

EXPLORING PHASE STABILITIES IN FCC TERNARY INTERSTITIAL ALLOYS USING THE CUBE APPROXIMATION OF CVM

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The combination of the Cluster Variation Method (CVM) and *ab initio* calculations has opened the pathway towards *a priori* predictions of thermodynamic properties and phase stabilities in systems that show order-disorder transitions. In this work we introduce a thermodynamic model for interstitial alloys since many technologically important materials consist of binary or higher order host metal lattices containing interstitials. Typical examples are N and C in steels, B or C in aluminum alloys, and hydrogen in Pd- or Mg-based alloys for separation and storage materials. On both sublattices, the substitutional host and the interstitial sublattice, order-disorder transitions could occur. Moreover the presence of interstitial atoms could induce ordering in the metal lattice, or vice versa, the presence of alloying atoms in the metal host lattice could induce the ordering of the interstitial atoms. For example, experiments indicate that in the presence of hydrogen a disordered Pd-33at%Mn alloy orders at temperatures where no ordering occurs in vacuum, and that the dissolved hydrogen suppresses the short-range ordering of Pd-9at%Y alloys [1].

A sound thermodynamic model for such systems should be capable of predicting the presence of short- and (or) long-range order, as well as the occurrence of order-disorder transformations. In this work a unified approach that incorporates the coupling of the interstitial and substitutional lattices is put forward. The mutual interaction of the metal host and the interstitial atoms is accounted for by the appropriate choice of a basic cluster. Here FCC substitutional hosts with interstitial atoms residing in the octahedral interstices, that also form a FCC sublattice, are considered. These systems can be modeled by taking a simple cube as the basic cluster such that it includes sites belonging to both sublattices comprising the system. The proposed approach is applied to calculate phase boundaries for several hypothetical systems to illustrate the effects of mutual interactions between sublattices.

[1] T.B. Flanagan and Y. Sakamoto, *Platinum Metals. Rev.*, 1993, vol. 37, pp. 26-37.