

# Abstracta

Ano I - N. 04

Abstr.97



Trabalhos Aceitos para Publicação

A014-97 à A022-97

**[A014.97] "Structural and Optical Properties of Amorphous Hydrogenated Fluorinated Carbon Films Produced by PECVD"**

S. F. Durrant, S. G. C. Castro, L. Bolivar-Marinez, D. S. Galvão, M. A. Bica de Moraes

Fluorinated films were deposited from radiofrequency discharges of toluene/Trifluorotoluene and toluene/sulfur hexafluoride mixtures. Actinometric optical emission spectroscopy (AOES) was used to determine trends in the concentrations of the plasma species H, CH, and F as a function of the partial pressure of trifluorotoluene or sulfur hexafluoride present (expressed as a percentage of the total chamber pressure) designated  $R_T$  and  $R_S$ , respectively. Transmission infrared spectrophotometry ( $IR_S$ ) and electron spectroscopy for chemical analysis (ESCA) revealed that the films contain various fluorine-containing functionalities and that the degree of fluorination increases as  $R_T$  or  $R_S$  is increased. Ultraviolet-visible spectrophotometry (UVS) of films deposited at various values of  $R_T$  and of  $R_S$  is increased. Ultraviolet-visible spectrophotometry (UVS) of films deposited at various values of  $R_T$  and of  $R_S$  allowed the determination of the absorption coefficients of the films. From plots of as a function of photon energy it was possible to calculate the optical gap ( $E_{04}$ ). An intriguing result was a decline and subsequent rise in  $E_{04}$  as  $R_S$  was increased. Molecular modelling using ZINDO/PM3 calculations provided a semi-quantitative explanation of the dependence of  $E_{04}$  on  $R_S$ .

Thin Solid Films 304 (1-2), 149-156, 1997

**[A015.97] "Structural and Optical Properties of Plasma-deposited Amorphous Hydrogenated Oxygenated Carbon Films"**

S. F. Durrant, R. T. de Oliveira, S. G. C. Castro, L. E. Bolivar-Marinez, D. S. Galvão, M. A. Bica de Moraes

Amorphous hydrogenated oxygenated carbon (a-C:O:H) films were deposited from  $C_6H_6O_2H_e/Ar$  mixtures in a deposition system fed rf power. The principal variable was the percentage of oxygen in the feed,  $R_{ox}$ . Film structure and composition were investigated as a function of  $R_{ox}$  using transmission infrared and X-ray photoelectron spectroscopy. Greater values of  $R_{ox}$  lead to greater incorporation of oxygen functionalities such as OH, C-O and C=O in the deposited material. As revealed by ultraviolet-visible spectrophotometry (UVS), the optical gap  $E_{04}$  increased from about 3.1 to about 3.5 eV as  $R_{ox}$  was increased from 0 to about 50%. Semi-empirical methods (PM3) and ZINDO-S/CI allow modeling of the dependence of  $E_{04}$  on  $R_{ox}$ . Broad agreement between the results of the experimental and theoretical analyses was obtained.

Journal of Vacuum Science &amp; Technology A-Vacuum Surfaces and Films 15 (3), 1334-1339, 1997

**[A016.97] "Extended States in Interacting Disordered Polyacetylene-Like Chains"**

B. Laks, D. S. Galvão

In spite of the enormous amount of theoretical and experimental work on conducting polymers, the actual mechanism involved in the transition to a metallic regime is still an open and polemical question. Recently, Galvão et al. have proposed, based on the study of long, disordered, one-dimensional chains, that disorder is in the origin of the metallic transition in conducting polymers. They suggest that disorder induces the appearance of extended (conducting) states near the Fermi level. Since in actual samples there are interactions among chains one important question is whether this kind of states could survive when interactions among chains are taken into account are taken into account in the calculations. In this work we show that extended states can

exist even when the interaction among chains is taken implicitly into account. These results strongly support disorder as the physical mechanism behind the metallic transition in conducting polymers. The density of states (DOS) of long chains were obtained through the use of the Negative Factor Counting (NFC) technique coupled to a tight-binding Hamiltonian.

Physical Review B 56 (3), 967-970, 1997

**[A017.97] "Hinged and Chiral Polydiacetylene Carbon Crystals"**

R. H. Baughman, D. S. Galvão, C. Cui, S. O. Dantas

Structure and properties are calculated for hinged and chiral polydiacetylene carbon phases, which consist entirely of periodic biaxial and triaxial arrangements of the carbon chains found in organic polydiacetylenes. These theoretical results are compared with experimental reports for claimed carbyne carbon phases. The polydiacetylene carbon phases are predicted to be large bandgap semiconductors, which are expected to undergo a semiconductor-to-metal transition upon doping with alkali metals. Also, these phases are predicted to have spectacularly high third-order non-linear optical susceptibilities. The hinged phases have a soft deformation mode that results in negative linear and area compressibilities, negative Poisson's ratios, and expected shape-memory and ferroelastic behavior. In contrast, the chiral polydiacetylene carbon phase is mechanically rigid and has a predicted density-normalized bulk modulus that nearly equals that of diamond. This phase should be optically active and display second harmonic generation and torsional and transverse compressional piezoelectricity. We show consistencies between the predicted properties for the chiral polydiacetylene and those for reported carbon phases of unknown structure, and provide a plausible route by which the chiral phase might have been accidentally synthesized from a predicted phase of (-C C-)n.

