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Dynamics of cluster induced sputtering in gold

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Abstract

Impacts of 0.13–1.4 MeV Au_{13} clusters onto Au(1 1 1) target are investigated in molecular dynamics simulations. The evolution of sputtered Au atoms and clusters are simulated up to 10 ns. The total sputtering yield, angular and velocity distributions of the sputtered material, as well as dimensions of impact induced craters are compared to recent experimental results. It is shown that the experimental observations can be explained by a flow of atoms from the craters. Secondary cluster ejection from crowns formed around the craters is found to be one of the main mechanisms of sputtering. The results are summed up in an empirical model.
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1. Introduction

Impacts of energetic atomic clusters on solid targets create craters on the surface and release material from the target, which is usually called sputtering. The number of atoms ejected per incoming cluster (sputtering yield) depends on the target material, as well as cluster composition, nuclearity, angle of incidence and kinetic energy. The physics of cluster induced sputtering is not yet fully understood, but in recent years many new significant advances have been made and a consistent model of cluster impacts is emerging. The progress is reviewed in [1–5]. This will promote development of applications like chemical analysis of nanodomains [6] and surface smoothing [7]. In addition to the application point of view, the cluster impacts are also an interesting example of a phenomenon in the border of quantum and continuum domains, allowing to investigate and model the emergence of continuum phenomena out of the interactions between atoms.

The aim of this work is to show that simulated results of Au cluster impacts on a crystalline Au(1 1 1) target are in good agreement with the recent experimental sputtering measurements, which proves that the *flow model* of sputtering can explain the experimental results. In the model, the impact energy deposited from the projectile to the target lattice forms a rapidly expanding cascade of hot atoms. The cascade is surrounded by the crystal lattice and, therefore, has high pressure. The pressure is released when the cascade disrupts the surface of the lattice forming a crater. A flow of gaseous and liquid material from the crater walls forms a crown around the crater, and the lattice atoms and clusters are ejected out to the vacuum. Eventually, the system cools down to the ambient temperature and the crown collapses to form a rim around the crater.

The idea of the flow model is not new. For example, Birtcher and Donnelly showed in 1996 that ion impact on Au surface induce nanoscale flows of liquid material. Recently, Samartsev et al. [8] have shown experimentally that cluster induced sputtering cannot be explained to be thermal evaporation from a heated surface. Instead, based on insights gained from molecular dynamics simulations, they conclude that a gas flow model, where the crown is an important source of sputtering, better explains the results. Also other researchers have observed cratering as well as velocity and angular distributions of sputtered

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material that support the flow model [9,7,10,11]. The flow of material after impact is not exclusively connected to cluster impacts. Also impacts of single high-energy ions can induce cratering [12]. Craters, crowns and flows are seen in the molecular dynamics simulations, which also supports the flow model. Already in 1991, Urbassek and Waldeer observed the material flow in their simulations of Ar ion impacts [13]. Ghaly and Averback showed in 1994 that local melting and viscous flow of hot liquid onto the surface caused the surface modifications in ion bombardment of Au surface [14]. Some more recent results of simulated impacts of various types of clusters on metal targets are in [15–24,18,25–29].

Formation of exotic structures due to the flow of liquid metal out of the craters during ion irradiation is reported in an earlier study of our group including transmission electron microscope (TEM) images of these structures taken by Birtcher and Donnelly [20]. Similar results are also reported in [18]. Now we have reached higher energies and longer simulations times than what has been previously possible. This gives on opportunity to use atomic clusters as projectiles and to compare the calculated results to experimental data and verify that several quantities like the total sputtering yield as well as velocity and angular distributions of the sputtered material are in agreement with the observations.

2. Methods

2.1. Interatomic potentials

High-energy cluster impacts were simulated using classical molecular dynamics. The quality of the interatomic potential used in the simulations is one of the most important factors affecting the results [19,30]. Especially in cluster collision simulations, the potential should describe well both the solid and liquid phases as well as crystalline and liquid surfaces.

The potential used in this study is based on the corrected effective medium theory (CEM) [31,32]. We have found that it describes single Xe ion induced sputtering from an Au(1 1 1) surface in agreement with experiments [30]. Other researches have found that it also gives good results in many other respects, for example, in metal surface relaxations [33–36] and in sputtering phenomena [37,38].

The correctness of the surface energy is very important for this study because ejection of large clusters is based on liquid droplet formation, as will be shown in Section 3.1. The CEM potential reproduces the surface energy of Au reasonably well [39,40]. We have obtained that for Au the simulated surface energy with the CEM potential is 1.4 J/m^2 [41]. The experimental value of the surface energy is difficult to determine, but a recent study [42] indicates that 1.51 J/m^2 is a good value.

Another important quantity is the melting temperature that affects collision cascade development after the cluster energy has deposited in the surface layers of the target. The melting temperature for the CEM potential has been determined in an earlier study in our group [41]. The result 1635 ± 5 K is higher than the empirical melting temperature for Au, 1337 K [43]. The volume of the melted region and the crater sizes decreases when the melting temperature increases [30]. Therefore, we can conclude that the CEM potential does not overestimate the fluid phenomena reported here. In reality, however, the volume of liquid Au could be larger and the cooling of the crater region may take longer than in the simulations.

At small interatomic distances, the CEM potential was smoothly joined to the universal Ziegler–Biersack–Littmark interatomic repulsive potential [44] to realistically describe strong collisions that occur when the cluster penetrates in the lattice and also when some high-energy recoil atoms collide with other target atoms. Electronic stopping was applied to all atoms having a kinetic energy larger than or equal to 5 eV [45,44]. The particular version of the CEM potential used in this study is discussed in [41].

2.2. Molecular dynamics simulations

The methods used in the molecular dynamics simulations have been described in detail elsewhere [46–48], so here we only summarize the features which are essential for this study.

The clusters were targeted perpendicular to the Au(1 1 1) surface. The impact point on the surface as well as the spatial orientation of the cluster were varied randomly between the simulation runs. The size of the rectangular target lattice was almost seven million atoms ($48.5 \times 49.0 \times 49.0$ nm), which ensured that the simulated cascades were not distorted by artificial boundaries. Techniques applied to prevent shock waves to reflect back and to disturb the cascade are described in [30]. Berendsen temperature control was used to cool the sides and the bottom of the simulation cell to 100 K. The thickness of the cooled region was 2.5 nm.

The simulation times were chosen to be long enough to reach the phase when the sputtering was over and the crater walls recrystallized. Times between 30 and 170 ps were used depending on the projectile energy. After that, the sputtered atoms were simulated an additional 4–10 ns without cooling, to find out how much material will deposit back to the surface after some large sputtered clusters have fallen apart. Although parallel processing was used, the large number of atoms and long simulation times limited the number of simulations. However, the crater formation at these energies is almost a continuum phenomenon and three simulations are enough to get reasonably small error of average for most quantities.

According to *ab initio* calculations, planar Au cluster structures are energetically favorable up to $N = 13$ [49], whereas with the CEM potential the stable Au_{13} structure is icosahedral. However, our test simulations with planar Au_5 clusters show that the cluster shape does not affect very

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