

# Abstracta

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## Trabalhos Aceitos para Publicação

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**A 064- 98 LMM and LMN Auger Transitions of 4d Metals: comparison of experiment and theory.**

A. de Siervo, R. Landers, G. G. Kleiman, S. G. C. de Castro, and J. Morais

In recent years, there has been considerable theoretical and experimental interest in the study of Auger transitions, specially with respect to: hole-hole interactions, electron correlation effects and screening processes. Auger transitions involving only core levels are particularly interesting because in this case the quasi-atomic model of screening is strictly applicable. In this limit, theoretical models are applicable to the calculation of both the energy and line shape. Comparisons with experimental results are a crucial test of atomic theories. Here we present the measured LMM and LMN Auger spectra of Ru, Rh, Pd, Ag, In, Sn and Sb, excited with the Ka radiation ( $h\nu = 4510.9$  eV) of Ti. In all cases, we compare the spectra with results of atomic calculations in the closed shell approximation, assuming the initial state in the jj coupling scheme and the final state in the intermediate coupling (IC) scheme. This comparison permits a study of the applicability of these atomic theories.

Journal of Electron Spectroscopy and Related Phenomena 101-103, 751-755, Jun 1999

**A 065 - 98 Line Shape Variations of Ag Auger Shake-up Satellites Outside the Resonance Regime.**

J. Morais, A. de Siervo, R. Landers, S. G. C. de Castro, M. Abbate and G. G. Kleiman.

In recent publications, unambiguously identified shake-up satellites have been observed in the L123M45M45 spectra of 4d metals, studied with conventional X-ray sources and, in the L3 threshold region, with Synchrotron radiation. There remain questions concerning the origin of these satellites and their relation to the corresponding XPS spectra. We report here a study of the Ag L23M45M45 spectra as a function of photon energy and demonstrate the evolution of the line shapes of the satellite spectra. The transition from the adiabatic to sudden approximation regimes appears to occur at around 80eV above threshold, which is much less than expected for plasmon satellites. These results may reflect the influence of quasi-atomic screening, as opposed to metallic screening. The experiments were performed using the SXS-beamline at the National Synchrotron Laboratory of Brazil (LNLS).

Journal of Electron Spectroscopy and Related Phenomena 101-103, 661-664, Jun 1999

**A 066 - 98 High Energy Auger Line Shapes of Pd and Rh: experiment and theory G.**

G. Kleiman, R. Landers, S. G. C de Castro and A. de Siervo.

We compare non-relativistic atomic multiplet calculations of the L1,2,3M4,5M4,5 spectra of Rh and Pd in the jj-intermediate coupling scheme with high resolution experimental spectra excited with a Ti anode, indicating general, good agreement even for these open valence shell metals: the simplicity of the calculations indicates their suitability for experimental analyses. Comparison with relativistic calculations, including configuration interaction, for Rh indicates that the non-relativistic spectra appear to agree better with the experimental data than do the relativistic ones. The influence of relativistic and correlation effects on the intensities do not seem to be important. The major influence on the forms of the spectra is that of the relative positions of the multiplet components. Satellites of all three spectra would seem to be produced by shake-up, rather than Coster-Kronig processes. The positions and forms of these satellites are consistent with a model in which spectator vacancies in the 4d band exist in both the initial and final-states of the Auger transition.

Physical Review B 58 (24), 16103-16109, 1998

**A 067 - 98 Electrochromism in MoOx Films Characterized by X-Ray Electron Spectroscopy.**

Tersio G. Souza Cruz, A. Gorenstein, Richard Landers, George G. Kleiman, Sandra C. de Castro.

