Abstracta

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P 254-05 à P 298-05

TRABALHOS PUBLICADOS

P 254-05 "A regular semiclassical approximation for the propagation of wave packets with complex trajectories"

Parisio, F. and de Aguiar, M. A. M.

The semiclassical propagation of Gaussian wave packets by complex classical trajectories involves multiple contributing and noncontributing solutions interspersed by phase space caustics. Although the phase space caustics do not generally lie exactly on the relevant trajectories, they might strongly affect the semiclassical evolution depending on their proximity to them. In this paper, we derive a third-order regular semiclassical approximation which correctly accounts for the caustics and which is finite everywhere. We test the regular formula for the potential V (x) = 1/x(2), where the complex classical trajectories and phase space caustics can be computed analytically. We make a detailed analysis of the structure of the complex functions involved in the saddle point approximations and show how the changes in the steepest descent integration contour control both the contributing and noncontributing trajectories and the type of Airy function that appears in the regular approximation

Journal of Physics A-Mathematical and General 38[42], 9317-9339. 2005.

P 255-05 "Broad temperature operation and widely tunable high dynamic range high-speed amplified electroabsorption modulator"

Foulk, H., O'Brien, S., Gebretsadik, H., Frateschi, N., Choi, W. J., and Bond, A. E.

In this work, we demonstrate high analog performance of an eleetroabsorption (EA) Jumped-element modulator monolithically integrated with a semiconductor amplifier over a broad temperature and wavelength range. Using the Stark effect (bandedge tuning with bias), the amplified EA modulator exhibits minimal changes in second- and third-order spur-free dynamic range (SFDR) as well as link gain over a 45 degrees C range in chip temperature. We further demonstrate tunability of the amplified modulator over 25 nm of wavelength from 1530 to 1555 run with little-to-no degradation in SFDR, link gain, and noise figure

Ieee Photonics Technology Letters 17[10], 2191-2193. 2005.

P 256-05 "Chitosan membrane with patterned surface obtained through solution drying"

Torres, M. A., Aimoli, C. G., Beppu, M. M., and Frejlich, J.

Chitosan membranes with self-organized lines on surface were obtained. SEM and laser diffraction techniques showed that structures with peak-valley periods of about 5 +/- 2 mu m were observed in both porous and dense chitosan membranes. These unique patterns may be of special interest for applications where micro-mechanical interactions are important such as for biomaterials. The procedure used to produce these membranes consisted of casting, drying of a 2.5% chitosan solution, followed by coagulation using 1.0M NaOH solution. The analyses indicate that the drying step is the most important to shape the organized surface pattern. This is in agreement with literature that cites that when layers of polymer solutions undergo solvent evaporation and/or heating from below, the interface can become unstable, generating patterns, depending on the surface tension differences and density effects, fluid motion can be generated and amplified, through the known Marangoni effect. (c) 2005 Elsevier B.V. All rights reserved

Colloids and Surfaces A-Physicochemical and Engineering Aspects 268[1-3], 175-179. 2005.

P 257-05 "Comment on "Contaminants in suspended gold chains: An ab initio molecular dynamics study""

Hobi, E., da Silva, A. J. R., Novaes, F. D., da Silva, E. Z., and Fazzio, A.

***Physical Review Letters* 95[16]. 2005.**

P 258-05 "Comment on "Contaminants in suspended gold chains: An ab initio molecular dynamics study" - Reply"

Legoas, S. B., Rodrigues, V., Ugarte, D., and Galvao, D. S.

***Physical Review Letters* 95[16]. 2005.**

P 259-05 "Computer simulations of gold nanowire formation: the role of outlayer atoms"

Sato, F., Moreira, A. S., Coura, P. Z., Dantas, S. O., Legoas, S. B., Ugarte, D., and Galvao, D. S.

Metallic nanowires (NWs) have been the object of intense theoretical and experimental investigations in the last years. In this work we present and review a new methodology we developed to study NW formation from mechanical stretching. This methodology is based on tight-binding molecular dynamics techniques using second-moment approximations. This methodology had been proven to be very effective in the study of NWs, reliably reproducing the main experimentally observed structural features. We have also investigated the problem of determining from what regions the atoms composing the linear atomic chains come. Our results show that similar to 90% of these atoms come from outmost external layers

***Applied Physics A-Materials Science & Processing* 81[8], 1527-1531. 2005.**

P 260-05 "Computer simulations in the study of gold nanowires: the effect of impurities"

Novaes, F. D., da Silva, A. J. R., Fazzio, A., and da Silva, E. Z.

Suspended gold nanowires have recently been made in an ultra-high vacuum ambient and were imaged by electron microscopy. Two puzzles were presented: one atom thick wires are produced and some of the atomic distances between these atoms before their breaking were too large. Simulations using realistic molecular dynamics method were able to unveil some processes to explain the mechanisms of formation, evolution, and breaking of these atomically thin Au nanowires under stress. The calculations showed how defects induce the formation of constrictions that eventually will form the one-atom chains. Atomically thin chains, five atoms long were obtained, before breaking. The results were in excellent agreement with experimental results except for the large Au-Au distances. In fact no theoretical calculation of pure gold nanowires have been able to produce such large distances. Light impurities that cannot be imaged in these experiments may be responsible for these large Au-Au distances. Using ab initio total energy calculations based on the density functional theory, we have studied the effect of H, C, O, N, B, S, CH, CH2, and H-2 impurities on the nanowire's electronic and structural properties, in particular how they affect the rupture of the nanowire. We find that the impurities tend to locally increase the nanowire's strength, in such a way that its rupture always occurs at an Au-Au bond and never at an Au-X bond (X being an impurity). In particular, oxygen seems to form very stable bonds that may be used to pull longer Au chains. Regarding the observed large Au-Au bond lengths, it was found, based on quasi-static calculations, that the best candidate to explain the large distances is H. However, some particular experimental conditions may lead to different results

***Applied Physics A-Materials Science & Processing* 81[8], 1551-1558. 2005.**

P 261-05 "Dependence of transition probabilities for non-linear photo-ionization of He atoms on the structure of the exciting radiation pulses"

Castro, A. R. B. de, Moeller, T., Wabnitz, H., and Laarmann, T.

