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EQUILIBRIUM PROPERTIES OF THE Cu-Au ALLOY SYSTEM AT T=0 K

H.M. Polatoglou, K. Magoutis and G.L. Bleris
Physics Department, Aristotle University of Thessaloniki, GR-54006 Thessaloniki, Greece

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Abstract

The T=0 K equilibrium properties of the Cu-Au alloy system have been studied using a random-alloy and a supercell calculation employing an N-body potential. The interaction parameters for Cu have been taken from literature while the ones for Au have been adjusted to the experimental data. The cross-interaction parameters have been determined according to two procedures. a) taking them as the geometric average of their respective atomic b) by adjusting them to the experimental data of the ordered Cu_3Au phase. In the former case it is found that the random-alloy and the supercell calculations give similar but quantitatively different results. Using adjusted cross-interactions in the supercell calculations gives better agreement with experiment.

Introduction

Modeling alloy systems is very interesting in the prospect of studying their thermodynamical properties, such as order-disorder transformation, the effect of temperature on the Grain Boundary properties, melting at the Grain Boundary e.t.c, using methods such as Monte Carlo or Molecular Dynamics [1]. The Cu-Au alloy is a prototype system because it is possible to study experimentally many of its properties by electron microscopy [2]. It has been recently found that the N-body potentials can give quite accurate description of the bulk and surface properties of metalic systems such as Cu [3]. Also it has been found that is possible to model the equilibrium properties of metalic alloys by using a random-alloy model [4]. The aim of the present work is to search for an appropriate potential to study the thermodynamic properties of the Cu-Au system.

Potential and the random-alloy model

The potential we employ in the present work is given by the following formula [5]:

$$E = \sum_{\alpha} \sum_{i_\alpha=1}^{N_\alpha} \{ \sum_{\beta} \sum_{\substack{j_\beta=1 \\ j_\beta \neq i_\alpha}}^{N_\beta} A_{\alpha\beta} e^{-p_{\alpha\beta}[\frac{r^{\alpha\beta}}{d_{\alpha\beta}}-1]} - \{ \sum_{\beta} \sum_{\substack{j_\beta=1 \\ j_\beta \neq i_\alpha}}^{N_\beta} \xi_{\alpha\beta}^2 e^{-2q_{\alpha\beta}[\frac{r^{\alpha\beta}}{d_{\alpha\beta}}-1]} \}^{\frac{1}{2}} \}, \qquad (1)$$