

Abstracta

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Trabalhos Aceitos para Publicação

A023-98 à A033-98

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C003-98 à C006-98

A 023-98 Influence of Nitrogen Ion Implantation on the Properties of Polymer Films Deposited in Benzene Glow Discharges.

E.C. Rangel, N. C. da Cruz, M.A. Bica de Moraes and L. C. Kretly

Investigations of the structural, optical and electrical properties of plasma-polymerized benzene films were carried out as a function of the ion fluence. The films were obtained from rf (40 MHz, 70 W) plasmas of benzene and afterwards implanted with 170 keV molecular nitrogen ions (N₂⁺) with fluences F ranging from 1017 to 1021 m⁻². Infrared (IR) and ultraviolet-visible (UV-VIS) spectroscopy were used to analyze the chemical and the electronic structure of the films, respectively. Further structural informations were obtained from etching experiments using an oxygen plasma. Electrical resistivity measurements were performed by the two-point probe technique. With rising ion fluence, the IR spectra of the implanted films reveal an increasing loss of hydrogen, the formation of new single and condensed aromatic structures and oxygen-containing functional groups. The latter are formed from reactions between the free radicals created upon ion implantation and oxygen from ambient air. The optical gap EG, calculated from the UV-VIS spectra of the films, showed a decrease from 1.6 to 0.9 eV as F increased from 0 to 1019 m⁻². The electrical resistivity r of the films decreases significantly with the fluence. The decreases in EG and r are attributed to an increase in the overlap of the p-orbitals. The plasma etching experiments show that at low ion fluences, polymer chain degradation prevails. The highly chemically resistant polymer surface developed under high fluences suggests a strongly cross-linked structure.

Nuclear Instruments and Methods in Physics Research B 141 (1-4), 211-215, 1998

A 024-98 Thin Film Deposition from Plasmas of Tetramethylsilane-Helium-Argon Mixtures with Oxygen and Nitrogen.

N. C. da Cruz, S.F. Durrant and M. A. Bica de Moraes

Films were produced by plasma enhanced chemical vapor deposition (PECVD) of tetramethylsilane mixed with either oxygen or nitrogen in a vacuum system fed with radiofrequency power. Actinometric optical emission spectrometry was used to determine trends in the concentrations of plasma species of interest (H, CH, CO and CN) as a function of the ratio of the inorganic reactive gas (oxygen or nitrogen) to the monomer (TMS) in the system feed. As the ratio of oxygen to TMS in the feed is increased, the degree of oxygenation of the deposited material, as revealed by transmission infrared spectroscopy, is also increased. Similarly, the degree of nitrogenation of the films increases with increasing nitrogen to monomer ratio in the feed. Strong correlations exist between the plasma concentrations of the above-mentioned plasma species and the film structure and composition.

Journal of Polymer Science Part B: Polymer Physics 36 (11), 1873-1879, Ago 1998

A 025-98 Annihilation Dynamics of Positrons in Molecular Environments.

Silva, E. P. , Germano, J. S. E. , Lino, J. L. S. , de Carvalho, C. R. C., Natalense, A. P. P. and Lima, M. A. P.

We present recent results for positron-molecule scattering obtained with the Schwinger multichannel method. Our calculations include integral, differential and momentum transfer cross sections and the annihilation parameter Zeff for C₂H₂ and C₂H₄ molecules. We discuss a mechanism for annihilation of positrons in low-energy positron-molecule scattering. We interpret the annihilation process through virtual electronic excitation of the target combined with electronic cloud relaxation and virtual positronium formation. We study the influence of the first electronic state of the

target on the cross section and on the annihilation parameter in e⁺-C₂H₂ scattering.

Nuclear Instruments & Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 143 (1-2), 140-148, 1998

A 026-98 PECVD of Amorphous Hydrogenated Carbon Films Containing Oxygen and Nitrogen.