We discuss the expected dependence of the probability transitions for 2-photon and 3-photon absorption in Helium gas on the spatial and temporal structure of the exciting radiation pulses. Regarding spatial structure, we assumed a Gaussian radial intensity distribution; we find, as expected, that the 2-photon and 3-photon processes become negligible at distances D away from the focus, where D is of the order of the beam waist FWHM. Regarding temporal structure, we compared transition probabilities for square, Gaussian and cosine squared temporal profiles; we find that for the same FWHM, Gaussian and cosine squared pulses give essentially the same transition probabilities, but the square pulses are about twice as efficient. We finally studied the effect of sharp versus smooth rise and fall edges in the light pulse; we find negligible correlation with the shape of the pulse edges, and strong correlation with the pulse FWHM, i.e., with pulse total energy, as might be expected

***Brazilian Journal of Physics* 35[3A], 632-635. 2005.**

P 262-05 "Disorder-driven non-Fermi liquid behaviour of correlated electrons"

Miranda, E. and Dobrosavljevic, V

Systematic deviations from standard Fermi-liquid behaviour have been widely observed and documented in several classes of strongly correlated metals. For many of these systems, mounting evidence is emerging that the anomalous behaviour is most likely triggered by the interplay of quenched disorder and strong electronic correlations. In this review, we present a broad overview of such disorder-driven non-Fermi liquid behaviour, and discuss various examples where the anomalies have been studied in detail. We describe both their phenomenological aspects as observed in experiment, and the current theoretical scenarios that attempt to unravel their microscopic origin

Reports on Progress in Physics **68[10], 2337-2408. 2005.**

P 263-05 "Double optical tweezers for ultrasensitive force spectroscopy in microsphere Mie scattering"

Fontes, A., Neves, A. A. R., Moreira, W. L., de Thomaz, A. A., Barbosa, L. C., Cesar, C. L., and de Paula, A. M.

We used a double tweezers setup to perform ultrasensitive force spectroscopy and observe the forces due to light scattering in a single isolated particle. We demonstrate how to selectively couple the light to the transverse electric (TE), transverse magnetic (TM), or both TE and TM microsphere modes by means of the beam polarization and positioning, and to observe correspondent morphology-dependent resonances (MDR). The results show how the usually assumed azimuthal symmetry in the horizontal plane no longer holds because of the symmetry break caused by the beam polarization. Also, the MDR resonances can change the force values by more than 30-50%. (c) 2005 American Institute of Physics

Applied Physics Letters **87[22]. 2005.**

P 264-05 "Dynamics of the antimicrobial peptide PGLa action on Escherichia coli monitored by atomic force microscopy"

Silva, A. da and Teschke, O.

Atomic force microscopy (AFM) images of living cells in physiological solution were used to monitor the different stages involved in the interaction between Escherichia coli and the antimicrobial peptide PGLa. Damage on bacterial membranes was observed in the past using standard electron microscopy; stiffness measurements and images scanned in physiological solution demonstrate the advantage of AFM for such studies. From force versus separation curve measurements it is possible to determine the variation of the cellular stiffness. PGLa action on components of the cell structure like the outer membrane, the bacterial pili, the peptidoglycan wall and the inner membrane was determined by the comparison of AFM images of bacteria before and after PGLa addition. The interaction of Escherichia coli with PGLa in the culture medium has two stages. The first is characterized by the loss of surface stiffness and the formation of micelles probably originating from the disruption of the outer membrane and the loss of the bacteria's ability to adhere to the substrates. In the second stage there is further damage, which resulted in total cell rupture. AFM images of bacteria in air and surface roughness measurements were also used to estimate peptide damage

World Journal of Microbiology & Biotechnology **21[6-7], 1103-1110. 2005.**

P 265-05 "Electric potential due to an infinite conducting cylinder with internal or external point charge"

Hernandes, J. A. and Assis, A. K. T.

We utilize the Green's function method in order to calculate the electric potential due to an infinite conducting cylinder held at zero potential and a point charge inside and outside it. We calculate and plot the net force upon the point charge as a function of its distance to the axis of the cylinder. We show that this force goes to zero when the radius of the cylinder goes to zero, no matter the distance of the external point charge to the conducting line. (c) 2005 Published by Elsevier B.V.

Journal of Electrostatics **63[12], 1115-1131. 2005.**

266-05 "Ensemble formalism for nonequilibrium systems and an associated irreversible statistical thermodynamics"

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

It is reviewed what can be considered as the present research trends in what regards to the construction of an ensemble formalism -Gibbs' style-for the case of far-from-equilibrium systems. The main questions involved are presented accompanied with brief discussions. The construction of a nonequilibrium statistical operator is described and its applications commented, and, particularly, it is presented the derivation of an Irreversible Thermodynamics based on the statistical foundations that the nonequilibrium ensemble formalism provides

Brazilian Journal of Physics **35[3A], 689-717. 2005.**

P 267-05 "Entanglement versus mixedness for coupled qubits under a phase damping channel"

Cardoso, E. S., de Oliveira, M. C., and Furuya, K.