The ability of molybdenum oxide thin films to reversibly exchange lithium ions (with an electrolyte) and electrons (with an external circuit) has been explored in optical electrochromic devices. The as-grown films are either transparent or slightly blue and show a deep blue color upon Li<sup>+</sup>/e<sup>-</sup> insertion. The thin film electronic band and crystallographic structure govern the kinetics of insertion reaction and the charge capacity of the material, as well as the optical behavior of the system. In this work, molybdenum oxide thin films were produced by r.f. reactive sputtering of a metallic molybdenum target in an O<sub>2</sub>-Ar atmosphere. Thin films with distinct compositions, were obtained by varying the oxygen flow ( $f$ ) during deposition and maintaining all other deposition parameters constant. Lithium intercalation was promoted by electrochemical means, from an aprotic, Li<sup>+</sup> containing electrolyte. The films of distinct compositions were analysed by x-ray photoelectron spectroscopy in order to investigate the relation between MoO<sub>3</sub> reduction and the electrochromic effect reported in the literature<sup>1</sup>. Data obtained on high oxygen flow samples show narrow Mo 3d lines, with binding energies characteristic of the 6+ state. Lowering the oxygen flow results in very broad 3d lines, indicating the presence of Mo<sup>6+</sup>, 5+ and 4+. This broadening of the 3d lines is also observed upon Li intercalation in high flow samples both on as-grown films and on films intercalated with Li<sup>+</sup>/e<sup>-</sup>.

Journal of Electron Spectroscopy and Related Phenomena 101-103, 397-400, Jun 1999

**A 068 - 98 Photon Energy and Core Hole Lifetime Dependences of Ag High Energy Auger Satellites.**

J. Morais, A. de Siervo, R. Landers, S. G. C. de Castro and G. G. Kleiman.

Understanding metallic response to the presence of a dynamic, localized perturbation, such as a finite lifetime core hole, has been the theme of many studies. Although, in XPS of such metals as Ni and Pd, shake-up satellites are common, in Auger spectroscopy, an intrinsic laboratory of many-body effects, the most extensively studied metal, Cu, manifest LVV satellites which are associated with Coster-Kronig (CK) transitions. Unambiguously identified shake-up satellites have been observed in the L123M45M45 spectra of the 4d metals, studied with conventional X-Ray sources and, in the L3 threshold region, with synchrotron radiation. There remain questions concerning the origin of these satellites and their relation to the corresponding XPS spectra. Here, we report a study of the Ag L23 M45M45 spectra as a function of photon energy and demonstrate the evolution of the satellite spectra. The change of the satellite shapes with photon energy is directly related to the validity of the sudden approximation. Correlation of the satellite spectra with core level lifetime indicates the influence of core hole dynamics. From the experimental systematics, it becomes clear that isolation of Ck effects is very difficult.

Surface Science 433-435, 878-881, Ago 1999

**A 069 - 98 Search for Disoriented Chiral Condensate in cosmic g - hadron families.**

C. R. A. Augusto, S. L. C. Barroso, V. Kopenkin, M. Moriya, C. E. Navia and E. H. Shibuya.

We present a systematic study on large asymmetries in neutral pion fraction distribution in high energy cosmic ray families ( $100 \text{ T eV} < E_{\text{vis}} < 700 \text{ T eV}$ ) detected at high mountain altitude at the Pamirs (4300m, 595g/cm<sup>2</sup>). With this purpose we have constructed robust observables, ratios of factorial moments, in experimental and simulated families in a similar way. We have found that our experimental data do not exclude the possibility of DCC formation mechanism in high energy interactions.

**A 070 - 98 Weighted Oscillator Strengths and Lifetimes for the Si VI Spectrum.**

L. H. Coutinho and A. G. Trigueiros.

The weighted oscillator strengths (gf) and the lifetimes for Si VI 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-squares 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 lifetime values that are closer to the experimental ones. In this work we presented all the experimentally known electric dipole Si VI spectral lines.

**The Astrophysical Journal Supplement Series 121 (2), 591-597, Abr 1999**

**A 071 - 98 Weighted Oscillator Strengths and Lifetimes for the Si X Spectrum.**

G. H. Cavalcanti, F. R. T. Luna, and A. G. Trigueiros

The weighted oscillator strengths (gf) and the lifetimes for Si X 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-squares 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 lifetime values that are closer to the experimental ones. In this work we presented all the experimentally known electric dipole Si X spectral lines.

