Electronic Structure of $PbZr_{0.52}Ti_{0.48}O_3$ Thin Films by X-ray Absorption Spectroscopy

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The electronic structure of RF magnetron sputtering grown variously oriented [i.e. <001> (tetragonal), <101> (monoclinic) and <111> (rhombohedral)] $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) thin films have been studied by the Polarization-dependent x-ray absorption near edge structure (XANES) spectroscopy using the Ti *K*-edge, Ti & Zr $L_{3,2}$-edge. The photo induced XANES intensities at Ti *K*-edge and Ti/Zr $L_{3,2}$-edges shows clear difference in between absorption spectra taken at = 0^0 (normal incidence) and 70^0 (near parallel incidence) corresponds to the polarization in the *ab* and *c* plane polarizations respectively. In Ti *K*-edge XANES spectrum of <001> oriented PZT film shows that the edge is slightly shifted at higher energy (~1.4 eV) from the <101> and <111> oriented PZTs that reflects the change of effective valence of the Ti atom due to the influence of the electric charge on the surrounding oxygen as the ligand. Different pre-peaks and their intensity variations in Ti *K*-edge XANES spectra of all PZTs, clearly accompany the degree of ferro-electricity in the perovskite structure, signature of quadrupolar transitions to the localized e_g and t_{2g} *d*-like states. Splitting of e_g and t_{2g} sub-bands in the L_3- and L_2-edge respectively is also observed at the Ti and Zr $L_{3,2}$-edge XANES spectra that gives direct measurements of crystal field splitting.

Reference: Ray *et al.* Mater. Lett. **60**, 1714 (2006).

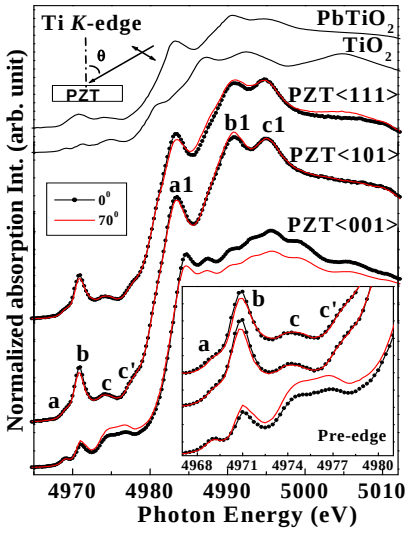

Figure 1. Ti *K*-edge XANES spectra

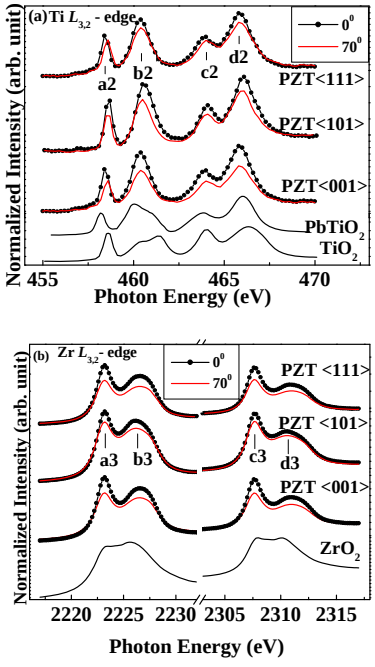

Figure 2. (a) Ti $L_{3,2}$-edge XANES and (b) Zr $L_{3,2}$-edge XANES Spectra