Quantification of entanglement against mixing is given for a system of coupled qubits under a phase damping channel. A family of pure initial joint states is defined, ranging from pure separable states to maximally entangled states. An ordering of entanglement measures is given for a well-defined initial-state amount of entanglement

Physical Review A **72[4]. 2005.**

P 268-05 "Feynman identity: A special case revisited"

Da Costa, G. and Variane, J.

It is proved that a special case of Feynman identity is a consequence of the generalized Witt identity of some Lie algebra

Letters in Mathematical Physics **73[3], 221-235. 2005.**

P 269-05 "Growth and characterization of cubic InxGa1-xN epilayers on two different types of substrate"

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

We report on the growth and characterization of cubic InGaN epilayers on two different types of substrates: GaAs (0 0 1) and 3C-SiC (0 0 1). The films are grown by RF plasma-assisted molecular beam epitaxy (MBE). The crystalline quality and state of stress in these films were assessed by performing Raman scattering and X-ray diffraction experiments. Both types of measurements complement one another as techniques to determine crystalline quality and the state of biaxial strain present in the alloy layers. Our experiments show that, for the same In molar fraction, samples deposited on SiC Substrates are more uniformly strained and have better crystallinity than those deposited on GaAs Substrates. (c) 2005 Elsevier B.V. All rights reserved

Journal of Crystal Growth **284[3-4], 379-387. 2005.**

P 270-05 "Growth and morphological characterization of Al-Cr-Nb eutectic alloys"

Souza, S. A., Rios, C. T., Coelho, A. A., Ferrandini, P. L., Gama, S., and Caram, R.

Directional solidification of eutectic alloys attracts considerable attention, when in situ composites are concerned. The eutectic alloys are regarded as presenting regular morphology (lamellar and fibrous structures). Besides, when directionally solidified they show high microstructure stability at high temperatures. This work reports a morphological study of an Al-Cr-Nb eutectic alloy. The solidification morphology of the alloys was studied both in the as-cast and in the directionally solidified conditions. The samples were first obtained in an arc furnace and then directionally solidified using Bridgman equipment. During the directional solidification process, the growth rates utilized varied from 5.0 to 30.0 mm/h. Optical (OM) and scanning electron microscopy (SEM) was used in order to determine the influence of the solidification conditions on the microstructure. The results obtained indicated that the eutectic transformation temperature is near 1347.9 degrees C with formation of Al-3(Nb,Cr) and Cr(Al,Nb) phases. Also, it was noted that the Cr(Al,Nb) phase undergoes a polymorphic transformation (similar to 892.3 degrees C) forming the Al(Nb)Cr-2 compound, followed by eutectoid decomposition Cr(Al,Nb) -> Al(Nb)Cr-2 + Al8Cr5. (c) 2005 Elsevier B.V. All rights reserved

Journal of Alloys and Compounds **402[1-2], 156-161. 2005.**

P 271-05 "Heterometallic manganese/zinc-phytate complex as a model compound for metal storage in wheat grains"

Rodrigues-Filho, U. P., Vaz, S., Felicissimo, M. P., Scarpellini, M., Cardoso, D. R., Vinhas, R. C. J., Landers, R., Schneider, J. F., McGarvey, B. R., Andersen, M. L., and Skibsted, L. H.

Myo-inositol-1,2.3,4,5.6-hexakisphosphate, also known as phytate, is a natural metal chelate present in cereals, an important feedstock worldwide. This article reports the characterization of three metal storage model complexes: the homometallic Mn(II) myo-inositol-1,2,3,4,5,6-hexakisphosphate (IP6), the heterometallic Zn(II), Mn(II) analogue Na4MnZn4(C6H6O24P6) (NO3)(2)-8H(2)O (MnZn(4)IP6) and the homometallic Zn(II) metal complex Na3Zn5(C6H6O24P6)OH-9H(2)O (Zn(5)IP6). The techniques of high-resolution Na-23, C-13 and P-31 NMR, electron paramagnetic resonance (EPR) and X-ray photoelectron spectroscopy (XPS) were applied in this study. The complexation of Zn(II) and Mn(II) by phosphate groups of IP6 is demonstrated by NMR and XPS results. C-13 NMR results show a conformation for IP6 consisting of five equatorial phosphate groups to one axial group showing only one chemical environment for Zn and two for Mn, when characterized by XPS and EPR, in both Mn complexes. These results support, for the first time, a probable supramacromolecular structure for phytate complexes of transition metals. Based on the similarity between the EPR spectra of wheat seeds and that of the MnZn(4)IP6 compound, the manganese storage centers in wheat grains can be assigned to similar heterometallic phytate complexes. (c) 2005 Elsevier Inc. All rights reserved

Journal of Inorganic Biochemistry 99[10], 1973-1982. 2005.

P 272-05 "Highly integrated laser-modulator module for high-speed high dynamic range analog transmission"

O'Brien, S., Foulk, H., Gebretsadik, H., Frateschi, N., Choi, W. J., Bond, A. E., and Robertson, S.

