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Temperature dependence of XANES spectra for BaTiO3, SrTiO3 and TiO2 with structural phase transitions

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BaTiO3 is perovskite structure and has good physical properties as industrial material. The main constituent (MgSiO3CaSiO3) of the lower mantle is the same structure. Therefore, BaTiO3 has been intensively studied for a long time. But BaTiO3 had not been so researched by using X-ray absorption near edge structure (XANES) spectra. XANES spectra of BaTiO3, SrTiO3 perovskite and TiO2 rutile and anatase were measured at various temperatures. The composition, structure and temperature dependence of XANES spectra was investigated especially on the phase transition. The appropriate amount of fine powder sample and boron nitride powder was mixed and pressed into pellet of <0.2 mm I thickness and 10.0 mm in diameter. All samples had edge-jumps with 0.7 . The measurements of Ti k-edge XANES spectra were carried out in transmission mode at beam line BL-9A of the Photon Factory in KEK, Tsukuba. X-ray absorption measurements in the temperature range from 20K to 800K were made under a helium atmosphere. The XANES spectra for TiO2 were largely different between anatase and rutile structure, although these two compounds have the same composition. Ti K-edge XANES spectra changed largely with different compositions, while the temperature dependence of XANES spectra is small in each compound even if undergoing structural phase transition. Perovskite-type ATiO3 compounds reveal several phase transitions. SrTiO3 and BaTiO3 perovskite undergo several structural phase transitions in the temperature ranges in this study, SrTiO3; rhombohedral-tetragonal-cubic, BaTiO3; trigonal-orthorhombic-tetragonal-cubic, the distinct changing of pre-edge XANES spectra was observed near transition points. Ti atoms are located in TiO6 octahedral site for the all samples, but Ti k-edge XANES spectra changed largely with different compositions

Keywords: XANES, BaTiO3, Perovskite, Phase transition