Electric-field-induced Polarization Rotation in $PbZb_{0.5}Ti_{0.5}O_3$ Revealed by *in-situ* Pair Distribution Function Study

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$PbZb_{1-x}Ti_xO_3$ (PZT) shows excellent piezoelectric and dielectric properties near the morphotropic phase boundary (MPB). Electric-field-induced polarization rotation is thought to be one of the mechanisms explaining such a large piezoelectricity [1-2]. This type of polarization rotation was experimentally observed in Pb-based single crystals of different compositions [3-4]. However, evidence for the polarization rotation in polycrystals has not yet been reported. In order to observe polarization rotation in PZT ceramics, we investigated the local structural behavior of $PbZb_{0.5}Ti_{0.5}O_3$ (PZT 50/50) piezoceramics during application of electric fields using pair distribution function (PDF) analysis. In the present work, *in-situ* synchrotron X-ray total scattering was conducted, and the PDFs were converted from the total scattering pattern. The PDF refinement of the zero-field data suggests a model with [001] Ti displacement and negligible Zr displacement is in good agreement with the experimental data. The directional PDFs of different fields indicate the bond length of the nearest Pb-*B* pair changes significantly with the field (Figure 1). We suggest the changes in Pb-*B* bond length can be dominantly caused by the polarization rotation, by calculating the radial distribution functions (RDFs) of a model with the Ti displacement rotating in (110) plane and comparing the trend in the calculated and the experimental RDFs. Peak fitting of the RDFs was also conducted, which suggests that Zr atoms start to displace under the electric field besides the polarization rotation.

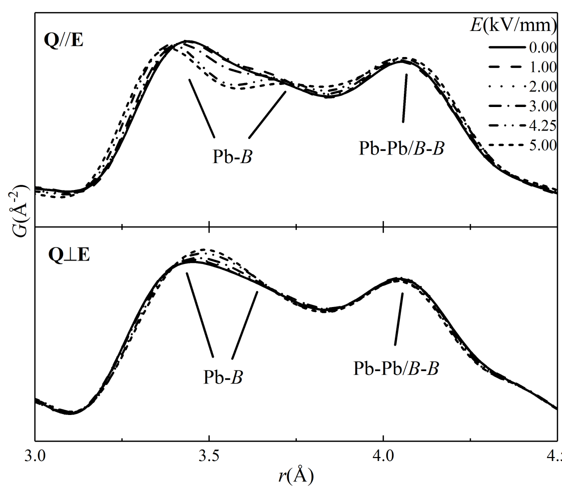

Figure 1. Low-*r* part of the directional PDFs in the directions parallel and perpendicular to the field. **Q** denotes the momentum transfer, and **E** represents the electric field.

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