Chemical Physics Letters 269 (3-4), 356-364, 1997

**[A018.97] "Photosynthetic Energy Storage and Oxygen Evolution Determined Through open Photoacoustic cell Technique"**

P. R. Barja, A. M. Mansanares

Recently a new open photoacoustic cell (OPC) has been developed for the determination of both optical and thermal properties of the sample. The OPC can also be applied for the determination of photosynthetic parameters as energy storage and oxygen evolution for in vivo and in situ plant leaves. However, the membrane of the microphone used in this cell inserts a spurious component in the photoacoustic signal of non-opaque samples as plant leaves. The membrane signal is added to the sample signal, making the analysis more complicated. In the present work we discuss this problem and propose a simple method to eliminate it.

Instrumentation Science and Technology 26 (2-3), 209-219, 1998

**[A019.97] "Photothermal and electroreflectance images of biased metal-oxide-semiconductor field-effect-transistors: six different kinds of sub-surface microscopy"**

J. A. Batista, A. M. Mansanares, E. C. Silva, D. Fournier

Six different configurations for MOSFET reflectance microscopy are presented, each one revealing a particular contrast of the operating structure. These different images are obtained by interchanging the modulation of gate-source and drain-source potentials, as well as by varying the probe beam intensity. Three main components were identified in the signal, their relative importance depending on the experimental configuration: the electroreflectance component, the photo-injected carrier (probe induced)

component and the bias current (Joule effect) component. The high ability of the technique to detect defects in these structures is also demonstrated.

**Journal of Applied Physics 82 (1), 423-426, 1997**

[A020.97] "Diamagnetic Peaks in Magnetization Versus Temperature Curves Caused by Flux Trapped Relaxation Observed in  $\text{Yb}_2\text{Cu}_3\text{O}_7$ - samples"

O. F. de Lima, R. A. Ribeiro

We present the results and interpretations for two types of diamagnetic peaks observed in magnetization versus temperature curves, taken for field cooled on warming (FCW) experiments in  $\text{Yb}_2\text{Cu}_3\text{O}_7$  samples. The high field data ( $2.0 < H < 4.5$  T), for a high quality twinned crystal, presents a universal behavior described by the collective flux creep theory.

**Physica C: Superconductivity 282 (4), 2251-2252, 1997**

[A021.97] "Study of Paramagnetic Frozen States in Superconducting Nb and Ta samples"

O. F. de Lima, M. A. Avila, C. A. Cardoso

Experimental evidence of paramagnetic frozen states (or paramagnetic Meissner effect) for Nb and Ta samples is presented. A surface layer of higher  $T_c(H)$ , caused by a higher  $k$  shell in Nb and by surface superconductivity in Ta, is the mechanism proposed to explain flux trapping and its compression when cooling the sample.

**Physica C: Superconductivity 282 (4), 2201-2202, 1997**

[A022.97] "The Basic Principles of Irreversible Thermodynamics in the Context of an Information-Statistical Approach"

R. Luzzi, A. R. Vasconcellos

We consider on the light of information statistical thermodynamics the basic principles of phenomenological thermodynamics theories, namely, the principles of equipresence, objectivity, and memory, as well as, the characteristics of Physica A (march 1997) Complex Behavior in Condensed Matter: morphological ordering in dissipative carrier systems A. R. Vasconcellos and R. Luzzi (contact us) We study the dissipative thermodynamic regime of an electron system in bulk matter under the action of an external source of energy, which generates electron-hole pairs with a nonequilibrium distribution in energy space. It is shown that with increasing values of the source power (furthering the distance from equilibrium), and strictly in the case of a p-doped material, the carrier system displays complex behavior characterized by undergoing a succession of transitions between synergetically self-organized dissipative structures. the sequence goes from the homogeneous steady state (or stochastic thermal chaos), to sinusoidal spatial deviations

(morphological ordering) to intricate ordered states (subharmonic bifurcations), to deterministic turbulent-like chaos (large amount of nonlinear periodic spatial organization of the Landau-Prigogine's type). the phenomenon may arise, for example, in semiconductor systems, molecular polymers, and in protein molecular chains in biosystems. Complexity Journal (april 1997) entropy production. Informational statistical thermodynamics arises as a particular application of maximum-information-entropy inference. We discuss how in this perspective, in conjunction with the property of contraction of description based on Bogoliubov's hierarchy of relaxation times, it is possible to account for the above mentioned principles. Particular analyses are carried out on the basis of a model system. Moreover, selecting the basic set of thermodynamical variables in a closed and in truncated approaches, we assess the validity of the approximations. In particular we derive the limiting conditions under which one recovers the constitutive equations of linear Irreversible Thermodynamics. The associated equations of evolution for the basic macrovariables and a particular A-theorem are described and discussed.

**Physica A 241 (3-4), 677-703, 1997**

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