In this work, we demonstrate the integration of linear electroabsorption (EA) lumped-element modulator, a semiconductor optical amplifier (SOA), and a distributed feedback laser, resulting in high analog performance from a compact and highly integrated packaged module. The EA modulator is monolithically integrated on the same chip with an SOA resulting in cost-effective and high fiber-coupled optical power > 10 dBm. The resulting module exhibits robust performance over bias, frequency, and temperature and is telco-qualifiable. Some operating characteristics of the module are spur-free dynamic range (SFDR) of 108 dB. Hz(2/3), 15-GHz bandwidth, relative intensity noise (RIN) of -159 dB/Hz, as well as constant and high SFDR over > 1-V bias range and 30 degrees C variation in chip temperature

Ieee Photonics Technology Letters 17[10], 2188-2190. 2005.

P 273-05 "Inter-comparison of three techniques for radon activity measurements"

Neman, R., Hadler, J. C., Junes, P. J., Paulo, S. R., Guedes, S., and Curvo, E. A. C.

In this paper the results of an inter-comparison employing three distinct techniques for measuring indoor radon activities are discussed: (i) NRPB-SSI dosimeter, a diffusion chamber, CR-39 based, calibrated in a controlled radon chamber; (ii) a diffusion chamber, CR-39 based, calibrated via nuclear emulsion; (iii) canister with activated charcoal. Totally 39 dwellings of Pocos de Caldas city (Minas Gerais State, Brazil), located in a high natural radioactivity region, have been monitored during a six months period. Dosimeters (i) and (ii) were exposed continuously in all of 39 dwellings and dosimeter (iii) was exposed in 10 of them, randomly chosen. In this case the individual exposures lasted around 5 days and 4 equally time spaced exposures were made in each dwelling. Results produced by techniques (i) and (ii) show a great level of concordance. Individual results of technique (iii) for each residence show great fluctuations, but their mean results statistically agree with the other techniques. So our results indicate that active charcoal technique can be used to study average term radon variation (in few days), but its individual results cannot reflect long-term indoor radon activity. (c) 2005 Published by Elsevier Ltd

Radiation Measurements 40[2-6], 295-298. 2005.

P 274-05 "Investigation of red blood cell antigens with highly fluorescent and stable semiconductor quantum dots"

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

We report a new methodology for red blood cell antigen expression determination by a simple labeling procedure employing luminescent semiconductor quantum dots. Highly luminescent and stable core shell cadmium sulfide/cadmium hydroxide colloidal particles are obtained, with a predominant size of 9 nm. The core-shell quantum dots are functionalized with glutaraldehyde and conjugated to a monoclonal anti-A antibody to target antigen-A in red blood cell membranes. Erythrocyte samples of blood groups A(+), A(2)(+), and O+ are used for this purpose. Confocal microscopy images show that after 30 min of conjugation time, type A(+) and A(2)(+) erythrocytes present bright emission, whereas the O+ group cells show no emission. Fluorescence intensity maps show different antigen expressions for the distinct erythrocyte types. The results obtained strongly suggest that this simple labeling procedure may be employed as an efficient tool to investigate quantitatively the distribution and expression of antigens in red blood cell membranes. (C) 2005 Society of Photo-Optical Instrumentation Engineers

Journal of Biomedical Optics 10[4]. 2005.

P 275-05 "Kinetic model for the annealing of fission tracks in zircon"

Guedes, S., Hadler, J. C., Iunes, R., Oliveira, K. M. G., Moreira, R. F. P., and Tello, C. A.

A model for the annealing kinetics of fission tracks is proposed based on a simplified track. The principal hypothesis is that the atoms displaced during the passage of the fission fragment have to transmit through a potential barrier to occupy the vacant sites left. The resulting model equation is applied to zircon data both from laboratory and geological sources. The model succeeded in fitting the data and the addition of the geological data during the fitting procedure improved the extrapolation of the model to the timescale of millions of years, which is the timescale of interest in geology applications. (c) 2005 Elsevier Ltd. All rights reserved

Radiation Measurements 40[2-6], 517-521. 2005.

P 276-05 "Magnetic field effect on the volt-equivalent of arc spot heat flux"

Essiptchouk, A. M., Marotta, A., and Sharakhovsky, L. I

The results of an experimental study of the are spot heat flux on the copper cathode of a coaxial Electric Arc Heaters (EAH), with magnetically driven arc, in air are presented. The three rings method was used for indirect separation of arc spot heat flux from total heat entering the electrode. As a result of joint generalizing new and previously published data, the linear dependence of the volt equivalent of arc spot heat flux on magnetic field was obtained for the range B = 0.01 - 1 Tesla and atmospheric pressure. A method, which allows to improve the measurement of the volt equivalent in highly unsteady arc spots, is proposed

Contributions to Plasma Physics 45[7], 522-530. 2005.

P 277-05 "Metallic submicrometer sieves fabricated by interferometric lithography and electroforming"

Gutierrez-Rivera, L. E., de Carvalho, E. J., Silva, M. A., and Cescato, L.

We propose and demonstrate a low cost technique to fabricate submicrometer sieves using the association of laser interference lithography and nickel electroforming. The sieves are fabricated on glass substrates and are released from the substrate by adding a hexagonal sustaining structure, electroformed in nickel, using conventional lithography. The resulting sieves are free self-sustained membranes similar to those used in filtration devices, with typical diameters of the holes of about 250 nm and areas of about I cm(2)

Journal of Micromechanics and Microengineering 15[10], 1932-1937. 2005.

P 278-05 "Modification of electrode materials for plasma torches"

Jankov, I. R., Szente, R. N., Goldman, I. D., Carreno, M. N. P., Valle, M. A., Behar, M., Costa, C. A. R., Galembeck, F., and Landers, R.

