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Finite-Temperature Predictions of Inhomogeneous Chemical Correlations using Self-consistent KKR-DCA[1] DOMINIC A. BIAVA, DUANE D. JOHNSON, University of Illinois at Urbana-Champaign — The optimal-basis[2] Korringa-Kohn-Rostoker (KKR) electronics-structure method combined with the dynamical cluster approximation (DCA) provides a first-principles framework to predict accurately the electronic, structural, chemical short-ranged order (SRO) effects in disordered alloys. We perform subspace restricted, ensemble averaging over Betts[3] clusters with probability distributions preserving higher-order sum rules and show that the resulting electronic grand potential has simple dependence on SRO. We then predict directly the chemical SRO by minimizing the electronic grand potential with chemical entropy with respect to the probability distribution at temperature. We correlate the atomic degrees of freedom over Betts[2] clusters and investigate the electronic and structural effects arising from the SRO in various disordered alloys, showing good agreement to observed SRO.

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[2]Phys. Rev. B 80, 125123 (2009)
[3]Can. J. Phys. Rev. 75, 47-66 (1997)

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