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Determining fundamental properties from diffraction: electric field induced strain and piezoelectric coefficient

Piezoelectric ceramics exhibit the remarkable property to couple elastic strain and polarization under the influence of an applied electric field. Among the various types of piezoelectric devices, especially actuators rely on high electric fields to generate high strains and forces. Prominent examples for actuators are multilayer stack actuators used for nanopositioning or in modern combustion engines for automobiles to control injection cycles. The two most important characteristics of this class of materials are macroscopic strain and piezoelectric coefficient. Despite extensive studies and elaborated measurement techniques, the correlation between macroscopic strain and structural response is still not fully understood. Most of the relevant systems found up to now are compositions close to phase boundaries linking highly correlated phases. This results in major challenges for structural analyses due to overlapping reflections. Apart from the well-known field induced structural responses such as domain switching and the converse piezoelectric effect we recently identified field induced phase transitions in different systems as an additional poling mechanism [1,2]. In order to resolve all three involved poling mechanisms within only one experiment we developed a structural analysis technique with in situ X-ray and neutron powder diffraction data [3]. The results not only separately reveal the contributions of each poling mechanism to the macroscopic strain, but also different behaviours of the individual phases. The calculation of the elastic strain perfectly matches the macroscopic observations, confirming the accuracy of the applied models. Since this method yields fundamental information such as the crystal structure as a function of applied electric field, we were able to calculate the piezoelectric coefficient for the individual phases based on information on the atomic scale. In this contribution we present the latest research on the elucidation of strain mechanisms and fundamental properties in piezoceramics.

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