Crystal symmetry and domain structure of morphotropic Pb(Zr,Ti)O$_3$-ceramics

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Abstract

For technical applications based on the piezo- and ferroelectric effect the most common material used is PZT (Pb(Zr$_{1-x}$Ti$_x$)O$_3$). While the processing and tuning of the material for different applications is mastered, there is still ambiguity in the understanding of the origin of the strong piezoelectric effect in this material. So far the coexistence of tetragonal and rhombohedral structure in proximity of the morphotropic phase boundary (MPB) [1] and the possible field induced phase transition was supposed to be responsible for the excellent properties. About ten years ago [2], based on high resolution x-ray powder diffraction data, a monoclinic structure proposal was made, the monoclinic phase. Nevertheless coexistence of different phases is observed.

**Crystal structures:**

To the left the phase diagram by Jaffe et al. [1] is shown. In the middle the crystal structures R3m (rhombohedral), Cm (monoclinic) and P4mm (tetragonal) as determined by XRD [2] are displayed with their mirror planes shown in transparent grey. The tetragonal-90° domains were found (1-x)/x ranging from 0/40 to 45/55 have been examined. The compositions up to 60/40 up to 55/45 showed rhombohedral symmetry. For PZT 54/46 tetragonal as well as monoclinic symmetry were observed. With increasing Ti-content the monoclinic phase diminishes. For neighboring monoclinic domains in PZT 54/46 the determined orientations lead to a twin operation which is expected for Cm as a subgroup of P4mm. The inverse transition from monoclinic to tetragonal symmetry was observed for the same composition in an in situ heating experiment accompanied by vanishing of those nanodomains. Therefore the nanodomains are attributed to the monoclinic phase. Nevertheless coexistence of different phases is observed.

**Convergent-Beam Electron Diffraction**

**Fig. 4:** Domains and the relationship between PZT 54/46 and 45/55. Rhombohedral-like (left) and tetragonal-like Domain configuration coexist in this composition at RT [5].

**Fig. 5:** Fourfold symmetry in a c-domain and the (110) - and (100) mirror plane proved by zone axis and dark field patterns.

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**References:**


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