New Graphical User Interface for Calculating Structural Distortions using the ISOTROPY Software

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ISOTROPY (http://stokes.byu.edu/isotropy.html) is a set of computer programs which use group-theoretical methods for solving a variety of crystallographic problems dealing with structural phase transitions in crystalline materials. One of the most useful features is the association of distortions (patterns of atomic displacements) with the reduction of space-group symmetry in a transition. We have designed a new interface for ISOTROPY which guides the user through the process of choosing a distortion mode based on considerations such as initial and final space group symmetry, distortion k-vector, irreducible irrep, etc., and subsequently returns the distorted structure which the user can import into a 3rd-party package for analysis or visualization.

Keywords: structural change associated with phase transitions, group theory, graphical interfaces