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Mode parameterization of structures with very low symmetry: PZT and magnetite

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The parameterization of distorted structures in terms of symmetry modes is an effective and efficient method for both their description and refinement [1]. A basis of symmetry-adapted modes transforming according to irreducible representations not only provides a hierarchical division of the degrees of freedom consistent with the mechanism at the origin of the distorted phase, but it allows the avoidance of false refinement minima, typical of highly pseudo-symmetric phases. A reduction of the number of free parameters by setting to zero negligible marginal modes is also possible. The mode description is nowadays easily applicable through freely available programs [2,3], while direct single crystal and powder diffraction refinements under this parameterization are possible combining these programs with some of the most popular refinement codes. The mode description is especially effective when dealing with distorted structures of very low symmetry compared with that of the parent phase. In these cases, the hierarchy between strong primary modes and weak marginal ones is specially pronounced, minimizing the role of many secondary modes. The physical origin of each primary distortion is usually a set of unstable degenerate normal modes. This introduces correlations among the different phases in the phase diagram that become patent in a mode description and can be used both to characterize the evolution of the relevant order parameters and as a stringent test of proposed structural models. Furthermore, the fact that each of the primary mode distortions is basically associated with the activity (instability) of a single normal mode can yield a “single mode” signature in the mode decomposition, which represents a set of subtle additional structural constrains beyond conventional crystallography. We will illustrate these considerations using the examples of the monoclinic phases of ferroelectric PbZr1-xTixO3 (PZT) and the Verwey phase of magnetite.

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