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Molecular dynamics simulations of low energy ion sputtering of copper nano-dimensional clusters on graphite substrates

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Abstract

Molecular dynamics simulations have been performed of sputtering of copper clusters, which consisted of 13, 39, 75 and 195 Cu atoms, on a (0001) graphite surface by 200 eV Ar ions. The role of multiple Ar–Cu and Ar–C interactions in the polar distributions of backscattered Ar ions was investigated. Yields, energy and angular distributions of sputtered cluster atoms were examined. The azimuthal angular distribution of sputtered Cu atoms exhibit periodic maxima every 60°. The polar angular distributions of sputtered Cu atoms have maxima in directions parallel to the substrate surface for all clusters. The obtained sputtering yields are for a surface with a single Cu cluster deposited. A solution to the problem of comparing the sputtering yield for such a single surface cluster with the yield from a surface with a given cluster coverage is presented.

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Keywords: Sputtering; Cluster; Molecular dynamics

1. Introduction

Binary systems of metal nano-dimensional clusters on metal and carbon-based substrates [1–9] are of considerable technological interest in the field of heterogenous catalysis, new materials for electronic devices, thin film growth, epitaxy and

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the fabrication of nanostructured materials. A number of computer simulations of such cluster/substrate systems have been performed during the last decade for carbon systems [10–13], deposition of metal clusters [14–18], sputtering of metal and non-metal surfaces initiated by energetic clusters [19–23], as well as cluster [24] and molecular fragment [25] sputtering mechanisms. So far no detailed simulations of sputtering of nano-dimensional clusters on a substrate have been performed. Especially the interplay of substrate and cluster in ion scattering, the angular and energy distributions of sputtered atoms from such a binary system under ion bombardment as well as the sputtering yield values have not been investigated, but can be studied within the framework of classical molecular dynamics (MD) [26].

The present investigations are devoted to MD simulations of low energy ion backscattering from and sputtering of binary systems, consisting of copper nano-dimensional clusters of different sizes on a (0001) graphite surface. We analyzed the penetration depth of implanted ions as well as the polar angular and energy distributions of backscattered bombarding ions. Furthermore for sputtered Cu cluster atoms angular (azimuthal and polar) and energy distributions were obtained. The relevant mechanisms are discussed for Ar ion backscattering from the clusters and sputtering of Cu cluster atoms on graphite substrates. The results for the copper–graphite systems are compared to the MD calculated sputtering yield of a pure Cu (100) surface and are used to estimate effective sputtering yields for such Cu clusters on graphite systems.

2. Model

Simulations were performed for Cu clusters consisting of 13, 39, 75 and 195 Cu atoms on (0001) graphite substrates, which consisted of 1584, 2288, 3000 and 5880 carbon atoms, respectively. Additionally, a cluster with 27 Cu atoms on a graphite substrate with 1920 carbon atoms was used for sputtering yield estimations. Carbon atoms were arranged in two layers with an interlayer distance of 3.35 Å and a nearest neighbor distance of 1.46 Å between carbon atoms in the layer. The Tersoff potential [27] with a cut-off radius of $R_{cf}^{(C)} = 2.1$ Å, splined to the Ziegler–Biersack–Littmark potential [28], was applied to the C–C interactions. A tight binding many body potential, directly connected to the Born–Mayer potential [29,30] with a cut-off radius of $R_{cf}^{(Cu)} = 5.5$ Å, was used for the Cu–Cu interatomic interactions. C–Cu interactions were simulated using a Lennard–Jones potential [31]. Different parameter estimates exist in the literature for the C–Cu Lennard–Jones potential [32–34]. We have used the values given by Dorfman et al. [32] and $R_{cf}^{(Cu-C)} = 3.75$ Å. The C–Cu potential was splined to the Ziegler–Biersack–Littmark potential. Trajectories of particles were calculated in accordance to Newton's equations of motion using the Verlet algorithm [26]. The variable time step for the integration of the equations of motion was in all cases less than 4 fs. Conservation of energy was in all cases better than 1%. Every ion impact was calculated for 2 ps.

The initial copper clusters were also obtained from molecular dynamics calculations. Copper lattice fragments of the appropriate size were heated to 1700 K at a heating velocity of 0.25°/ps. At 1700 K the fragments were allowed to relax freely during 10^4 ps. Afterwards clusters were cooled at the same velocity to 0 K in accordance to an algorithm, suggested in [19]. The obtained copper clusters exhibit a lattice structure similar to the structure of free model nickel clusters obtained in [35]. For the preparation of the cluster/substrate systems these copper clusters were located close to the C surfaces in the range of, at least, a few Cu–C pair interactions. Then the relaxation of the cluster/substrate system was calculated for 20–40 ps, depending on cluster size. The final kinetic energies of Cu atoms in the binary system after relaxation were less than 0.02 eV/atom. The substrate graphite (0001) atomic planes were allowed to relax freely only in the lateral directions during this relaxation process, to avoid distortions of the graphite structure [36]. An energy dissipation layer [37] as well as periodic boundary conditions [26] were put at all lateral borders of the carbon substrates.

Calculations were performed for 200 eV Ar ions, impinging normally to the substrate surface.