NANOPARTICLE HETEROCOALESCENCE INDUCED BY DEPOSITION

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Cobalt in nanocrystalline form is an attractive system because it displays a wealth of size-dependent structural, magnetic, electronic, and catalytic properties [1]. From a technological viewpoint, Co nanoparticles have applications in magnetic storage media. Below a certain size (≤20 nm of diameter), clusters of cobalt crystallize in the face-centered cubic (fcc) phase and most particles possess crystalline structures made up of multiply-twinned icosahedra [2]. Besides, these nanoparticles are converted into single-crystal Wulff polyhedra above 300ºC.

The general process of intercluster coalescence has been extensively studied using molecular dynamics [3-5] or by macroscopic models of sintering [6]. This process is driven by capillarity since it reduces the surface free energy. Specifically, the coalescence of supported clusters is of great importance in the field of surface nanostructuring [7]. Kellet and Lange [8, 9] indicated that, in the case of the presence of grain boundaries between particles, a further lowering of the free energy would require the recrystallization of some particles. Therefore, atomistic models describing coalescence must account for changing crystallographic mismatch. Many groups have performed crystallite rotation techniques in order to investigate the reorientation during sintering for metals [10- 14] and oxide particles [15, 16]. For metals, the mechanism of reorientation may then include the formation or migration of grain-boundary dislocations.

In the present work, the coalescence between Co and Cu clusters on Cu(001) substrate is studied by constant-temperature molecular dynamics simulations. Cobalt clusters embedded or supported in a copper matrix constitute an attractive system, because it displays important magnetic properties [17,18]. Atomic interactions are mimicked by a many-body potential based on the second-moment tight-binding approximation (TB-SMA). Initially, Co clusters of about half a thousand of atoms in their more stable form were deposited on a Cu (001) substrate at 250 meV/atom and room temperature. Next, a randomly oriented Cu cluster of the same size at 250 meV/atom with icosahedral or cuboctahedral form and fcc phase was deposited on the former colliding with this at room temperature. The center-of-mass separation between the projectile and target clusters was varied uniformly. The degree of epitaxy of the two clusters has been investigated as a function of this separation, and of the type of material. The effect of the temperature as activation of grain-boundary movement to get the complete epitaxy has been also analyzed in the projectile cluster.

Nanoparticle coalescence has theoretically as well as experimentally been shown to be a two-step process: first a reorientation of adjacent nanoparticles, and second a complete or incomplete adhesion depending on the matching of the crystallographic orientations [16]. This work is mainly focused on the first process, since the appearance, movement, and disappearance of grains after the collision has been described. The evolution of the number of atoms and energy in each grain plays an important role in the alignment of the second cluster with the substrate [19], and define a trend in the final internal morphology of the system.

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