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Applications of the KKR-DCA: A Finite-Temperature Density Functional Theory to Predict Chemical Short-Range Order Effects in Disordered Metallic Alloys[1] D.A. BIAVA, D.D. JOHNSON, University of Illinois — Short-range order (SRO) is ubiquitous in metallic alloys, affecting changes in their electronic, thermodynamic, mechanical, magnetic, and structural properties. For example, SRO is responsible for the yield-strength anomalies observed in Cu-Al at high temperatures, i.e., the materials is more resistant to dislocation motion at high temperature than it is at room temperature. Within the Korringa-Kohn-Rostorker (KKR) electronic-structure method, we present results using the dynamical cluster approximations (DCA) to obtain the temperature-dependent SRO in disordered alloys. We obtain the KKR-DCA SRO energetics versus local neighbor SRO parameters and minimize it at fixed temperature to predict the SRO. We show that the calculated SRO at fixed temperature compares well with available experimental results, and then correlate the results to the electronic structure. We discuss how an accurate analytic estimate can be made for the SRO in most metals due to the dependence of the grand potential on SRO.

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