Poster Session Afternoon (14h30 - 16h)

INSTRUMENTATION

[13/05/10 - P016]
Pressure cell for XPD, XAS and SAXS experiments using Synchrotron Light, C. A. C. Passos, M. T. D. Orlando, V. A. Rodrigues Jr., J. L. Passamai Jr., *Universidade Federal do Espírito Santo, Vitória, ES, Brasil*, L. G. Martinez, J. L. Ross, *Instituto de Pesquisas Energéticas e Nucleares, SP, Brasil*, H. P. S. Corrêa, *Universidade Federal do Mato Grosso do Sul, Campo Grande, MS, Brasil*, F. Garcia, *Laboratório Nacional de Luz Síncrotron, Campinas, SP, Brasil*, F. C.L.de Melo, *Centro Técnico Aeroespacial - IAE - São José dos Campos - SP - Brasil*, F. G. Souza Jr., *Instituto de Macromoléculas Professora Eloisa Mano - IMA/UFRJ* ■ A high pressure CuBe cell with B4C anvil has being developed since 2004 for small- and wide-angle synchrotron x-ray scattering experiments under hydrostatic pressure up to 2GPa, at room temperatures. Recently, an optimized version of this cell was used to measure the pressure effect on structure of Cardanol-Furfural-PAni Green Blend in SAXS beam line at Laboratório Nacional de Luz Sincrotron - LNLS - Campinas . This cell has also been applied to investigate solid samples behaviour under external hydrostatic pressure since 2007 at LNLS. Moreover, it might also be used to investigate biological system as lipid-water dispersions without changes in its design. Magnetic field up to 1.6 kGauss can be applied together the hydrostatic pressure in this cell, taken into account there is no magnetic signal from de CuBe, B4C anvil, and CuBe gasket used. Investigations about ReO2 behaviour under hydrostatic pressure up to 1.6 GPa were performed at LNLS-XPD and XAFS Synchrotron beam line, and the results revealed to be the ReO2 a good inner gauge pressure for 8keV-13keV energy range. This project has been developed by LNLS, UFES, IPEN/CNEN and IEA/CTA collaboration.

Acknowledgements: We would like to thank CNPq Grant 471536-2004-0, CT-Energ 504578-2004-9, and CAPES for financial supports. Thanks also to Cia. Vale do Rio Doce (CVRD), Cia Siderurgica de Tubarao (AcelorMittal), and National Laboratory of Synchrotron Light - LNLS, Brazil (XPD 2950-04, XPD 4742-05, XPD 5720-06, DXAS 2950-04, DXAS 2952-04, DXAS 5741-06, D02A - SAXS2 8519/09).

[13/05/10 - P017]
Frequency Raman Shift due to edge/surface effect, Sanclayton Geraldo Carneiro Moreira, Cláudio Márcio Rocha Remédios, Jordan Del Nero, Petrus Alcântara Jr., *Universidade Federal do Pará* ■ The Raman spectroscopy is worldwide used in the several scientific areas as an important technique to characterization of the materials. Many theoretical models were developed to obtain the observed vibrational modes in the materials. Due to microscope to be coupled to Raman spectrometer it was possible to do surface and edge effect analysis with more precision through MicroRaman spectroscopy. Here we present the experimental results by MicroRaman spectroscopy in KDP crystals applied to investigate the Raman spectrum differences, between internal and external parts of the sample. The KDP crystal was chose due to high crystalline quality and also because its modes to be very good known, as well. To Raman Spectroscopy we have used a iHR-320 System (non-polarized) manufactured by HORIBA Jobin Yvon. The system has, internally, a He-Ne laser at 632 nm with 17 mW of power and a thermoelectric cooled CCD camera (model synapse) as a detector of the signal. The KDP sample was cut and polished in parallelogram shapes with 3 x 4 x 4 mm3. The Raman spectra were obtained at different parts of the sample, starting (external part) up to bulk. The internal molecules of the sample has under different potential from that external molecules because of it molecules are trapped differently in the crystalline lattice. The crystal is formatted by um repetitive primitive cell but in the edge region crystal all molecules have one side free that is the end of the limited sample. The molecules situated around the edge region not are trapped with the same potential of them situated in the bulk region. Therefore, the phonons relate close to edge molecules present a shift to low frequencies. Analyzing the Raman spectra we observe a frequency decrease of the 7 cm-1 approximately only for PO4 stretching. For other Raman mode none was observed any shift. Simple mass-spring models applied to the molecules explain very well the observed result.

[13/05/10 - P018]
Characterization of crystal structure with simultaneous X-ray topography and rocking-curve, Irineu Mazzaro, , Kelin Regina Tasca, Cesar Cusatis, *Universidade Federal do Paraná* ■ Crystal characterization is of great importance for use and application in the recent technological advances as well to improve the process of obtainment and growth. In this work we present a method for crystal characterization and defect analysis, that can be performed with conventional x-ray tube, up o micrometer spatial resolution. The method is based on the combination of X-ray diffraction topography and rocking curve analysis, a method called "rocking-curve imaging". It's a non-destructive method which can be applied, for example to semiconductors wafers. For each angular position of the rocking curve an image (topography) of the sample illuminated by the X-ray beam is obtained. The intensities registered by each pixel corresponds to a small sample area and it can be used to show the kind of defects, on each point of the sample, like local d-spacing variations, strains and curvature. It's possible to determine the maximal and integral peak intensities, the peak angular position and the half width of the rocking-curves of the whole sample with micrometer resolution depending on the CCD camera resolution. It's possible to establish a correlation between the microscopic defects and the macroscopic effects. It can be done with conventional sources and the limitation is due the CCD camera resolution used as a detector. The first