As part of the studies of new materials to be used as electrodes for plasma torches, polycrystalline copper thin film substrates, obtained by depositing copper on silicon wafer using the Electron Beam technique, were implanted with low energy (20-50 keV) alkali ions. The samples, before and after implantation process, were analysed in terms of surface composition and work function changes. Although the implantation doses were low (3 x 10(15) ions/cm(2)), relatively high concentrations of alkali metals were detected on the surface, which yielded a work function decrease of 3-9% in relation to the copper value. (c) 2005 Elsevier B.V. All rights reserved

Surface & Coatings Technology 200[1-4], 254-257. 2005.

P 279-05 "Modification of plasma-polymerized organosiloxane films by irradiation with He+, Ne+, Ar+, and Kr+ ions"

Gelamo, R. V., de Moraes, M. A. B., Trasferetti, B. C., Rouxinol, F. P., and Davanzo, C. U.

The effects of ion irradiation on the composition, structure, compactness, and surface hardness of polyorganosiloxane films synthesized by plasma-enhanced chemical vapor deposition were investigated as a function of the ion mass and fluence. The films were obtained from a glow discharge plasma of a hexamethyldisiloxane (HMDSO)-O-2-Ar mixture, and the irradiations were carried out with 170 keV He+, Ne+, Ar+, and Kr+ ions at fluences between 1 x 10(14) and 1 x 10(16) cm(-2). To characterize the film elemental composition, two ion-beam analysis techniques were used: Rutherford backscattering spectroscopy (RBS) and forward recoil spectroscopy (FRS). The ion-beam-induced hydrogen loss from the films was significant. For the He+-irradiated samples, a H loss of about 50% with respect to the pristine or unirradiated film was observed for the highest fluence. The surface hardness measurements, performed with a nanoindenter, in films irradiated at a fluence of 1 x 10(16) cm(-1) were 8.1, 6.0, 4.7, and 1.6 GPa for He+, Ne+, Ar-,(+) and Kr+, respectively. To examine the ion-induced structural transformations in the films, infrared reflection-absorption spectroscopy (IRRAS) was employed. From analysis of the spectra of the irradiated samples several conclusions could be drawn. For example, as the ion fluence increased, (i) the densities of methyl- and Si-O-related groups changed, (ii) film disorder increased, and (iii) groups such as Si-CH2-Si, and Si-OH, which were not present in the pristine film, were formed at lower fluences but disappeared when the latter attained their highest values. Furthermore, some of the absorption peaks that appeared at low fluences and increased with increasing fluence strongly indicate formation of carbon domains in the film. Finally, differences in the ion-induced modifications produced by the different ion species were analyzed in terms of the electronic and nuclear collisions of the ions traversing the film using the well-known SRIM simulation program

Chemistry of Materials 17[23], 5789-5797. 2005.

P 280-05 "Molecular dynamics simulations reveal multiple pathways of ligand dissociation from thyroid hormone receptors"

Martinez, L., Sonoda, M. T., Webb, P., Baxter, J. D., Skaf, M. S., and Polikarpov, I.

Nuclear receptor (NR) ligands occupy a pocket that lies within the core of the NR ligand-binding domain (LBD), and most NR LBDs lack obvious entry/exit routes upon the protein surface. Thus, significant NR conformational rearrangements must accompany ligand binding and release. The precise nature of these processes, however, remains poorly understood. Here, we utilize locally enhanced sampling (LES) molecular dynamics computer simulations to predict molecular motions of x-ray structures of thyroid hormone receptor (TR) LBDs and determine events that permit ligand escape. We find that the natural ligand 3,5,3'-triiodo-L-thyronine (T-3) dissociates from the TR alpha 1 LBD along three competing pathways generated through i), opening of helix (H) 12; ii), separation of H8 and H11 and the Omega-loop between H2 and H3; and iii), opening of H2 and H3, and the intervening beta-strand. Similar pathways are involved in dissociation of T-3 and the TR beta-selective ligand GC24 from TR beta; the TR agonist IH5 from the alpha- and beta-TR forms; and Triac from two natural human TR beta mutants, A317T and A234T, but are detected with different frequencies in simulations performed with the different structures. Path I was previously suggested to represent a major pathway for NR ligand dissociation. We propose here that Paths II and III are also likely ligand escape routes for TRs and other NRs. We also propose that different escape paths are preferred in different situations, implying that it will be possible to design NR ligands that only associate stably with their cognate receptors in specific cellular contexts

Biophysical Journal 89[3], 2011-2023. 2005.

P 281-05 "Negative charged excitons in double barrier diodes"

Camps, I., Vercik, A., Gobato, Y. G., Brasil, M. J. S. P., Marques, G. E., and Makler, S. S.

We have studied the effects of excitonic complexes formation, such as excitons and trions, on the optical and on transport properties of GaAs-GaAlAs n-i-n double barrier diodes, by measuring the current-voltage characteristics and the photoluminescence emission, as function of bias. The observation of a pre-resonance shoulder in the I(V) curves, under high laser intensities, and a negative charged excitons in the photoluminescence spectra, under the same bias conditions, were associated to the dissociation of these complexes either by thermal excitation or by scattering with 'free' carriers in the quantum well layer. A simple rate equation model allows us to explain the kinetics of the excitonic complexes in double barrier devices. (c) 2005 Elsevier Ltd. All rights reserved

Microelectronics Journal 36[11], 1038-1040. 2005.

