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Revisiting the segregation driving forces rule: the Coupled Three Effects Model JÉRÔME CREUZE, ISABELLE BRAEMS, FABIENNE BERTHIER, LEMHE/ICMMO, UMR 8182, Universite Paris Sud-XI, Bat. 410, F91405 Orsay cedex, France., CHRISTINE MOTTET, GUY TRÉGLIA, CRMCN-CNRS, Campus de Luminy, Case 913, 13288 Marseille cedex 9, France., BERNARD LEGRAND, SRMP-DMN, CEA Saclay, F91191 Gif-sur-Yvette cedex, France. —
Separating the surface segregation enthalpy into three elementary contributions (cohesive, alloy and size) has been proposed by many authors, but rarely tested quantitatively. Such a separation rule, derived from a tight-binding Hamiltonian years ago, has yielded very satisfying results for various environments (surfaces, grain boundaries and clusters) for the Cu-Ag system and for many other alloys, but recently stumbled over the Co-Pt system. We propose a new approach based on a systematic study of the permutation enthalpies, both in the bulk and in the surface, as a function of the mixed interaction involved in the N-body interatomic potentials derived from the electronic structure. We then show that both the disagreement observed for Co-Pt and the agreement mentioned for Cu-Ag can be explained by the variation of the effective pair interactions in the surface and by the existence of coupling coefficients between the three effects. Finally, we introduce a new decomposition, the Coupled Three Effects Model (CTEM), that is valid for systems with both size and cohesive effects.

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