

# Abstracta

Ano III - N. 10

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Trabalhos Aceitos para Publicação

A058-99 à A063-99

Trabalhos Aceitos para Publicação em Conferências

C006-99

**[A058 -99] "A Nonequilibrium Ensemble Formalism: criterion for truncation of description."**

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

In the framework of a nonequilibrium statistical ensemble formalism, consisting in the so-called Nonequilibrium Statistical Operator Method, we discuss the question of the choice of the space of thermo-hydrodynamic states. We consider in particular the relevant question of the truncation of description (reduction of the dimension of the state space). A criterion for justifying the different levels of truncation is derived. It depends on the range of wavelengths and frequencies which are the relevant ones for the characterization, in terms of normal modes, of the thermo-hydrodynamic motion in a nonequilibrium open system. Applications to the cases of thermal-sensitive resins and of n-doped polar semiconductors are done, numerical results are presented, and experimental observation is discussed.

Journal of Chemical Physics 112 (6), 2692-2700, 2000

**[A059 - 99] "On the Thermodynamics of Far-from-Equilibrium Dissipative Systems."**

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

We consider the question of the concepts of entropy and temperature in arbitrary nonequilibrium conditions in the framework of the so-called Informational Statistical Thermodynamics. This is the approach to Thermodynamics based on the statistical-mechanical foundations provided by a Gibbs ensemble-like algorithm in nonequilibrium situations. The resulting nonequilibrium temperature-like variable-dubbed as quasitemperature - is shown to be a quantity measurable with appropriate "thermometric devices". A comparison of quasitemperatures that arise in different approximated nonequilibrium statistical-thermodynamic descriptions of the dissipative systems is done. The validity of these different approximations is evaluated, and (in the framework of the theory) generalized Gibbs, Clausius, and Boltzmann's relations, as well as properties of the corresponding entropy-like function (or informational entropy in Jaynes-Shannon sense), that the theory introduces, are presented. Conceptual and physical aspects of the question are also discussed, and a partial comparison of these concepts with those arising in other approaches to irreversible thermodynamics is briefly attempted.

Fortschritte der Physik - Progress of Physics 47 (9-10), 937-964, 1999

**[A060 -99] "Hysteresis-like behaviour in meta-nitroaniline (mNA) crystals."**

L. H. Avanci, R. S. Braga, L. P. Cardoso, D. S. Galvão and J. N. Sherwood

In the present work we report for the first time an experimentally observed hysteresis-like variation of lattice parameter of the organic crystal mNA under the influence of an externally applied DC electric field. Calculations have been made to determine whether the main features of the hysteresis-like behavior can be explained in terms of the geometrical distortions of isolated mNA molecules or are dominated by molecular interactions. The results show that the main features of the non-linearity can be explained in terms of changes in the acceptor-donor properties of isolated mNA molecules.

Physical Review Letters 83 (24), 5146-5149, 1999

**[A061 - 99] "Early Cosmic Background."**

A. K. T. Assis, M. C. D. Neves

We discuss the measurements and calculations leading to early estimatives of the cosmic background radiation prior to Penzias and Wilson in 1965. These works were not based on the big bang nor on the expansion of the universe.

Astronomy &amp; Geophysics, accepted on October 1999.

**[A062 - 99] "Synchrotron Radiation X-ray Multiple Diffraction Applied to the Study of Electric Field Induced Strain in MBANP Organic Non-linear Optical Material."**

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

In this work, distortions produced in the unit cell of a MBANP [(-)-2-(a -metilbenzilamina)-5-nitropiridina] nonlinear organic crystal under the influence of an applied electric field, are investigated by using synchrotron radiation x-ray multiple diffraction (XRMD). 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 XRMD pattern (Renninger scan). The (hkl) 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 give rise to a corresponding variation in the (hkl) peak position and the observed strain is related to the piezoelectric coefficients. The advantage of this method is the possibility of determining more than one piezoelectric coefficient from a single Renninger scan measurement [L. H. Avanci, L. P. Cardoso, S. E. Girdwood, D. Pugh, J. N. Sherwood and K. J. Roberts, Physical Review Letters 81(24), 5426-5429 (1998)]. The method has been applied to the MBANP (monoclinic, point group 2) crystal and we were able to determine four piezoelectric coefficients:  $|d_{21}| = 0,2(1) \times 10^{-11}$  CN<sup>-1</sup>,  $|d_{22}| = 24,8(3) \times 10^{-11}$  CN<sup>-1</sup>,  $|d_{23}| = 1,3(1) \times 10^{-11}$  CN<sup>-1</sup> and  $|d_{25}| = 5,9(1) \times 10^{-11}$  CN<sup>-1</sup>. The measurements have been carried out at the SRS station 16.3, Daresbury Laboratory, Warrington, UK.