P 282-05 "New pathways in plasma nitriding of metal alloys"

Figueroa, C. A. and Alvarez, F.

In this paper, we report the effects of oxygen, hydrogen, and deuterium on nitrogen implanted stainless steel AISI 316. The samples were studied in situ by photoemission electron spectroscopy (XPS), nano-indentation (hardness), and scanning electron microscopy (SEM). At relative higher oxygen partial pressures, a surface potential barrier for nitrogen implantation is created by the oxygen absorption. The absorption process obeys a Langmuir isothermal law. The surface barrier is formed by the oxidation of metallic nitrides. The bulk properties such as nitrided layer thickness can be modeled by studying the surface properties. Hydrogen improves the nitrogen content on surface and, consequentially, the hardness in-depth. Surprising efficient oxygen elimination was detected using deuterium instead of hydrogen. This is due to the fact that deuterium improves the nitrogen chemical potential, augmenting the material hardness in depth up to 30% compared to the case when hydrogen is used. This phenomenon is interpreted by an increasing isotope residence time. These novel results suggest that new pathways can be opened in plasma nitriding processes using deuterium in industrial equipment for treatments of metal alloys with stable oxides on the surface. (c) 2005 Elsevier B.V All rights reserved

Surface & Coatings Technology 200[1-4], 498-501. 2005.

P 283-05 "Random magnetic fields inducing solar neutrino spin-flavor precession in a three generation context"

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

We study the effect of random magnetic fields in the spin-flavor precession of solar neutrinos in a three generation context, when a nonvanishing transition magnetic moment is assumed. While this kind of precession is strongly constrained when the magnetic moment involves the first family, such constraints do not apply if we suppose a transition magnetic moment between the second and third families. In this scenario we can have a large nonelectron antineutrino flux arriving on Earth, which can lead to some interesting phenomenological consequences, as, for instance, the suppression of day-night asymmetry. We have analyzed the high-energy solar neutrino data and the KamLAND experiment to constrain the solar mixing angle, theta, and solar mass difference, Delta m(2), and we have found a large shift of allowed values. Also, sizable effects in the Borexino experiment are expected which can discriminate this scenario and standard large mixing angle solution to the solar neutrino problem

Physical Review D 72[7]. 2005.

P 284-05 "Real-time atomic resolution study of metal nanowires"

Bettini, J., Rodrigues, V., Gonzalez, J. C., and Ugarte, D

The conductance of atomic-size wires generated by mechanical stretching is determined by the preferred atomic structure, and atomistic descriptions are essential to interpret the quantum transport behavior of metal nanostructures. Here, we present a thorough analysis of real-time in situ high resolution transmission electron microscopy studies of atomic-size metal nanowires (NWs). By associating careful image processing with image simulation, we have been able to derive detailed information of the atomic arrangement evolution of rod-like NWs. This shows that the atomic resolution imaging can provide quantitative information of the atomic-size NW structure

Applied Physics A-Materials Science & Processing **81[8], 1513-1518. 2005.**

P 285-05 "Real trajectories in the semiclassical coherent state propagator"

Novaes, M.

The semiclassical approximation to the coherent state propagator requires complex classical trajectories in order to satisfy the associated boundary conditions, but finding these trajectories in practice is a difficult task that may compromise the applicability of the approximation. In this work several approximations to the coherent state propagator are derived that make use only of real trajectories, which are easier to handle and have a more direct physical interpretation. It is verified in a particular example that these real trajectories approximations may have excellent accuracy. (c) 2005 American Institute of Physics

Journal of Mathematical Physics **46[10]. 2005.**

P 286-05 "Semiclassical propagation of spin-coherent states"

Novaes, M.

The semiclassical propagation of spin-coherent states is considered in complex phase space. For two time-independent systems, we find the appropriate classical trajectories and show that their combined contributions are able to describe quantum interference with great accuracy. Not only the modulus but also the phase of the quantum propagator, both dynamical and geometric terms combined, are accurately reproduced

Physical Review A **72[4]. 2005.**

P 287-05 "Semiclassical propagation of coherent states using complex and real trajectories"

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

A semiclassical approximation to the time evolution of coherent states may be derived from a saddle point approximation to the exact quantum propagator, and in general it involves complex classical dynamics. We generalize previous one-dimensional results to d dimensions, and for the case d=2 we present several applications. We also consider other simple approximations that depend only on real classical trajectories, but are not initial value representations. These approximations are able to reproduce interference and tunneling effects and involve propagating a few classical initial conditions compatible with the quantum uncertainties

Physical Review A **72[3]. 2005.**

P 288-05 "Semiclassical propagation of wavepackets with complex and real trajectories"

Aguiar, M. A. M. de, Baranger, M., Jaubert, L., Parisio, F., and Ribeiro, A. D.

We consider a semiclassical approximation, first derived by Heller and coworkers, for the time evolution of an originally Gaussian wave packet in terms of complex trajectories. We also derive additional approximations replacing the complex trajectories by real ones. These yield three different semiclassical formulae involving different real trajectories. One of these formulae is Heller's thawed Gaussian approximation. The other approximations are non-Gaussian and may involve several trajectories determined by mixed initial-final conditions. These different formulae are tested for the cases of scattering by a hard wall, scattering by an attractive Gaussian potential and bound motion in a quartic oscillator. The formula with complex trajectories gives good results in all cases. The non-Gaussian approximations with real trajectories work well in some cases, whereas the thawed Gaussian works only in very simple situations

Journal of Physics A-Mathematical and General **38[21], 4645-4664. 2005.**

P 289-05 "Sensitivity enhancement in thermoreflectance microscopy of semiconductor devices using suitable probe wavelengths"

Freitas, L. R. de, da Silva, E. C., Mansanares, A. M., Tessier, G., and Fournier, D.

