

MS44 Total scattering: pdf analysis and diffuse scattering in X-Ray, neutron and electron diffraction

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MS44-P1 Cooperation or competition? Multiprobe PDF analysis of local and long-range instabilities in A-site doped SrTiO₃

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Local structural order in perovskites can take a number of forms, and its relationship to both the crystallographic structure and the physics of the material lends itself to an even greater number of interpretations. Recent pair distribution function (PDF) approaches to disorder in perovskites have managed to explain some relations between short-range order and electric behaviour and to give new views on structural phase transitions [1,2].

We present a multiprobe PDF study of Sr_{1-x}Pr_xTiO₃ (0<x<0.150), a perovskite with a significant relaxor ferroelectric response at room temperature. A composition-driven phase transition occurs via gradual stabilization of the nonpolar antiferrodistortive mode with doping [3]. Also, the continuous temperature dependence of the TiO₆ octahedral tilt resembles the SrTiO₃ critical behaviour. But although the ferroelectric and antiferrodistortive instabilities are commonly regarded as competitive, in this case the onset and magnitude of the dielectric permittivity peak are insensitive to high Pr concentration, which should promote antiferrodistortion. In fact, recent theoretical work proposed cooperation between the ferroelectric and antiferrodistortive instabilities in large-tilted structures [4]. The increased tetragonal strain observed alongside octahedral tilt, moreover, might prompt an analogy to the polar strain in ferroelectric SrTiO₃ films (e.g.[5]).

To assess the compatibility of local atomic displacements and long-range antiferrodistortive structure, we have undertaken a combined X-ray and neutron total scattering study. We collected PDF-quality XRPD data at the ID22 beamline (ESRF) and neutron TOF data at GEM (ISIS). Large-box models were provided by Reverse Monte Carlo joint refinement of

real- and reciprocal-space neutron data. The resulting atom displacement and tilt angle distributions were compared to the results of small-box modelling on both X-ray and neutron PDF data. Besides a possible picture for the coexistence of local atomic displacements and antiferrodistortive structure, we discuss reliability and downsides of the joint analysis method used.

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