Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Phase Transitions of Boron Carbide: Pair Interaction Model of High Carbon Limit SANXI YAO, MICHAEL WIDOM, Carnegie Mellon University, WILLIAM HUHN, Duke University, QIN GAO, Carnegie Mellon University
— Boron carbide is a structure that exhibits a broad composition range, implying a degree of intrinsic substitutional disorder. While the observed symmetry is rhombohedral, the enthalpy minimizing structure has lower, monoclinic, symmetry. With high melting temperature, it is difficult to experimentally study its phase transition at low temperature and there is discrepancy among different research groups. Moreover, the widely-accepted phase diagram suggests substitutional disorder at low temperature, implying a non vanishing entropy. Here we use computational method to study its phase transition. We implement a pair interaction model and fit to a database of structural energies. Utilizing histogram methods to analyze Monte Carlo simulations of this model, we investigate the symmetry-restoring phase transition that explains the observed rhombohedral symmetry at high temperatures.

Sanxi Yao
Carnegie Mellon University

Date submitted: 12 Nov 2014 Electronic form version 1.4