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Impact and spreading behavior of cluster atoms bombarding substrates

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ABSTRACT

The purpose of this study is to investigate the behavior of copper cluster atoms bombarding a substrate using molecule dynamics based on tight-binding second moment approximation (TB-SMA) potential. The simulated results show that a crater on the substrate surface was created by the impact of the clusters. The variations of kinetic energy of cluster bombardments can be divided into three stages. At the initial impact level, the kinetic energies of the clusters and the substrate were constant. Then, the system went into a sluggish stage of energy variation, in which the kinetic energy of the clusters reduced. In the final stage, the kinetic energy of the system became stable. The high slip vector region around the crater had a disorder damage zone. The symmetry-like cross-slip occurred beneath the top layer of the substrate along the ⟨1 1 0⟩ orientations. The spreading index, temperature, and potential functions that affect the bombardments are also discussed.

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1. Introduction

In recent years, cluster bombardment and sputtering technology have been increasingly used for various applications in thin films, surface science, and nanotechnology [1–3]. The interaction of cluster bombardment on surfaces has achieved to etch for surface modification applications [4,5].

Deposition field techniques, such as the ionic beam sputtering (IBS) method, plasmonic fields, and molecular beam epitaxy (MBE), have potential applications in creating nanostructures on solid surfaces [6]. The contact and optical properties of the nanostructures can be controlled by the impact energy of the cluster and cluster size. The mechanism of cluster bombardment is difficult to investigate with traditional experimental methodology, but it can be easily solved by using molecular dynamics (MD) simulation. Ratner et al. [7] studied the collision between Cu dimer and Ar film and found that the dense surroundings of the Ar film could confine the Cu dimers. Bromann et al. [8] showed that Ag clusters could be deposited nondestructively on Pt substrates by using Ar buffered layers. Jiménez-Sáez et al. [9] studied structural changes in Cu clusters softly landing on Au substrates at various energies and temperatures. Zang et al. [10] found that collision dynamics were dominant in the early stages of single cluster deposition. Lee et al. [11] found that cluster atoms activated copper substrate atoms through collective collisions in the impact region.

The effect of the impact energy of the cluster and cluster size on the surface and mechanical properties of the metallic nanoparticle interface is still not fully known. In this paper, the impact and spreading behavior of copper cluster atoms bombarding copper substrates were investigated. The influences of the cluster size, temperature, and potential energy on the bombardments were investigated on a nanometer-scale.

2. Molecular simulation

The simulated model consisted of an impacted cluster and a Cu substrate. The Cu (1 0 0) substrate consisted of 16000 atoms perpendicular to the *z*-axis. The substrate, a face-centered-cubic (FCC) crystal, had dimensions of $7.24 \times 7.24 \times 3.62$ nm. The two lowest layers of the substrate were fixed to prevent the substrate from being moved by the incident atoms during impact. The two layers above the fixed layer were called thermal layers. The velocities of atoms in these layers were rescaled at every ten time steps according to the prescribed substrate temperature. The velocities of the thermal control layer atoms were constantly adjusted by the Boltzmann distribution [12] of the prescribed substrate temperature. Other layer atoms of the substrate were Newtonian atoms. The kinetic energy of incident cluster atoms may be affected during the cluster bombardment process. Periodic boundary conditions (PBC) [12] were imposed in the *x* and *y* directions; there was no periodic boundary condition along the *z* direction. The incident clusters were Cu atoms and their incident velocities were calculated by the incident energy. The *x* and *y* positions of the incident atoms were assigned and the height of the

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Table 1
parameters of TB-SMA potential function for copper.

Parameters	Values
r_0 (Å)	2.566
A (eV)	0.0855
ζ (eV)	1.2440
p	10.960
q	2.2780

incident atoms was placed at the 15-fold lattice length above the substrate surface, i.e., the distance between the substrate and cluster was 15a (lattice constant a). The impacted clusters considered in this work were composed of 32, 108, and 256 atoms after thermal relaxation. The shape of the cluster was spherical. The substrate temperatures considered were 100, 300, 600, and 1000 K. The incident angle was fixed at 0°, i.e., perpendicular to the substrate surface.