**Journal of Quantitative Spectroscopy and Radiative Transfer 64 (1), 5-13, 1998**

**A 072 - 98 The Subimplantation Model for Diamond-like Carbon Films Deposited by Methane Gas Decomposition.**

R. G. Lacerda and F.C. Marques.

In this work, the formation of hard a-C:H films deposited on the cathode of a rf-sputtering system through the methane gas decomposition was explained using the subimplantation model. Even though in a rf plasma deposition the ions striking the films surface are not monoenergetic, the stress data matches the theoretical model proposed by C. A. Davis. The stress vs. bias plot shows a behavior similar to those already obtained for ta-C and ta-C:H films, which are prepared using monoenergetic ion beam.

**Diamond and Related Materials 8, 495-499, 1999**

**A 073 - 98 Cross Sections for Rotational Excitations of NH<sub>3</sub>, PH<sub>3</sub>, AsH<sub>3</sub> and SbH<sub>3</sub> by Electron Impact.**

Marcio T. do N. Varella, Marcio H. F. Bettega, Antonio J. R. da Silva, and Marco A. P. Lima

We report elastic and rotationally inelastic cross sections for e<sup>-</sup> - XH<sub>3</sub> collisions (X: N, P, As, Sb), at the static-exchange level of approximation. The energy range was from 7.5 up to 30 eV. Our fixed-nuclei scattering amplitudes were obtained through the Schwinger Multichannel Method with Pseudopotentials (SMCPP) (M. H. F. Bettega et al. Phys. Rev. A 47, 1111 (1993)). The rotational cross sections were obtained with the help of the adiabatic-nuclei-rotation approximation. There is good agreement with available experimental elastic cross sections. In order to improve rotational cross sections at small scattering angles for the dipole-allowed 00 → 10 rotational excitation, we have combined the SMCPP and the First Born Approximation of the full interaction potential and also of the dipole moment potential. To our knowledge this is the first time that rotational excitation cross sections for these molecules are reported.

**A 074 - 98 Observation of Coherent Hybrid Reflection with Synchrotron Radiation.**

S. L. Morelhão, L. H. Avanci, M. A. Hayashi, and L. P. Cardoso.

High resolution synchrotron radiation has been used to investigate the occurrence of coherent hybrid reflections (CHR) in the In<sub>0.49</sub>Ga<sub>0.51</sub>P/GaAs(001) structure. Several f scans at the 002 layer reflection were carried out. The scanned f intervals are correlated by the [001] axis symmetry and should present the same pattern. A break in the symmetry is observed due to constructive/destructive interference of the hybrid amplitudes with the amplitude from the 002 layer reflection. The effects of substrate miscut and interface distance are taken into account to explain the observed patterns. The application of CHR as a high sensitive tool to analyze epitaxial growth is discussed.

**Applied Physics Letters 73 (15), 2194-2196, 1998**

**A 075- 98 High Resolution Synchrotron Radiation Renninger Scan to Examine Hybrid Reflections in InGaP/GaAs(001).**

M. A. Hayashi, L. H. Avanci, L. P. Cardoso, J. Bettini, M. M. G. de Carvalho, S. L. Morelhão and S. P. Collins.

High resolution Synchrotron radiation Renninger scans (RS) have been used in the analysis of hybrid reflections in the InGaP/GaAs structure. Four-beam cases involving two Bragg (primary and secondary) and one Laue (secondary) reflections of the 002 Renninger scans for the GaAs substrate and the InGaP layer were analyzed in detail. Different structures of asymmetry regarding the in-plane directions [110] and [10] were observed from the measurements of the same three families of four beam cases, {1}/13, {20}0/{20}2 and {3}/33, at several f positions. The comparison between the experimental and MULTX simulated scan clearly shows a marked asymmetry observed on the {20}0/{20}2 contributions. An asymmetric peak instead of the simulated dip appears due to the layer Laue secondary beam {20}0 crossing the layer/substrate interface to generate a hybrid peak. The break in the lattice coherence for this heterostructure is shown by the occurrence of an unexpected dip in the layer RS, which does not obey the mirror symmetry.

