Simulating Order Parameters for Phase Transitions in Alloys

RICHARD R. VANFLEET, CONRAD W. ROSENBROCK, GUS L.W. HART, BRANTON J. CAMPBELL, Department of Physics and Astronomy, Brigham Young University Provo — When determining the structure of alloys using diffraction patterns, possible distortions that lower the symmetry of the parent phase can be limited by group-theoretical arguments as long as a group-subgroup relationship exists between the parent and distorted phases. Order parameters are vectors in representation space where each dimension corresponds to a specific superlattice vector in reciprocal space (e.g. \( L = [0.5,0.5,0.5] \) or \( X=[1,0,0] \)); such order parameters determine the distortions that may arise during a phase transition. By measuring the Fourier transform of the structure at each relevant superlattice vector during a Monte Carlo simulation for CuPt\(_3\), we were able to extract these thermodynamic order parameters and qualitatively confirm distortions in the L and X order parameters observed in experiment. The methodology presents a highly effective avenue for comparing simulated phase transitions with experimental results.

[1] Harold T. Stokes, Branton J. Campbell and Dorian M. Hatch. Order parameters for phase transitions to structures with one-dimensional incommensurate modulations


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Date submitted: 13 Nov 2014
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