

Oral Contributions

[MS34 - 03] In-situ neutron diffraction on ferroelectrics under electric field

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Neutron diffraction studies on technical ferroelectric ceramics under the influence of electric field were performed to establish correlations between the macroscopic poling behaviour and corresponding structural changes. Investigations were carried on bulk samples of lanthanum doped lead zirconate titanate ($\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$) with different Ti/Zr ratios as well as on different compositions of the system $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3 - \text{BaTiO}_3 - \text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$. Neutron diffraction studies were performed at the high-resolution powder diffractometer SP0DI (FRM II) and the materials science diffractometer STRESS-SPEC (FRM II). Different set-ups were used with the electric field direction either perpendicular to the scattering plane or within the scattering plane. The first set-up is suitable for conventional Rietveld refinement of structure parameters while the latter configuration allows the analysis of texture and strain effects. Using the “vertical set-up”, changes in the response to the electric field were observed for different compositions. Distributions of atomic displacements in the electric field were

reflected by thermal displacement parameters. The data corresponding to the “horizontal set-up” allow Rietveld analysis by taking into account texture and strain parameters besides the structural parameters and phase fractions (space groups R3m, P4mm). For a more specific study of domain switching processes in a commercial actor (based on lead zirconate titanate, space group P4mm), pole figures were collected under the influence of an electric field. A robot was used to orient the sample cell. A fibre texture could be deduced from the radial symmetries in the pole figures of (002) and (200) reflections. In two compositions of the system $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3 - \text{BaTiO}_3 - \text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$, the large field induced macroscopic strain could be explained by a phase transformation during the poling process. In both cases the transition to a rhombohedral phase was identified by corresponding superlattice reflections, arising from a superstructure in the tilting angles of the oxygen octahedra around Ti/Nb atoms.

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