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Chemical Correlations in Atomic Size-Mismatch Disordered Alloys Predicted from KKR-DCA[1] D.A. BIAVA, Dept. of Physics, University of Illinois, Urbana, IL 61801, D.D. JOHNSON, Ames Laboratory/US DoE and the Dept. of Materials Science & Engineering, Iowa State University, Ames, Iowa 50011 — The dynamical cluster approximation (DCA) has been implemented in a Korringa-Kohn-Rostoker (KKR) electronic-structure method to predict electronic and structural properties of disordered alloys, in particular, chemical short-range order (SRO). We adapted an optimal-basis method[2] to the KKR-DCA to account for variations in atomic size due to different configurations present in size-mismatch alloys. In comparison to experiment, we find excellent agreement for predicted lattice constants and SRO, with origins identified in the electronic structure and affecting mechanical properties at finite temperatures. We also show how coarse-grained symmetry of the DCA can be exploited to reduce memory and computation time, allowing us to perform for the first time self-consistent KKR-DCA calculations with 2^{16} or more configurations (and atoms) on a single compute node.

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[2]A. Alam and D.D. Johnson, Phys. Rev. B 80, 125123 (2009)

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