[MS23-P02] A Survey of PbZrxTi1-xO3 Structural Models Using Symmetry Mode Analysis.

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Numerous structures have been reported for the different phases of the lead zirconate titanate system $PbZr_xTi_{1-x}O_3$ (PZT). Symmetry mode analysis allows a quantitative comparison of different structures, even having different space groups, separating the effect of the different distortion modes present, and distinguishing variations of mode amplitudes from changes in the relative weight within the distortion modes.
A detailed systematic quantitative analysis of amplitudes and polarization vectors [1,2] of the frozen modes at different temperatures, compositions and phases of PZT, shows the consistency of some of the reported models and puts into question others. The fact that the distortions in any of the phases have their ultimate origin in the existence of a 3-fold degenerate polar polarunstable mode, plus in some cases a 3-fold unstable octahedral tilting mode (of the ideal cubic perovskite structure) introduces approximate correlations between the different structures, which are beyond conventional crystallographic rules, and can be detected and quantitatively assessed if the structures are described in terms of symmetry-adapted distortion modes. These correlations were used as a stringent test of the self-consistency of the models proposed in the literature. In the case of the elusive monoclinic Cm phase, the analysis allows to do a quantitative comparison between the various structural models that have been proposed and crosscheck their consistency with those reported for the rhombohedral and tetragonal phases. The much lower symmetry of this phase also allows to perform an additional self-consistency test of the monoclinic structural models, by checking if they can be described by the presence of a single polar distortion mode along a low symmetry direction of a free parameter. A structural distortion of this type implies additional non-crystallographic constraints, and its fulfillment by the different models has been evaluated.

The analysis of the polarization vector components of one phase allows to theoretically predict the polarization vector components of other phase. The result show high concordance in deriving the vector elements of Cm phase from the R3c.

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