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Molecular-Dynamics Simulation of Metal Atomic Clusters under Low-Energy Bombardment

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The evolution of free copper atomic clusters under low energy Ar ion bombardment is simulated using the classical molecular dynamics. The clusters consisting of 26, 78, and 390 atoms have been studied at a impact energy ranging from 1 to 800 eV. Interatomic interactions between copper atoms were described by the many body Ackland potential, whereas the interaction of copper atoms with argon ions has been described using the Ziegler–Biersack–Littmark potential. Time dependences of the temperature and potential energy as well as values of sputtering yields of free clusters under the ion bombardment have been simulated.

Keywords: Molecular dynamics, atomic clusters, copper, Ackland potential.

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1. INTRODUCTION

The study of metal clusters has been growing steadily in the last three decades because of their importance in understanding catalytic processes on one hand, and they may serve as a useful model for studying a chemisorption process on a solid surface on the other hand [1]. Various methods to investigate the characteristics and properties of atomic clusters have been employed, both theoretical and experimental [2]. We have used the classical molecular dynamics approach for the simulation of Cu clusters (26, 78, 390 atoms) under low-energy Ar ion bombardment.

2. MODEL

The model clusters used in the calculations were obtained by the arrangement of two equal initial copper clusters consisting of 13, 39, and 195 atoms at a distance of 2 nm between the nearest surface atoms. As a result of the interactions between atoms, the clusters merge, forming a unified cluster. To stabilize its structure, the model temperature was uniformly increased from 0 to 500 K for 20 ps and, during the next 20 ps, the temperature did not change; then, during the following 20 ps, the temperature was uniformly reduced to the initial value. As a result, stable clusters near the minimum of their potential energy at a temperature about 0 K were formed. The obtained clusters were bombarded by argon ions placed in the arbitrary point in space at the distance of 6-7 Å from the target surface. The initial velocity vector of the ion was directed to the mass center of the cluster. The evolution of the atomic cluster–bombarding ion system was simulated for 5 ps. The bombarding ion energy in different experiments varied from 1 to 800 eV. For each initial energy 500 experiments with different randomly chosen initial coordinates of the Ar ion were executed. The simulation was performed in the framework of the method of classical molecular dynamics (MD) [3]. The interatomic interaction of copper atoms was described by the Ackland potential [4].

To describe the interaction between argon ions and copper atoms, we used the universal Ziegler–Biersack–Littmark (ZBL) repulsive potential [5].

3. SIMULATION RESULTS

The results of the simulation of the time variation in the potential energy of clusters under the influence of bombarding argon ions are presented in Fig. 1. An abrupt variation in the potential energy takes place at the instant of time when a bombarding ion collisionally interacts with the target. The value and the amplitude of oscillations of the potential energy increase with the cluster size. In this case, collective coherent oscillations of atoms in the clusters at the initial time period of the interaction gradually, for 0.1–0.15 ps, evolve to the state of random oscillations in which the potential energy curve passes to the saturation.

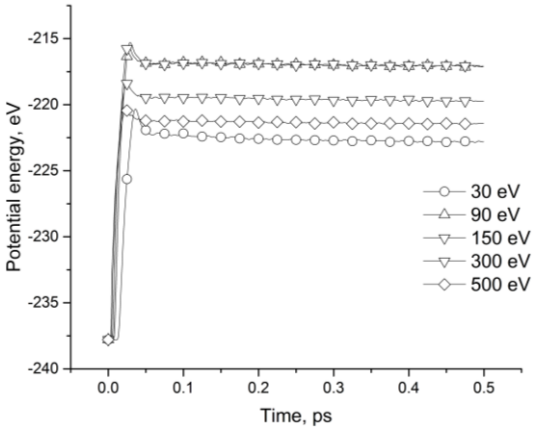

Fig 1 – Time dependences of the potential energy for the cluster consisting of 78 atoms under ion bombardment with energies of 30–500 eV.

As a whole, functional dependences of the sputtering yield from the bombardment energy agree with the conceptions of the sputtering theory, and the increase in the number of sputtered atoms in the given conditions at high energies can be explained by the direct dislodging of atoms from a cluster (Fig. 2).

