Integrated Density of States Lloyd’s Formula for Disordered Alloys with Short-Range Order via a KKR-based Dynamical Cluster Approximation

D. A. BIAVA, SUBHRADIP GHOSH, W. A. SHELTON, D. D. JOHNSON, Physics and Materials Science and Engineering, University of Illinois Urbana Champaign — Within Korringa, Kohn and Rostoker (KKR) multiple scattering theory, we have formulated a static version of the Dynamic Cluster Approximation (DCA), which is a cluster (or non-local) generalization of the coherent potential approximation (NLCPA) that includes environmental effects, including short-range order. Within our KKR-DCA/NLCPA we present an analytic expression for configurationally-averaged integrated density of states $<N(E)>$, or generalized Lloyd’s formula. We show also that this Lloyd’s formula is stationary with respect to changes in the DCA/NLCPA effective medium, providing a rigorous electronic density functional theory and total-energy formalism for (partially) disordered alloys with(out) short-range order that is exact for infinite sized clusters and reduces to the single-site CPA for a cluster size of one. We show applications to various alloys with(out) short-range order.

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