MS41.O05

Electron density, d-p hybridization and dipole moment of PbTiO3 and BaTiO3

T. Yamanaka[1,2], Y. Nakamoto[2], M. Ahart[1], H. Mao[1], R. Hemley[1]

[1]Carnegie Institution of Washington, Geophysical Laboratory, Washington DC, USA, [2]Osaka University, Quantum Science Technology under Extreme Conditions, Osaka, Japan

Present experiment first reveals electron density (ED) distributions and split atomic displacements of ferroelectrics PbTiO3 (PTO) and BaTiO3 (BTO) by high-resolution x-ray single crystal diffraction study under high pressures using maximum entropy method (MEM). Diffraction measurements were carried out using a four-circle diffractometer installed at BL-10A Photon Factory, KEK, Japan. *** ED observed by FMEM(h) illustrates the d-p pai-bond resulting from the hybridization of Ti 3d and O 2p orbitals. The split atom distribution is generated from the dynamical disorder (static time and space average) due to the thermal vibration of atoms in the [001] direction of these crystal structures. The split distributions of Ti and O are clearly disclosed in the tetragonal ferroelectric PTO and BTO. The ferroelectric pseudo-particle occupies double-well potential. The feature disappears in the cubic paraelectric phase and electron density is more localized with increasing pressure in the cubic phase. *** Effective charges of atoms in PTO and BTO are evaluated from the least-squares refinement based on diffraction intensities. Using the pseudopotential model, inner-core electrons are frozen with bonding effects, but only valence electron clouds are deformed due to coordination and thermal vibration of atoms. The pressure dependence of the dipole moment (l) is calculated by the effective charge (q) and atomic deformation Δr. The dipole moment of ferroelectric materials is derived from the spontaneous polarization Ps (= ρ l = ρNΔr). Pressure dependences of dipole moments of PTO and BTO are first experimentally determined by observed effective charge q and Δr from their structure refinements. The dipole moment of PTO is much larger than BTO, which implies the difference in the dielectricity of these ferroelectrics. The result is consistent with the dielectric measurement.

[1] *T. Yamanaka, T. Okada, and Y. Nakamoto, Phys. Rev. B 80, 094108 (2009).*

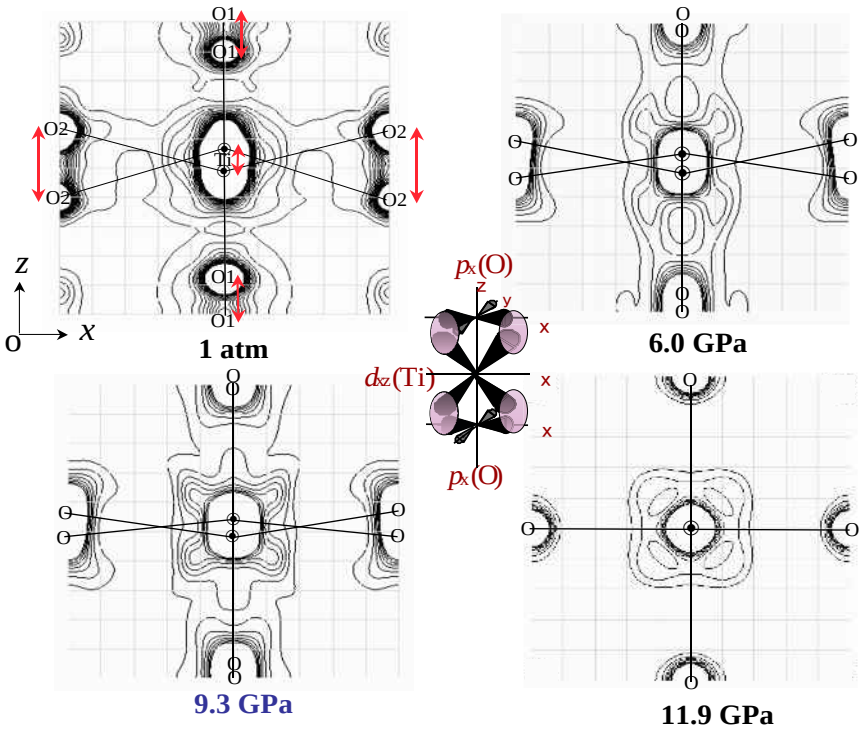

Fig. 2
Yamanaka

Keywords: ferroelectrics of PbTiO3 and BaTiO3, d-p hybridization, split atom distribution