Motivation

Functional materials which perform a designed action in response to an environmental stimulus are becoming increasingly valuable in the design of novel devices and technologies. An important class of functional materials are piezoelectric perovskites. Their extraordinary (and well-known) ability to couple elastic strain and polarization under the influence of an applied electric field is exploited in piezoelectric sensors, actuators and for energy harvesting. Prominent examples are multilayer stack actuators used in a large number of everyday and high-tech applications, e.g.: • In airbag systems to increase efficiency, • In modern combustion engines for control fuel injection cycles, • In trains, planes or cars they are used for active vibration damping to guarantee comfortable travelling, • In modern highly dynamic pressure transducers, piezoelectric actuators are used for active error compensation of structural oscillations at the tool centre point.

In the past decade in situ and in operando techniques for the investigation of piezoelectric advanced up significantly. However, to date the literature does not provide a method to correlate all structural mechanisms with the macroscopic observations. Here we present a comprehensive model, which is capable of describing the macroscopic behaviour based on a model on the atomic scale.

Experimental (measurement)

Special requirements are necessary for a successful X-ray or neutron diffraction analysis in order to resolve the coexisting and highly correlated phases, a high angular resolution is mandatory. At the same time a high Q-range is necessary to obtain enough information to correctly determine the orientation distribution function (ODF) of the tetragonal material. The requirements could be achieved with neutron diffraction measurements at high-intensity neutron diffractometers such as D20 (Institute Laue-Langevin, Grenoble) or WOMBAT (Australian Nuclear Science and Technology Organisation). For each measurement, a series of 13 complete diffraction patterns were collected with different orientations of the electric field with respect to the incident beam by moving the sample table in 15° steps. By this means, the relative orientation between the electric field vector and the scattering vectors of the individual reflections was varied.

Data analysis was carried out using the software package MAUD (Materials Analysis Using Diffraction)\(^*\). MAUD allows full pattern-refinement including full-profile analysis for multiple phases. Therefore, all data sets with different sample orientations contribute to the refinement. By assigning the Euler angles to the experiment to each diffraction pattern, the orientation dependent information can be exploited. For this additional information the extended Willkomm-Matthies-Vinel (E-WIMV) algorithm was used for texture refinement\(^1\) and the weighted strain orientation distribution function (WSODF) strain model for refinement of the field-induced lattice strain\(^2\). The phase fractions can be obtained from Refinement.

Experimental (analysis)

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References
