

SMP044-08

Room:301B

Time:May 25 12:00-12:15

Comparison in temperature dependence of Ti K edge XAFS spectrum for PbTiO₃,PZT, ATiO₃ compounds (A=Mg,Ca,Sr,)

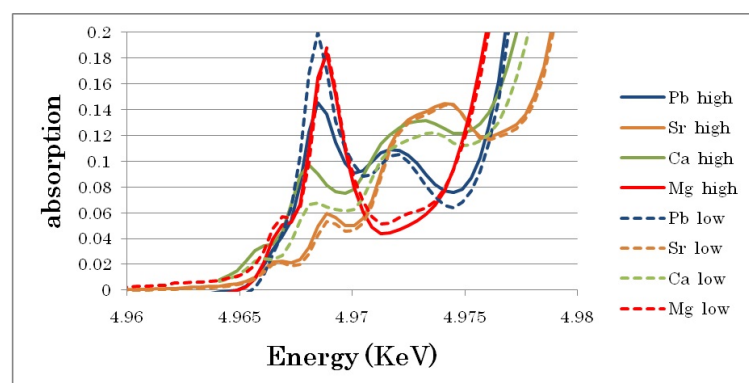
Tomotaka Nakatani^{1*}, Tatsuya Hiratoko¹, Maki Okube², Takashi Takeda³, Kei-ichirou Murai⁴, Akira Yoshiasa¹

¹Kumamoto University, ²Institute of Technology, ³National Institute for Materials Science, ⁴Tokushima University

Ti k-edge X-ray absorption near edge structure (XANES) spectra of PbTiO₃ and various titanates such as ATiO₃ (perovskite- and ilmenite-type structure, A=Mg,Ca,Sr,Ba,) were measured at various temperatures up to 1100 K. The composition, local structure and temperature dependence of XANES spectra was investigated especially on the phase transition. Ti atoms are located in TiO₆ octahedral sites for the all samples. Ti k-edge XANES spectra change largely with different compositions, while the temperature dependence of XANES spectra is small in the each compound even if undergoing structural phase transition. Perovskite-type ATiO₃ compounds reveal several phase transitions. SrTiO₃ and PbTiO₃ perovskite undergo structural phase transition in the temperature ranges in this study, SrTiO₃; rhombohedral-tetragonal-cubic, PbTiO₃; tetragonal-cubic, weak but distinct changing of the XANES spectra was observed near phase transition point. These structural transitions of perovskite are caused mainly by rotation and distortion of TiO₆ octahedron. Pre-edge feature and local structure around Ti atom is little changing by rotation of octahedron. The distinct changing of pre-edge XANES spectra was observed at some transition points. Five pre-edge peaks can be identified: pp(a) 4.9667eV, pp(b) 4.9687eV, pp(c) 4.9727eV, pp(d) 4.9747eV and pp(e) 4.9796eV. The temperature dependence for each pre-edge peaks is largely different in temperature and local structure [1]. The different behaviors of the pre-edge intensity suggest that the increase and decrease of X-ray absorptivity at various temperatures is fluctuated by the hybridized orbital proportion and local symmetry.

References

[1] Hashimoto T., Yoshiasa A., Okube M., Okudera H. and Nakatsuka A., Temperature dependence of XANES spectra for ATiO₃, A₂TiO₄, and TiO₂ compounds with structural phase transitions, The American Institute of Physics, Conf. Proc. Vol.882 AIP Melville, NY, (2007) pp. 274-276.



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