S.F. Durrant and M. A. Bica de Moraes

An actinometric optical emission spectroscopy (AOES) study of the trends in the concentrations of the plasma species H, CH, CO, OH and CN in film producing glow discharges of mixtures of isopropanol and nitrogen was undertaken. Conventional AOES was used to obtain the trends in the plasma concentrations of these species as a function of the proportion of nitrogen in the feed, RN. A dynamic variant of actinometry in which trends in the concentrations of the plasma species are measured as a function of time following the cutting of one of the principal gas flows was also employed to investigate the relative importance of gas phase and plasma/polymer-surface interactions in the production of the species of interest. Each of the above-mentioned species is produced, to some degree, by plasma/polymer surface reactions. As revealed by transmission infrared spectroscopy, the films deposited contain C-H, C=O and O-H groups. For RN > 0, the films become nitrogenated, with both N-H and C° N groups being present. Calculations of the index of refraction n , and the optical gap, EG, of the films, using ultraviolet-visible spectroscopy, show that n and EG fall as RN is increased.

Journal of Polymer Science Part B-Polymer Physics 36 (11), 1881-1888, 1998

A 027-98 Avalanchelike Magnetic Relaxation in the Peak-Effect regime of Nb-O Solid Solution.

Kopelevich, Y and Moehlecke, S.

An increase of the pinning of vortices near the upper critical field boundary, the peak-effect (PE), is studied in Nb-O solid solution by means of the magnetization measurements. The PE onset is understood as a disorder-induced transition between a relatively ordered vortex lattice and an entangled vortex state. It is found that a characteristic feature of the vortex state in the PE region is a relaxation occurring via a large size magnetization jump or avalanche. It is also found that the temperature and field dependent time $t_j(H,T)$, at which the jump occurs, quasi diverges at the peak field $H_p(T)$.

Physical Review B 58 (5), 2834-2837, 1998

A 028-98 Weighted Oscillator Strengths and Lifetimes for the Si IX Spectrum.

Orloski, R. V. , Cavalcanti, G. H. and Trigueiros, A. G.

The weighted oscillator strengths (gf) and the lifetimes presented in this work were carried out in a multiconfiguration Hartree-Fock Relativistic (HFR) approach. In this calculation, the electrostatic parameters were optimized by a least-square procedure, in order to improve the adjustment to experimental energy levels. This method produces gf values that are in better agreement with intensity observations and lifetimes values that are closer to the experimental ones. In this work we revised all the experimentally known electric dipole Si IX spectrum lines.

Journal of Quantitative Spectroscopy and Radiative Transfer, accepted on april 1998.

A 029-98 A Nonequilibrium Statistical Grand-Canonical Ensemble: description in terms of flux operator.

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

In the domain of Statistical Mechanics of nonequilibrium-nonlinear(dissipative) systems based on a generalized Gibbs-Boltzmann ensemble formalism, it may be highlighted the so-called Nonequilibrium Statistical Operator Method, and, particularly, Zubarev's approach. We report here a detailed analysis of a case consisting in a generalized nonequilibrium grand-canonical ensemble. Its construction requires to introduce besides the traditional densities of energy and the particle number their nonconserving-dissipative fluxes of all order. The description is quite appropriate to provide a framework for the construction of a nonclassical thermo-hydrodynamics, which is briefly described.

Journal of Chemical Physics 109 (6), 2099-2110, 1998

A 030-98 Relation between Huttner-Barnett's QED in dielectrics and classical electrodynamics: determining the dielectric permittivity.

Dutra, S. M. e Furuya, K.

In the Huttner-Barnett theory of QED in linear dispersive dielectrics with absorption, a certain function of frequency, $\epsilon(\nu)$, is interpreted as the dielectric permittivity of the medium. As the concept of permittivity is independent of the quantum nature of radiation, to fully justify their interpretation, it should be demonstrated that the Huttner-Barnett $\epsilon(\nu)$ coincides with the result of a classical calculation of the permittivity for the microscopic model adopted. We give such a demonstration here. In addition, we show that the expression for $\epsilon(\nu)$ given by Huttner and Barnett can be considerably simplified. The simplified expression makes evident what classes of dielectric permittivity can be described within the Huttner-Barnett theory.

