Symmetry change effect on dielectricity in KNbO3-perovskite under high-pressure

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Potassium niobate (KNbO3) is one of the most famous ferroelectrics belonging to the barium titanate (BaTiO3) family with perovskite-type structure and also has piezoelectricity. On heating at ambient pressure, the rhombohedral phase transforms to the orthorhombic, then to the tetragonal, and finally to the cubic phase at 263, 498 and 708 K, respectively. Under pressure, the results reported hitherto are complicated and contradict one another, which means that high-precision measurements are required for analyzing structure change.

Our powder diffraction experimental results locate the orthorhombic-tetragonal transition in the 5.5-7.0 GPa range and tetragonal-cubic transition in the 8.6-9.8 GPa range. Based on the single crystal X-ray structure analyses, we calculated observed tolerance factor and distortion parameter. From the relation between distortion parameter and the dipole moment, it was clarified that the distortion of NbO6 octahedron is important to the spontaneous polarization.