Pressure-induced Structure Change of Ferroelectric $KNbO_3$ using SR

Takamitsu Yamanaka[a], Taku Okada[a], Kenji Ohi[a], Yuki Nakamoto[b], [a]*Department of Earth and Space Science, Osaka University.* [b]*Kyokugen Extreme Research Center Osaka University*. E-mail: yamanaka@hpc.cmc.osaka-u.ac.jp

$KNbO_3$ is a perovskite-type ferroelectrics. It exhibits three structural transitions with increasing temperature at ambient pressure: rhombohedral -to- orthorhombic -to- tetragonal -to- cubic phase. The cubic phase is paraelectric, and the other three phases are all ferroelectric. The polymorphic structure transitions of $KNbO_3$ were studied under high pressure using synchrotron radiation at BL-18C, KEK with diamond anvil cell (DAC). These transition pressures were determined by profile analyses of powder diffraction data using a long wavelength . λ=0.92 Å and long film distance 500 mm. The orthorhombic -to- tetragonal transition takes place at about 6.0 GPa and the tetragonal-to- cubic transition causes at about 9.0 GPa. These transition pressures are consistent with the result of our previous dielectric measurement under compression[1]

Single crystal diffraction studies under various pressures using a new DAC [2] installed in four-circle diffractometer at BL-10A, KEK at ambient temperature: orthorhombic (Cm2m, z=2) at 0.0001, 1.6, 4.8, 5.7GPa; tetragonal (P4mm, z=1) at 6.5, 7.9GPa; cubic (Pm3m, z=1) at 9.4, 12GPa. Diffraction intensities were measured using wavelength λ=0.7004 Å, collimator 100 μm and Φ-fix mode. Reliabilities of all structure refinements including isotropic temperature factors are within R=0.04. Deformation and volume compressibility of polyhedra in each perovskite-type structure are finely analyzed in order to comprehend the dielectric property. Anisotropy in their ferroelectric property is clarified and an increase in the ferroelectricity with pressure is also elucidated.

[1] Kobayashi Y., et al., *Phys. Rev*., 2000, **B61**, 5819. [2] Yamanaka T., et al., *Rev. Sci. Inst*., 2001, **72**, 1458.

Keywords: $KNbO_3$, high pressure, ferroelectrics