**Journal of Synchrotron Radiation 6, Parte 1, 29-33, Jan 1999**

**A 076 - 98 Piezoelectric Coefficients of mNA Organic Nonlinear Optical Material Using Synchrotron Radiation X-Ray Multiple Diffraction.**

L. H. Avanci, L. P. Cardoso, S. E. Girdwood, D. Pugh, J. N. Sherwood and K. J. Roberts.

In this paper, distortions produced in the unit cell of a nonlinear organic crystal under the influence of an applied electric field, E, are investigated by using synchrotron radiation x-ray multiple diffraction (MD). The method is based in the inherent sensitivity of this technique to determine small changes in the crystal lattice which provide peak position changes in the MD pattern (Renninger scan). A typical Renninger scan shows numerous secondary peaks, each one carrying information on one particular direction within the crystal. The (h k l) peak position in the pattern, for a fixed wavelength, is basically a function of the unit cell lattice parameters. Thus, small changes in any parameter due to a strain produced by E give rise to a corresponding variation in the (h k l) peak position and the observed strain is related to the inverse piezoelectric effect. The advantage of this method is the possibility of determining more than one piezoelectric coefficient from a single Renninger scan measurement. The method has been applied to the mNA (meta-Nitroaniline, orthorhombic, point group mm2) crystal and we were able to determine three piezoelectric coefficients: |d<sub>31</sub>| = 7.3(1) x 10<sup>-11</sup> mV<sup>-1</sup>, |d<sub>32</sub>| = 16.5(7) x 10<sup>-11</sup> mV<sup>-1</sup> and |d<sub>33</sub>| = 10.3(8) x 10<sup>-11</sup> mV<sup>-1</sup>.

Physical Review Letters 81 (24), 5426-5429, 1998

A 077 - 98 Multilevel Granular Structure and its Coupling Distribution in Melt Textured YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-d</sub>.

F. M. Araújo-Moreira and W. A. Ortiz and O. F. de Lima.

We have performed AC magnetic susceptibility measurements as a function of the excitation magnetic field,  $h$ , for two YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-d</sub> polycrystalline samples using a high sensitivity homemade susceptometer, for fixed values of the temperature,  $T$ , and the external DC magnetic field,  $H$ . One of the samples is melt-textured and for  $H < 52.5$  Oe it presents features that can be associated with a multilevel granular structure. Using an effective medium model we have determined the critical current density distribution associated with the multilevel granular structure. The average critical current density in each intergranular region was then calculated by applying Bean's critical state model.

Physica C 311 (1-2), 98-106, 1998

### ACCEPTED PAPERS FOR CONFERENCE PRESENTATION

C 028 - 98 Decreasing the Superconductivity Suppression Power of Pr in RE:123 Compounds by Isolating the Same from Cu-O Conduction Band.

V. P. S. Awana and O. F. Lima

We present the results of structural (X-ray and Neutron diffraction), superconductivity (AC susceptibility), magnetic (DC moment) and thermal properties of several of Pr substituted distorted RE:123 compounds, such as (Y/Pr)BaSrCuO(YBaSr:123), (La/Pr)BaCaCuO(La:1113) and (Nd/Pr)BaCaCuO(Nd:1113). We observed that the suppression of superconductivity due to Pr in all these systems is less in comparison to their RE:123 counter parts, i. e in Pr substituted Y:123, La: 123 and Nd:123. Interestingly with full Pr substitution in RE:123 compounds, the Pr moments order antiferromagnetically at 17K, while in presently studied all three systems the same happens at around 10K, only. Antiferromagnetic ordering temperature of Pr moments, i. e the strength of Pr-4f orbital hybridisation with Cu-O conduction band has a direct relation to suppression of superconductivity. Our results show, that by various on-site substitutions or by modifying the parent unit cell of Pr:123 compound, in order to isolate Pr-4f magnetic interaction with Cu-O conduction band, one can achieve superconductivity. Several possible compounds are to be discussed as potential candidates to be superconducting with full Pr substitution in RE:123.

1999 University of Miami Conference on High Temperature Superconductivity, accepted on october 1998.

### BOOKS

L 001 - 98 On the Statistical Foundations of Irreversible Thermodynamics.

Roberto Luzzi, Áurea R. Vasconcellos, and J. Galvão Ramos

Berlin, TEUBNER VERLAG, 1998.

# Abstracta

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