Physical Review B - Condensed Matter 61 (10), 6507-6514, 2000

**[A063 - 99] "Effect of Zn Substitution on Para-Ferro Transition Temperature in La<sub>0.67</sub>Ca<sub>0.33</sub>Mn<sub>1-x</sub>Zn<sub>x</sub>O<sub>3</sub> CMR Materials."**

V. P. S. Awana, E. Schmidt, E. Gmelin, A. Gupta, A. Sedky, A. V. Narlikar, O. F. Lima, C. A. Cardoso, S. K. Malik, W. B. Yelon

Structural, magnetic and thermal measurements are carried out on the La<sub>0.67</sub>Ca<sub>0.33</sub>Mn<sub>1-x</sub>Zn<sub>x</sub>O<sub>3</sub> system with

X= 0.0 to 0.50. The structural characterisation of the samples is done in terms of their lattice parameters, site occupancies, atomic positions, oxygen content and bond lengths by Rietveld analysis of their neutron diffraction patterns. Zn substitutes at Mn-site isostructurally until x = 0.30. Oxygen content remains nearly invariant with x. Magnetic and thermal measurements as well as the electrical resistance show a para-to-ferro magnetic transition at T<sub>p</sub>, which decreases with an increase of x. For low Zn concentration (until x = 0,075) the decrease dT<sub>p</sub>/dx is smaller than for the larger concentrations of Zn. Relative decrease dT<sub>p</sub>/dx at higher concentrations (x > 0.10) is similar to that observed earlier for the La<sub>0.67</sub>Ca<sub>0.33</sub>Mn<sub>1-x</sub>Zn<sub>x</sub>O<sub>3</sub> system. For the transition at T<sub>p</sub>, the related change of magnetic entropy (D Strs) are calculated from the heat capacity data and indicate that for x = 0 the expected value D Strs = 12.8 J/mol K is recovered.

Journal of Applied Physics 87, 5034-5036, 1999

## Accepted papers for conference presentation

[C006 - 99] "Structure Ultrafast Carrier Drift Velocity in Photoexcited Zincblende GaN."

C. G. Rodrigues, A. R. Vasconcellos, R. Luzzi, V. Lemos, V. N. Freire

A theoretical study is performed on the ultrafast transient transport properties of photoexcited carriers in zincblende GaN subjected to electric fields up to 120 kV/cm. Depending on the photoexcitation degree, the subpicosecond electron and heavy-hole drift velocity evolution towards the steady state presents maxima and minima, e. g. a structured transient. Since nonequilibrium phonon effects are not included, the structured ultrafast carrier drift velocity is explained through the crossover of the evolution curves for the transport and momentum relaxation times, whose definition is based on the nonequilibrium variables used to describe the systems.

In: Proceedings of International Conference on Silicon Carbide and Related Materials, North Carolina, USA, Oct, 1999

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# Abstracta

Instituto de Física

Diretor: Prof. Dr. Carlos H. de Brito Cruz

UNICAMP

Cidade Universitária Zeferino Vaz

13083-859 - Campinas - SP - Brasil

e-mail: [secdir@ifi.unicamp.br](mailto:secdir@ifi.unicamp.br)

Fone: OXX 19 3521 - 5300

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Biblioteca do Instituto de Física Gleb Wataghin  
<http://webbif.ifi.unicamp.br>  
Diretora Técnica: Rita Aparecida Sponchiado

Elaboração  
Tânia Macedo Folegatti  
[abstract@ifi.unicamp.br](mailto:abstract@ifi.unicamp.br)

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