Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

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[1]. 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[2]. 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*
[2] Rokuro Miida and Denjiro Watanabe. *Electron Microscope and Diffraction Study on the Ordered Structures of Platinum-Rich Cu-Pt Alloys*

Richard R. Vanfleet
Department of Physics and Astronomy, Brigham Young University Provo

Date submitted: 13 Nov 2014 Electronic form version 1.4