Poster Presentation

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Pair distribution function analysis at the Brazilian synchrotron light source

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The XDS beamline of the Synchrotron Light National Laboratory (LNLS), was designed to take advantage of the 4T superconducting multipole wiggler inserted in the storage ring. This multipurpose beam line is employed for X-ray diffraction and X-ray absorption spectroscopy in the energy range between 5 and 30 keV. The X-ray diffraction patterns can be acquired in two different arrangements: a) Bragg-Brentano configuration, using a scintillation detector with an analyzer and b) Debye-Scherrer configuration, where the sample is mounted into capillaries and the diffraction pattern is acquired with an arrangement of 6 Mythen detectors or a scintillator. The sample can be measured at different atmospheres and temperatures. The viability of the beamline for pair distribution function analysis (PDF) was tested measuring two different standards: 1) Al2O3 and 2) BaTiO3. The patterns were acquired at room temperature using the two detection setups at an energy of 20 keV. The samples were mounted inside 0.3 mm boron-rich glass capillaries. In addition to the sample pattern, we also measured the empty capillary (background) to subtract it to the sample data. The acquired and normalized patterns were converted into total scattering PDF (G(r)) with the PDFgetX3.[1] The experimental G(r) was fitted with the PDFgui.[2] Both data sets were fitted in the corresponding structural phase with cell parameters close to the ones reported in the literature. In the special case of the BaTiO3 sample, it was very carefully modeled. We particularly focused in evaluating if we can discriminate the correct structural phase, as this sample presents different phases (orthorhombic, tetragonal and cubic). We could identify that the sample, at room temperature, was at the expected tetragonal phase. Finally, we will present a preliminary analysis of the following systems: Pb1-xRxZr1-yTiyO3 (R=La&Ba) and Ba1-xRxZr1-yTiyO3 (R=La&Ca) at the ferro- and paraelectric states by PDF.

[1] *P. Juhás, et al., J. Appl. Cryst., 2013, 46, 560-566,* ***[2]*** *C.L. Farrow, et al, J. Phys.: Condens. Matter, 2007, 19, 335219*

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