Poster

Lattice match between coexisting cubic and tetragonal phases in PMN-PT at the phase transition

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$(1-x)Pb(Mg2/3Nb1/3)O3-xPbTiO3$ (PMN-PT) are relaxor-ferroelectric perovskite-like solid solutions known for their exceptional electromechanical properties. Understanding their complex origins has been the subject of much academic research [1], especially for the compositions near the morphotropic phase boundary ($0.28 < x < 0.35$). In general, PMN-PT is described by the cubic and paraelectric phase above the Curie temperature (Tc). It undergoes structural phase transitions to tetragonal, monoclinic, or rhombohedral phases below Tc. The mechanisms of the phase transitions remain debatable.

This work aims to investigate the mechanisms of the phase transition between the cubic and tetragonal phases in 0.65PMN-0.35PT. We use high-resolution reciprocal space mapping on variable temperatures. The preliminary measurements at the four-circle X-ray diffractometer in Tel Aviv university [2] revealed an "intermediate state", a two-phase field, during the transition between the cubic and the tetragonal phases. More detailed studies at ID28 beamline [3] of the European Synchrotron Radiation Facility included the measurements of 3D reciprocal space maps - diffraction intensity distributions in the reciprocal space - around 32 different Bragg peaks at 25 temperatures with the temperature step as small as 1K in the anticipated phase transition range 424 K – 442 K. During the phase transition from the cubic phase to the tetragonal phase the Bragg peaks may split into sub-peaks, each diffracted from the corresponding ferroelastic domains formed during the phase transition (Fig. 1 (b-d)). We identified the two-phase field within a 4 K interval during both heating and cooling cycles, with a 1.8 K wide hysteresis between these two processes (Fig. 1 (a)).

Figure 1. The temperature dependence of the cubic phase fraction, $\eta C(T)$, during heating and cooling across the phase transition of 0.65PMN-0.35PT (a). Projection of the diffraction intensity distribution around the $7\bar{1}2$ reflection at different temperatures corresponding to the tetragonal phase (b), intermediate state (c) and cubic phase (d). The labels "C", "T1" and "T2" show the assignment of the sub-peaks to the cubic phase or the corresponding tetragonal domains.

Using the positions of the sub-peaks in the 3D reciprocal space maps, we evaluated the temperature dependence of the lattice parameters of both phases. We found that the two-phase field is characterized by the remarkable matching between the cubic lattice parameter (aC) and the orientationally average of the tetragonal lattice parameters ($2/3aT+1/3cT$). This finding may point at the presence of a strain-free connection between the two phases via low-index habit planes (HP). Usually, such a connection between the tetragonal and the cubic phases is possible only if one of the tetragonal lattice parameters is equal to the cubic lattice parameter. Alternatively, a HP may be formed between the cubic phase and the “adaptive” tetragonal phase. The adaptive tetragonal phase represents an assemblage of alternating tetragonal domains, with the longer axis changing its orientation, joined via strain-free domain walls of the {110} type. Miniaturization of these tetragonal domains results in the macroscopic averaging into monoclinic symmetry, with the effective monoclinic lattice parameters being explicitly dependent on the volumetric ratio of the micro tetragonal domains. If this volumetric ratio permits, the effective monoclinic lattice parameters will be nearly equivalent to the cubic lattice parameter. When this happens, it is possible for a habit plane to form on the (011) plane between the cubic and the adaptive tetragonal phases. Our results may be relevant to other perovskite-based ferroelectric materials, exhibiting similar phase transitions.

[1]Bokov A.A. & Ye Z-G. (2006) J. Mater. Sci. 41, 31–52.

[2]Gorfman S., Spirito D., Cohen N., Siffalovic P., Nadazdy P. & Li Y. (2021) J. Appl. Crystallogr. 54, 914–23.

[3] Girard A., Nguyen-Thanh T., Souliou S.M., Stekiel M., Morgenroth W., Paolasini L., Minelli A., Gambetti D., Einkler B. & Bosak A. (2019). J. Synchrotron Radiation. 26, 272–279.