

Surface Effects on the Ordering of A₃B Alloys

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We have simulated the surface segregation and the surface ordering on Cu₃Au(100) and Ni_{0.75}Pt_{0.25}(100) using Ising-type model Hamiltonian. Both alloys are known to show L₁₂ ordering at low temperatures and undergo first-order phase transition as temperature increases. Both surfaces are determined to be enriched with minority atoms (i.e., about 50 at.-% of Au or Pt atoms, respectively) and show the oscillatory depth profile from the previous experimental studies. However, it is not yet understood how the atomic ordering occurs in the surface region near the phase transition. Moreover, it is an important issue, from the theoretical point of view, to understand the surface effects on the first-order phase transition of a bulk. It is known that the surface of Cu₃Au(100) disorders first below the bulk phase transition, which is a so-called surface-induced disorder (SID) phenomenon. The similar conclusion for Ni_{0.75}Pt_{0.25}(100) might be drawn from the similarity of bulk and surface behaviors.

Therefore, we have investigated the surface ordering in addition to bulk phase transition and surface segregation using an Ising model through Monte Carlo simulation. It is appropriate to simulate both the bulk and surface behaviors of substitutional alloys with an Ising model Hamiltonian, which has short range interactions and renormalized surface interactions, and the surface confined segregation force terms. In our study, surface effects are described in Hamiltonian parameter space. Our results show that the surface-induced order (SIO), in that the surface maintains its orderedness somewhat above the bulk phase transition, can occur on Ni_{0.75}Pt_{0.25}(100) surface. However, the other features of surface segregation are not distinguishable from those of Cu₃Au(100) showing a surface-induced disorder. This result can be applied to give some guideline to the theoretical calculation on the Hamiltonian parameters on the basis of electronic structure calculation, while some of experimental features are not available.