STRUCTURE MAINTENANCE OF CU NANOCLUSTERS SOFTLY DEPOSITED ON AN Au(001) SURFACE

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The soft deposition of Cu clusters with Wulff-shape on an Au(001) surface is studied by constant temperature molecular-dynamics simulations. The influence of incident kinetic energy of the atoms in the low-energy limit, of the substrate as a result of the difference between lattice parameters (12.8%), of the cluster temperature and of its orientation is analyzed. Bombardment energy ranges between 1 and 100 meV/atom. These values are small enough compared to the binding energy of an atom in the cluster; due to this, no fragmentation of the clusters is expected upon impact on the substrate. The atomic interactions are mimicked by a many-body potential based on the tight-binding model. By depositing the clusters with low kinetic energies, one would like to conserve the memory of the free-cluster phase, retaining one of the peculiarities of the clusters, their high surface/volume ratio, which affects all their physical (structural, electronic) properties as well as their chemical reactivity (catalysis). We are researching growth kinetics, especially the equilibrium structure of deposited metallic clusters on a substrate highly distorting due to the great misfit in the lattice parameters. Previous results indicate that coherent and semi-coherent interfaces result for higher kinetic energies. Common neighbour analysis, CNA, and a centrosymmetry parameter have been used to analyze cluster structures.