Physical Review A: Atomic, Molecular, and Optical Physics 57 (4), 3050-3058, Abr 1998

A 031-98 Quantum Dynamical Manifestation of Chaotic Behavior in the Process of Entanglement.

Furuya, K., Nemes, M. C. e Pellegrino, G. Q.

Manifestation of chaotic behavior is found in an intrinsically quantum property. The entanglement process, quantitatively expressed in terms of the reduced density linear entropy, is studied for N-atom Jaynes-Cummings model. For a given energy, initial conditions are prepared as a minimum uncertainty wavepacket centered at regular and chaotic regions of the classical phase space. We find for short times a faster increase in decoherence for the chaotic initial conditions as compared to regular ones, which have oscillatory increase.

Physical Review Letters 80 (25), 5524-5527, 1998

A 032-98 Elastic Cross Sections and Annihilation Parameter for $e^+ - H_2$ Scattering Using the Schwinger Multichannel Method.

Jorge L. S. Lino, Jose S. E. Germano, Euclimar P. da Silva and Marco. A. P. Lima.

We report detailed results for positron - H_2 collisions obtained with the Schwinger multichannel method. Our calculations include annihilation parameter, differential, integral and momentum transfer cross sections for energies below the positronium formation threshold. The calculations were carried out in the static-plus-polarization approximation with symmetry resolved cross sections. Energy (temperature) dependence and symmetry resolved contributions for the annihilation parameter Z_{eff} are also reported. Our "ab initio" integral cross sections are found to be in good agreement with the experimental data.

Physical Review A 58 (5), 3502-3506, 1998

A 033-98 On the Hardness of a-C:H films Prepared by Methane Plasma Decomposition.

Marques, F. C. , Lacerda, R. G. , Odo, G. Y. and Lepienski, C. M.

Hard, thick, and almost stress free a-C:H films prepared by methane plasma decomposition are reported. The films were prepared on the cathode electrode of a conventional rf-sputtering system in the -100 to-1200 bias voltage. The properties of films were determined using optical transmission spectroscopy, Raman spectroscopy, hardness, and stress measurements. Films with high hardness (18 GPa) and very low stress (0.7 GPa) were obtained. It is proposed that the network rigidity of the films with low stress is mainly maintained by a matrix of dispersed sp² sites, in addition to some contribution of the sp³ C-C sites. The stress versus bias voltage dependence supports the subimplantation model, indicating that it also explains the origin of stress in films prepared by rf plasma decomposition.

Thin Solid Films 332 (1-2), 113-117, 1998

ACCEPTED PAPERS FOR CONFERENCE

C 003-98 A Numerical Model for Biomass Torrefaction.

Fonseca Felfli F., Luengo C. A., Bezzon G., Baeaton Soler P. and Suros Mora W.

Upgrading of biomass residues (agricultural and forest residues) by torrefaction, may be a good alternative for an efficient use of these material as fuels. For a good design and operation of a torrefaction plant, the influence of heat exchange, temperature, particle shape and size in the process must be analyzed. This analysis would allow to estimate process conditions and results, like temperature range, particle density and size, overall yield, residence time, and final products composition. A study of the influence of these parameters in the torrefaction of a biomass briquette is presented. A numerical model was developed for determination of best process conditions. The study of the physical and chemical processes during torrefaction involves the formation of three main species: gas, tar and char. The model also analyzes heat exchange by convection and conduction, the convective transport of gaseous species and overall mass balance, considering physical properties variation during the thermochemical reactions. Different briquette shapes can be used in this model, based on the ratio between diameter and length. The influence of heat exchange coefficient and temperature in the results is shown, defining best conditions for heat exchange, temperature and residence time, base on the weight yield and properties of the final products.