In this paper we present an experimental and theoretical study of the thermoreflectance response as a function of the probe wavelength for layered microelectronics structures. The investigated sample consists of a polycrystalline silicon conducting track grown on a SiO2-coated Si substrate. Thermoreflectance measurements were carried out in the wavelength range from 450 to 750 nm with the track biased in modulated regime. An oscillating pattern is observed in the spectral region where the upper layer is transparent. Such oscillations are due to the interference resulting from the multiple reflections at the interfaces. Using a thermo-optical model, we show that the optical constants (n and k) of the materials, which are wavelength dependent, as well as their temperature derivatives (dn/dT and dk/dT), strongly influence the thermoreflectance signal. The optical thicknesses of the layers, mainly determined by the real part of the refractive indices, define the period of oscillation. On the other hand, the imaginary part of the refractive indices establishes the cutoff wavelength of the oscillations. Below this cutoff wavelength, the probe light does not penetrate the material and the upper-surface reflectance dominates the signal. (c) 2005 American Institute of Physics

Journal of Applied Physics **98[6]. 2005.**

P 290-05 "Single chamber PVD/PECVD process for in situ control of the catalyst activity on carbon nanotubes growth"

Minea, T. M., Point, S., Gohier, A., Granier, A., Godon, C., and Alvarez, F.

In this paper, we studied the effect of oxygen on the catalyst activity and related influence on the nanotubes (CNTs) growth by low-pressure/high-density plasma. CNTs were prepared using a novel single vacuum chamber reactor combining (i) plasma assisted physical vapour deposition (PVD) for catalyst deposition under O-2, NH3 or Ar atmosphere with (ii) electron cyclotron resonance (ECR) C2H2/NH3 plasma enhanced chemical vapour deposition (PECVD) process for carbon nanotubes growth. The substrates are in situ prepared by controlled PVD allowing the deposition of sub-nanometric catalyst (Fe, Ni, Pd) films followed by ECR-PECVD CNTs growth. Transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) analysis of CNTs show that the volume oxidation of the nanometric catalyst particles partially inhibits the CNTs growth while the catalyst surface oxidation can be reduced by the atomic nitrogen during the PECVD process. The specially designed PVD/PECVD process preserves the catalyst from moisture contamination, reducing walls nanotube defects.

Surface & Coatings Technology 200[1-4], 1101-1105. 2005.

P 291-05 "Spallation physics and the ADS target design"

Mongelli, S. T., Maiorino, J. R., Anefalos, S., Deppman, A., and Carluccio, T.

This paper reviews the physics of the spallation which is a nuclear reaction in which a particle (e.g. proton) interacts with a nucleus. Given to the high energy of the incident proton, in a first stage it interacts with the individual nucleons in an intranuclear cascade which leads to the emission of secondary particles (neutrons, protons, mesons, etc.). In a secondary stage the nucleus is left in an excited state and can de-excite by evaporation and/or fission. Given to the high number of secondary neutrons produced (similar to 30 n/p for proton energy of I GeV), this reaction can be used as a source of neutrons, for example for ADS systems as external source to drive the sub critical reactor. The main codes used in the ADS target design and an example on the utilization of one of these codes (the LAHET code) for typical ADS target are given

Brazilian Journal of Physics 35[3B], 894-897. 2005.

P 292-05 "Spin-liquid behavior in electronic Griffiths phases"

Tanaskovic, D., Dobrosavljevic, V., and Miranda, E.

We examine the interplay of the Kondo effect and the RKKY interactions in electronic Griffiths phases using extended dynamical mean-field theory methods. We find that sub-Ohmic dissipation is generated for sufficiently strong disorder, leading to the suppression of Kondo screening on a finite fraction of spins, and giving rise to universal spin-liquid behavior

Physical Review Letters 95[16]. 2005.

P 293-05 "Statistical approach to fractal-structured systems: An illustration from the physics of semiconductor hetero structures"

Vasconcellos, A. R., Laureto, E., Meneses, E. A., and Luzzi, R.

Physico-chemical systems presenting fractal-like structures pose difficulties for their study within the scope of the standard statistical mechanics. A way around in order to make predictions for analyzing the system properties consists into resorting to auxiliary alternative statistics. We illustrate here one such a case in a study of luminescence spectra in nanometric quantum wells of semiconductor heterostructures which show anomalous behavior when compared with the usual one in bulk matter. This is a result of the occurrence of the phenomenon in constrained geometries (nanometer scales) with microroughened fractal-like boundaries. This sets practical difficulties for the theoretical treatment in that one does not have access to a proper description of certain relevant characteristics of the system. The situation becomes further hard to deal with when the system is in far-from-equilibrium conditions. A way around to perform a study of the phenomenon consists into the use of a formalism for dealing with nonequilibrium many-body systems based on auxiliary statistics, and we resort here to Renyi approach adapted to a nonequilibrium statistical ensemble formalism. (c) 2005 Published by Elsevier Ltd

Chaos Solitons & Fractals 28[1], 8-19. 2006.

P 294-05 "Structural and electronic properties of radialenes and related systems"

Konstantinova, E., Galvao, D. S., Barone, P. M. B., and Dantas, S. O.

