Effects of Partial Order in Alloys: Connecting Descriptions of Finite-T, Chemical Linear-Response and T=0 K Band-Structure Calculations

Duane D. Johnson and A.V. Smirnov, Department of Materials Science and Engineering,
University of Illinois Urbana-Champaign, USA
duanej@uiuc.edu

Electronic-structure-based thermodynamical linear-response calculations of atomic short-range order (SRO) in high-T random alloys using the multiple-scattering theory based on Korring-Kohn-Rostoker method and the Coherent-Potential Approximation (CPA) have been very successful in describing ordering instabilities and their origin in binary and multicomponent alloys (e.g., Phil. Mag. Letts, 79, 551 (1999)). This also holds generally for related methods, such as Generalized Perturbation Method. More recently, SCF KKR-CPA calculations for energetics for states of partially order have made a connection between high-T SRO calculations and T=0 K electronic-structure results, as well as explain discrepancies when comparing T=0 K results to data from high-T characterization experiments (see Phys. Rev. B 62, R 11 917 (2000)). I compare "Force Theorem" type results in partially ordered states and results from extrapolations using energetics from ASRO, and provide SCF results in states of partially order to show effects of symmetry breaking in the SCF. The effects of partial order may explain many discrepancies between calculations and experimental measurements, such as, e.g., B2 FeAl where a paramagnetic state is observed but T=0 K calculations obtain ferromagnetic state. Examples will be taken from a few cases, such as Ni-V, Fe-Al, Ni-Cr, Nb-Ti-Al, and Cu-Au-Zn.