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Predicting Short-Range Order in Multicomponent Alloys from an Improved Mean-Field Theory ZHUN-YONG ONG, DUANE JOHNSON, University of Illinois at Urbana-Champaign — In alloys the atomic short-range order (SRO) indicates the nascent ordering to which the disordered alloy is tending at high temperatures. Direct first-principles prediction based upon KKR-CPA and mean-field thermodynamics have been successful in predicting system-specific SRO [1], if, at a minimum, corrections are included to satisfy the diffuse scattering sum rule in k-space. However, such models do not account for k-dependence of the corrections. Here, we present an analytic generalization to multicomponent alloys that includes "cyclic diagrams" [2,3] for composition, temperature, and k-dependent corrections to SRO. We first explore the improvement to SRO in model fcc ternary alloys via the generalized Ising model. We find that there is much better agreement to Monte Carlo simulations than with standard Bragg-Williams with(out) Onsager corrections. Then we implement this within the KKR-CPA linear-response theory of SRO.Work was supported by DOE (Award DEFG02-03ER46026 and NSF (DMR-0325939).

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