The discovery of new allotropic forms of carbon gives rise to a great interest in carbon compounds as building blocks for novel nanostructure materials. Radialenes are homologous series of compounds with a cycloalkane nucleus bound to methylene side groups, with molecular formula CnHn. The series of expanded radialenes of molecular formulae C2nHn and C3nHn are obtained by inserting acetylene or diacetylene groups between each pair of methylene units. This paper is a report on the theoretical study of structural, electronic and spectroscopic properties of radialenes, expanded radialenes and related molecular systems. Using semiemperical methods we explore the behavior of pi-electrons along the carbon-rich skeleton. The results for structural parameters are in a good agreement with the available experimental data. The calculated electronic gaps and spatial distribution of frontier orbitals indicate to interesting electrical and nonlinear optical properties of the explored compounds, which may be useful for technological applications. (c) 2005 Elsevier B.V. All rights reserved

Journal of Molecular Structure-Theochem 729[3], 203-210.2005.

P 295-05 "The Stationary phase condition applicability to the study of tunnel effect"

Bernardini, A. E.

Some recent theoretical studies tended to employ analytically-continuous gaussian, or infinite-bandwidth step pulses to examine tunneling process. The stationary phase method is often employed to this aim. However, gaussian functions do not have a well-defined front, such that their speed of propagation becomes ambiguous. Also, infinite bandwidth signals cannot propagate through any real physical medium (whose transfer function is therefore finite) without pulse distortion, which also leads to ambiguities in determining propagation velocity during the tunneling process. In this manuscript, we appoint some incompatibilities with the application of the method of stationary phase in deriving tunneling times which, eventually, can ruin the superluminal interpretation of transition times

Modern Physics Letters B 19[18], 883-888. 2005.

P 296-05 "Ultrafast relaxation kinetics of photoinjected plasma in III-nitrides"

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

The ultrafast relaxation kinetics of photoinjected plasmas in blue-emitting highly-polar III-nitrides is analysed. The evolution of the nonequilibrium thermodynamic state of the 'hot carriers' and 'hot phonons' is studied. It is shown that the dissipative phenomena are orders of magnitude larger than in less strongly polar materials, such as GaAs. Moreover, the phenomena of 'phonon bottleneck' and 'hot-phonon temperature overshoot' are characteristically enhanced

Journal of Physics D-Applied Physics 38[19], 3584-3589. 2005.

P 297-05 "Volume of extracellular polymeric substance coverage of individual Acidithiobacillus ferrooxidans bacterium measured by atomic force microscopy"

Teschke, O.

The Acidithiobacillus ferrooxidans response to stress associated with the drying process is known to be the production of extracellular polymeric substance (EPS) coverage. Here, samples of A. ferrooxidans suspensions grown in 1.8 pH and 3.0 pH and dried on mica and silicon are shown to form a structure of isolated bacteria. Individual bacteria coverage patterns were imaged by atomic force microscopy (AFM) on hydrophobic (silicon) and hydrophilic (mica) substrates. A comparison of images of covered and uncovered bacteria establish the volume of individual EPS coverage. The EPS production for bacteria on hydrophobic substrates shows a substantial decrease (a factor of 30) in the EPS volume per bacterium when compared with the one on hydrophilic substrates. Shape and volume determination of EPS structures on bacteria as a function of hydrophobicity or hydrophilicity of the substrate may help to determine the functions of EPS on bacterial aggregates

Microscopy Research and Technique 67[6], 312-316. 2005.

P 298-05 "Water molecule clusters measured at water/air interfaces using atomic force microscopy"

Teschke, O. and de Souza, E. F.

During the tip approach to hydrophobic surfaces like the water/air interface, the measured interaction force reveals a strong attraction with a range of similar to 250 nm at some points along the interface. The range of this force is similar to 100 times larger than the measured for gold (similar to 3 nm) and 10 times larger than the one for hydrophobic silicon surfaces (similar to 25 nm). At other points the interface exerts a medium range repulsive force growing stepwise as the tip approaches the interface plane, consequently the hydrophobic force is a strong function of position. To explain these results we propose a model where the force on the tip is associated with the exchange of a small volume of the interface with a dielectric permittivity epsilon(int) by the tip with a dielectric permittivity epsilon(tip). By assuming a oscillatory spatial dependence for the dielectric permittivity it is possible to fit the measured force profiles. This dielectric spatial variation was associated with the orientation of the water molecules arrangement in the interfacial region. Small nanosized hydrogen-bond connected cages of water molecules present in bulk water at the interface are oriented by the interfacial electric field generated by the water molecules broken bonds, one broken hydrogen bond out of every four. This interfacial field orients small clusters formed by similar to 100 water molecules into larger clusters (similar to 100 nm). In the limit of small (less than 5 nm thick) water molecule cages we have modeled the static dielectric permittivity (epsilon) as the average response of those cages. In these regions the dielectric permittivity for water/air interfaces decreases monotonically from the bulk value epsilon similar to 80 to similar to 2 at the interface. For regions filled with medium size cages, the tip senses the structure of each cage and the static dielectric permittivity is matched to the geometrical features of these cages sized similar to 25 to 40 nm. Interfacial electric energy density values were calculated using the electric field intensity and the dielectric permittivity obtained by the fitting of the experimental points. The integration of the electric energy density along the interfacial region gives a value of 0.072 J m(-2) for interfacial energy density for points where the hydrophobic force has a range of similar to 250 nm. Regions formed by various clusters result in lower values of the interfacial energy density

Physical Chemistry Chemical Physics 7[22], 3856-3865. 2005.

Abstracta

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