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Influence of Microstructure on Symmetry Determination of Piezoceramics

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Frequently symmetry determination in studies is based on the discussion of agreement factors or the quality of the refinements, rather than on the basis of physical arguments. Especially in the field of piezoceramics this can be observed in the discussion whether monoclinic symmetry can be observed or not.

In this study we could show with temperature-dependent high-resolution X-ray and neutron diffraction that based on agreement factors alone the physical origin of observations cannot be revealed. Only in combination with additional electron microscopy and electron probe microanalysis we could elucidate that a segregation of substituents results in a complex reflection splitting and phase coexistence that can be misinterpreted as monoclinic symmetry. This single-phase monoclinic *Pm* model is able to perfectly reproduce the diffraction patterns and is known from literature [1,2]. A model with phase coexistence of two classical orthorhombic *Amm2* phases can reproduce the diffraction data with equal accuracy.

This demonstrates the need of comprehensive analyses with complementary methods to cover a broad range of length scales as well as considering both average and local structure. The conclusions drawn from this work will have an impact on a broad range of research areas where inhomogeneities cannot be ruled out. The underlying mechanisms of the extraordinary properties of some functional materials originate not just in their structures but also their complex microstructures. Consequently, knowledge of both features of materials may be essential for the exploitation and development of their functionalities as well as improvement of material properties.

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