In: 10th European Conference and Technology Exhibition "Biomass for Energy and Industry"- July 1998, Mai 1998

C 004-98 Bench Unit for Biomass Residues Torrefaction.

Fonseca Felfli F., Bezzon G. , Luengo C. A. and Beaton Soler P.

Charcoal industries throughout the world consume about 100 million tons of wood each year. Frequently, are inefficient and predatory. For example, in Brazil, around 48% is produced from native forest, causing serious environmental problems. An alternative to reduce those impacts consists of using new technologies to produce charcoal, or other solid fuel, which can be used for energy purposes. Torrefaction of biomass residues in an efficient alternative for this issue. Torrefaction basically is heating biomass in an inert environment, with low heating rates, until the maximum temperature 300°C. Torrefied biomass presents hydrophobic nature, high heating value and less smoke when burnt. It also has similar density and mechanical strength as the initial feedstock. A bench scale unit for biomass torrefaction was developed, aiming to improve energy properties of agricultural and forest residues. In some cases, torrefied residues may substitute firewood and charcoal, reducing costs and environmental impacts during forests exploitation. The unit is composed basically by a combustion and a thermal treatment chambers. The combustion chamber supplies process thermal energy, by burning part of biomass residues. Hot vapors and gases

produced in the torrefaction chamber are recirculated and burnt in the combustion chamber, improving overall energy efficiency and avoiding atmospheric pollution. Torrefied product of several experiments have presented low moisture and hydrophobic nature. According to the process conditions and properties of the starting material, fixed carbon content of the products was from 25 to 40% and overall yield in the range of 70-90%. Also, the average Heating Values were near 23 MJ/Kg, which is an intermediate value between biomass and charcoal. Torrefied biomass presents good quality for combustion and gasification purposes, with favorable characteristics for storage and transportation, mainly because of its low moisture, high density and hydrophobic nature

In: 10th European Conference and Technology Exhibition "Biomass for Energy and Industry"- July 1998, Mai 1998

C 005-98 The Chemical Environment of Er³⁺ IN a-Si:Er:H and a-Si:Er:O:H

Tessler, L. R., Piamonteze, C., Iñiguez A. N., Martins Alves, M. C. and 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 platelets. They present the characteristic Er³⁺ photoluminescence at 1.54 μm as deposited. The FFT of the Er EXAFS provides two well separated peaks. The characteristics of the first peak resemble those of Er₂O₃. We associate the first neighbor shell with oxygen atoms, even in non intentionally oxygenated samples. The average coordination and Er-O separation are significantly smaller than in Er₂O₃. This may be the reason why Er³⁺ luminescence in a-Si:H presents small temperature quenching. The second shell is interpreted as being composed of silicon atoms.

In: MRS Symposium Proceedings v.524 - Applications of Synchrotron Radiation Techniques to Materials Science IV, Mai 1998

C 006-98 Photo and Electroluminescence of a-Si:Er:H.

Tessler, L. R., Iñiguez, A. C.

Trivalent erbium (Er³⁺) presents a characteristic intra 4f optical transition 4I_{13/12} → 4I_{15/2} at 1.54 μm 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. Since the presence of oxygen impurities enhances the luminescence intensity, we studied the influence of oxygen added to the sputtering gas on the material properties. We found that oxygen reduces the erbium incorporation into the films. We obtained samples presenting 1.54 μm photoluminescence as deposited for a wide range of erbium concentrations. Maximum room-temperature photoluminescence efficiency is obtained for samples that contain ~ 1% [O] / [Si] concentrations. The

temperature quenching is small, mainly due to the temperature dependence of the luminescence lifetime. Room temperature electroluminescence at 1.54 μm was observed in reverse biased Si/a-Si:Er:O:H/Al structures.

In: MRS Symposium Proceedings v.507- Amorphous and Microcrystalline Silicon Technology, Mai 1998

Abstracta

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