Madelung energy for random metallic alloys in the coherent potential approximation

Within the conventional single-site coherent potential approximation (CPA) used to calculate thermodynamic properties of random alloys, the effect of charge transfer is neglected. We discuss a number of recent models based on the same mathematical form but with a different prefactor $\beta$ which allow one to include charge-transfer effects in the framework of the CPA. We show how the models work in actual calculations for selected metallic alloy systems, Al-Li, Li-Mg, and Ni-Pt, which exhibit charge transfer. We find that the so-called screened impurity model ($\beta=1$), which is derived completely within the mean-field single-site approximation, leads to the best agreement with experimental lattice parameter and mixing energy data for Al-Li and Li-Mg alloys. However, for the Ni-Pt system exhibiting strong ordering tendency this model seems to overestimate the Madelung energy of the completely random alloy, and in this case the screened-CPA method ($\beta=1/2$) gives more correct results. It is suggested that a comparison with the results obtained by the Connolly-Williams method may be used to determine an optimal value for $\beta$ depending on the alloy under consideration.

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