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Chemical and structural dynamical equilibrium in bimetallic nanoclusters JÉRÔME CREUZE, LEMHE/ICMMO, UMR 8182, Universite Paris Sud-XI, Bat. 410, F91405 Orsay cedex, France, LAURE DELFOUR, BERNARD LEGRAND, SRMP-DMN, CEA Saclay, F91191 Gif-Sur-Yvette cedex, France — Coupling the surface and finite-system thermodynamics is a challenging key point in modeling bimetallic clusters. This is particularly crucial when the alloy surfaces undergo first-order phase transitions. In this context, we have investigated the segregation of Ag atoms in the surfaces of Cu-Ag nanoclusters, using N-body interatomic potentials and the Monte Carlo method. The (111) and (100) surfaces of Cu-Ag alloys are known to exhibit first-order phase transitions coupling a jump in the surface concentration and structural rearrangements. For the Wulff polyhedron of 405 atoms, these phase transitions are replaced by a dynamical equilibrium (DE) in phase space. For the (100) facets, this DE affects both the composition and the structure of the facets. Furthermore, all the (100) facets are correlated during the DE, due to atomic relaxations which affect also the core region of the nanocluster. For the (111) facets, the DE concerns only the composition of the facets, the atomic structure remaining unchanged. Consequently, the (111) facets are not correlated each other, indicating that pure Ag and pure Cu (111) facets can be observed in a given nanocluster. These simulations allow us to propose a surface phase diagram for the studied Wulff polyhedron.

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