(l) are exploited to determine with precision the refractive index and the film thickness. The absorption coefficient is computed at the absorption edge using an efficient iterative method. At the transition zone between the interference region and the absorption edge artifacts in the absorption curve are avoided. A small absorption of the substrate is allowed for in the theory by means of a factor determined from an independent measurement, thus improving the quality of the results.Application of the method to a transmission spectrum of an a:SixN1-x:H film is illustrated in detail. Refractive index, despersion parameters, film thickness, absorption coefficient and optical gap are given with the help of tables and graphs.

Applied Optics 37 (22), 5262-5270, 1998

A 019-98 Flux Operators of Microdynamical Quantities in a Nonequilibrium Statistical Ensemble Formalism.

Madureira, J. R. , Vasconcellos, A. R. and Luzzi, R.

It is shown how the closure condition, for the set of kinetic equations in Zubarev's Nonequlibrium Statistical Operator Method, introduces a series of fluxes of a reference set of densities. These fluxes are the average values, over a Gibbs-like nonequilibrium generalized grand-canonical ensemble, of Hermitian operators for fluxes defined at the microscopic-mechanical level. The equations of evolution for these fluxes (or equivalently for their conjugated Lagrange multipliers that the variational method introduces - or intensive nonequilibrium thremodynamic variables) are described.

Brazilian Journal of Physics 28 (2), Jun 1998

A 020-98 On the Markovian Limit in a Kinetic Theory for Dissipative Systems.

Madureira, J. R. , Lauck, L., Vasconcellos, A. R. and Luzzi, R.

We reconsider a nonlinear quantum kinetic theory which is built within the context of a nonequilibrium statistical ensemble formalism. This is the Non-equilibrium Statistical Operator Method based on a variational principle, namely, the Maximization of the Informational-Statistical Entropy, and referred to as MaxEnt-NESOM. It may be considered as encompassed within the framework of E. T. Jayne's Predictive Statistical Mechanics. These theory has an ample domain of application covering a large class of experimental conditions. We consider a particular - and quit important - limiting case, consisting in the Markovian approximation. For illustration we applied it to the study of a spin system in interaction with the lattice. The presentation is an extended and detailed version of a Brief Report published in Phys. Ver. E (1998)

Brazilian Journal of Physics 28 (3), 169-182, 1998

A 021-98 On Entropy Production in Informational Statistical Thermodynamics.

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

We consider the question of the existence of a generalized H -theorem in the context of the variational method in the information-theoretical approach that generates the nonequilibrium statistical operator formalism. After briefly reviewing how the latter provides mechano-statistical foundations for phenomenological irreversible thermodynamics, we discuss how dissipative phenomena are accounted for by the procedure. Such effects are related to a generalized H -theorem and a weak criterion of positive entropy production. These results are a consequence of the definition of a coarse-grained statistical entropy, resulting from the projection of the full nonequilibrium distribution function on the subspace of the slow relaxing dynamical quantities, that are approapriate for the description of the irreversible evolution of the system from the initial preparation.

Brazilian Journal of Physics 28 (2), 97-110, 1998

A 022-98 On an Informational Statistical Approach in Sociology.

Luzzi, R.

It is considered the possibility of application of relatively recent modern statistical concepts to the study of general dynamical systems. Such approach is having an encouraging sucess in the natural sciences. It is also being tentatively tried in the disciplines of econometrics, history, sociobiology, archaeology, and others. We attempt ot describe in this paper an eventual application of such theory to the study of the dynamics of interacting social groups. For that purpose it is convenient to redirect the statistical theory (namely Jeffreys-Jaynes' Predictive Statistics), to derive an equivalent staochastic theory. The working of the theory is illustrated by applying it to the study of a quite simple oversimplified example. It describes the question of attitude forming in a scenery that grossly resembles the last presidential election in Brazil, taking only into account the two leading condidates FHC and LI(L)s. In the main body of the article it is discussed the fundamentals fo the formalism, with mathematical details reported in the Appendices.

Ciência e Cultura 50 (1), 29-44, 1998

ACCEPTED PAPERS FOR CONFERENCE PRESENTATION

C 001-98 The Chemical Environment of Er3+ in a-Si:Er:O:H.

Tessler, L. R. , Piamonteze, C., Iñiguez, A. C. Martins Alves, M. C. , Tolentino, H.

We have measured extended x-ray absorption fine structure (EXAFS) of the Er LIII edge in a-Si:Er:O:H with different concentrations of Er and O. The samples were prepared by reactive RF co-sputtering from a silicon target partially covered with metallic erbium chunks. They present the characteristic Er 3+ photoluminescence at 1.54 m m as deposited. The FFT of the Er EXAFS provides two well separated peaks at the distances corresponding to oxygen and silicon first neighbors. The relative areas correlate well with the relative oxygen contents. We assign the two peaks to different chemical environments of the erbium atoms. It is important to notice that the two environments are present in all samples studied.

In: MRS 1998 Spring Meeting, San Francisco, CA, Abril 1998

C 002-98 Photo and Electroluminescence of Er3+ in a-Si:H.

Tessler, L. R. and Iñiguez, A. C.

Trivalent erbium (Er3+ presents a characteristic intra 4f optical transition at 1.54 m m when incorporated in several solid hosts. Hydrogenated amorphous silicon (a-Si:H) is a good candidate as a host for applications in optical communications and photonic integration. We have studied Er3+ photo and electroluminescence in a-Si:H prepared by co-sputtering from a silicon target partially covered with metallic erbium chunks. The samples present 1.54 m m photoluminescence as deposited for a wide range of erbium concentration. Maximum room-temperature photoluminescence intensity is obtained for samples that are intentionally contaminated with oxygen. Similar results are found for nitrogen contaminated samples. Annealing at moderate temperatures can increase the photoluminescence intensity up to a factor 5. Photoluminescence excitation measurements show that the Er3+ ions are excited by energy transfer from the a-Si:H network.Room temperature electroluminescence at 1.54 m m has been observed in reverse biased Si/a-Si:Er:H/Al structures. A detailed study of electrical and optical properties will be presented.

In: MRS 1998 Spring Meeting, San Francisco, CA, Abril 1998

Abstracta

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Impressão
Gráfica Central - Unicamp