In this study, the tight-binding second moment approximation (TB-SMA) many-body potential function $U_{TB}(r_{ij})$ [13] was chosen to simulate the interaction force of copper. In the TB-SMA model, the cohesive band energy, which is described by the second moment of the d-band density of state, and the repulsive pairwise potential energy of the Born–Mayer term [13] are summed. For an atom i, the sum can be expressed as [13]:

$$U_{TB}(r_{ij}) = \sum_j A\exp\left[-p\left(\frac{r_{ij}}{r_0}-1\right)\right] - \left\{\sum_j \xi^2 \exp\left[-2q\left(\frac{r_{ij}}{r_0}-1\right)\right]\right\}^{1/2} \quad (1)$$

where r_{ij} is the separation distance between atoms i and j, ξ is the effective hopping integral, N is the number of atoms, and r_0 is the first-neighbor distance. The values of the parameters for Cu atoms are listed in Table 1. Parameters A, q, p, and ξ were fitted to the experimental values of various magnitudes. The Morse potential energy $U_{Morse}(r_{ij})$ is described with three parameters as:

$$U_{Morse}(r_{ij}) = D(e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}) \quad (2)$$

where D is the cohesive energy, α is fitted to the bulk modulus, r_0 is the equilibrium distance, and r_{ij} is the separation distance between atoms i and j. For Cu–Cu atoms, values of D, α, and r_0 are 0.3429 eV, 0.13588 nm^{-1}, and 0.2626 nm, respectively [14]. The Gear five-order predict-correct algorithm was used to calculate the position, speed, and acceleration after interaction among the microsystem atoms. To save computational time, the method also combined cell link and Verlet list to deal with the interaction among all atoms.

3. Results and discussion

Fig. 1(a–c) shows the behavior of copper clusters (red for cluster atoms) impacting the substrate surface at a temperature of 300 K. Before the bombarding the substrate, the cluster consisted of 108 copper atoms at 1000 fs, as seen in Fig. 1(a). The initial kinetic energy of the cluster was about 90 eV. Fig. 1(b) shows that the hopping atoms spread and transferred to the surface at 3000 fs. Some atoms of the solid sputtered out and formed a crater after the bombardment. These snapshots show a nearly round crater on the surface. This was due to the higher diffusivity and higher lattice energy of the {1 1 1} plane system [15]. The crater formation is an important plastic deformation of cluster bombardments and collisions on the solid surface. The region near the solid surface was compressed in the [1 0 0] direction and at the same time, the atoms around the crater were relaxed. The impact cluster atoms deformed and caused decrease in kinetic energy of the cluster

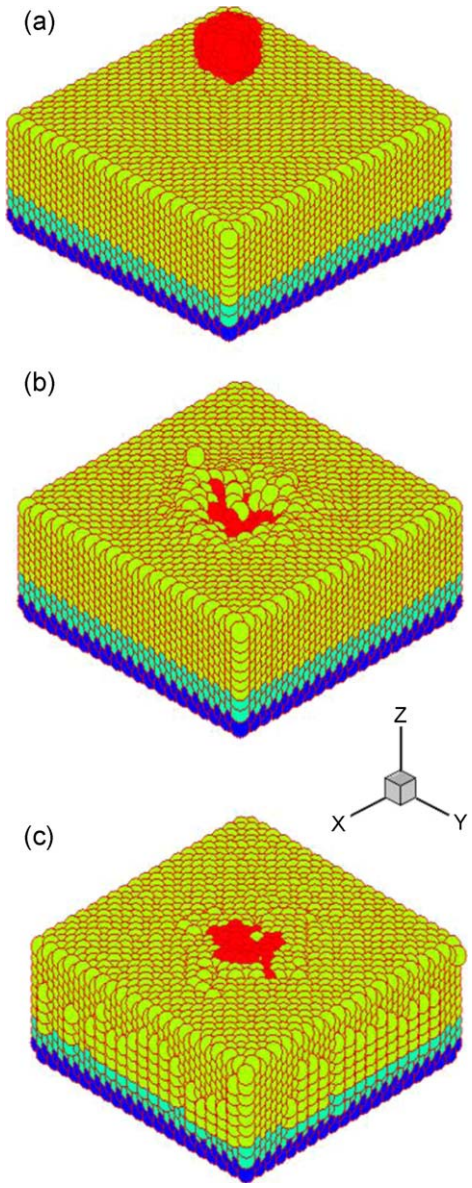

Fig. 1. Snapshots of a cluster impact on a Cu (1 0 0) substrate at different instants: (a)1000 fs; (b) 3000 fs; and (c) 6500 fs (red for cluster atoms). "For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article."

atoms then the atoms would disperse around the crater of the substrate. The shape of the crater became stable after the dislocations of the solid diffusion and structural stress relaxation, as seen at 6500 fs in Fig. 1(c).

Referring to Fig. 2, the simulation shows that the variation of kinetic energy of cluster bombardment can be divided into three stages. The first stage was at the initial impact level; the kinetic energy of the cluster and substrate were constant. In the second stage, called the sluggish change area of energy, the kinetic energy of the cluster decreased, but the kinetic energy of the substrate increased. In the final stage, the kinetic energy of the substrate became stable. Before impact, both the kinetic energy of the cluster and the solid substrate were in a steady state. At the moment of bombardment, the kinetic energy of the cluster decreased but that of the substrate increased. The lag of the energy removing phenomena occurred at the substrate between 1500 and 2500 fs time levels. Then, the kinetic energy of the cluster atoms decreased, and the atoms absorbed on the solid substrate. The

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