Atomic-Scale Modeling of Intergranular and Superficial Segregation in a Binary Alloy Exhibiting a Strong Size Effect

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The segregation of Ag in the Cu(Ag) solid solution domain has been studied at various interfaces: the $\Sigma = 5(310)\,[001]$ tilt grain boundary (GB) and the (001), (310) and (111) surfaces. The Cu-Ag system has been chosen because it has been the subject of many experimental works. It presents a strong tendency to phase separation in the bulk and an important size effect ($r_{Ag}/r_{Cu} = 1.13$). This system is described by empirical N-body potentials derived from the second moment approximation of the tight binding scheme.

In order to precisely analyze the driving forces responsible for the segregation as well as the chemical and structural interfacial transitions which follow, a mixed approach has been developed, including:

- grand canonical Monte Carlo simulations taking into account atomic displacements,

- an effective Ising model treated in the mean field approximation, the energetic parameters of which being obtained from realistic atomic simulations using the N-body potentials. Thus, the influence of atomic relaxations is incorporating in the model, which means that the segregation enthalpy (at infinite dilution) and the effective pair interactions are obtained consistently for each site and for each pair of sites of the interface.

This approach will be presented as well as some general results that it has allowed us to obtain. For example, the segregation driving forces have been extracted, which shows that the size effect is predominant in all considered cases. It has also been shown that the vibrational entropic effect on the interfacial segregation cannot be neglected for grain boundaries, contrary to the case of surfaces.

Results concerning more precisely the different studied interfaces will also be presented, particularly:

- multilayer transition, wetting with a structural transition at the $\Sigma = 5(310)$ [001] tilt GB.

- comparison between the segregation properties of the flat surface (100) and the open surface (310), this last one having the same orientation that the preceding GB.

- segregation and Ag deposit at the (111) surface.