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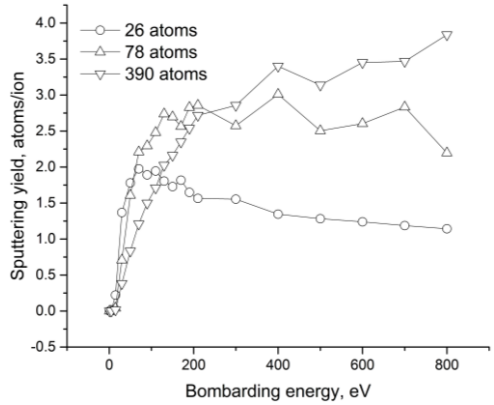

Fig 2 – Sputtering yield for clusters as a function of the initial energy of bombarding Ar ions

As it is evident from Fig. 3, the cluster is heated to the maximum temperature under the ion bombardment with energies of 30–400 eV. The large amount of the energy is carried away by sputtered atoms and the scattered Ar ion at more high initial energies.

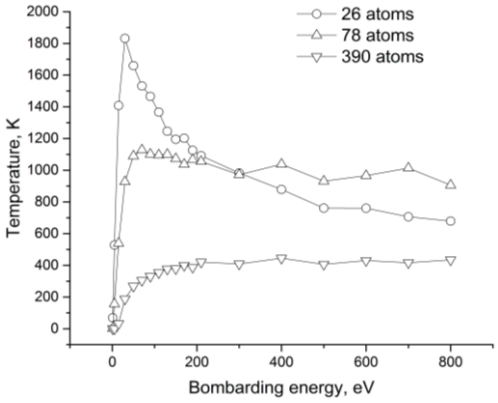

Fig 3 – Cluster temperature vs. the initial energy of bombarding Ar ions.

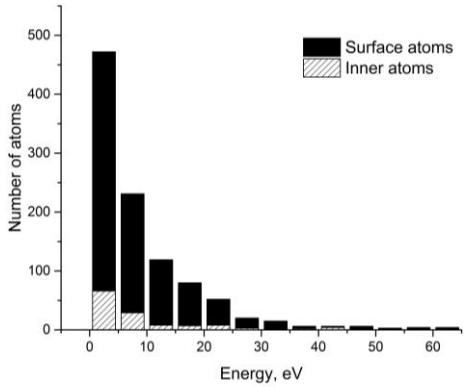

Fig 4 – Energy distributions of sputtered atoms for the cluster consisting of 78 atoms at the impact ion energy of 90 eV.

Fig. 4 presents the energy distribution of sputtered atoms for the 78-atom cluster at the bombarding Ar ions' energy of 90 eV. It is evidently that the maximum number of cluster atoms are sputtered at the energies under 5 eV. We can see that the atoms are sputtered mainly from the surface layer of atoms in the cluster.

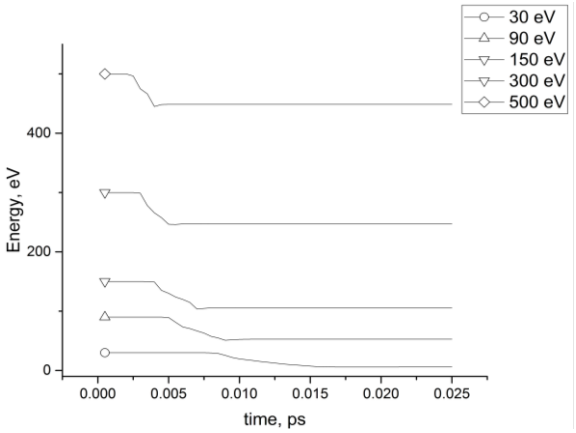

Fig 5 – Energy of bombarding Ar ions during the interaction with a 78_atom copper cluster at different ion impact energies.

The mean Ar ion energy in the process of the interaction with the 78-atom copper cluster was being observed (see Fig.5). The characteristic time of the interaction of a bombarding atom with the cluster does not exceed 0.15 ps, after which the incident ion leaves the cluster. The remaining model clusters demonstrate qualitatively the same dependences.

4. CONCLUSIONS

The molecular dynamics simulation of the free copper clusters of different sizes bombarded by argon ions at the energies from 1 to 800 eV with the use of the Ackland potential was performed. Dynamics of the potential energy as a function of the bombarding particle energy was considered. The maximum temperatures to which the clusters can be heated by such bombardment regime were obtained. These temperatures are 1832 K, 1128 K and 445 K at the energies of 30 eV, 70 eV, 400 eV for the clusters that consists of 26, 78 and 390 atoms correspondently. Single atoms from the cluster surface prevail in the sputtering material. The sputtered atom distribution reaches the maximum at the energies under 5 eV. The sputtering yield reaches its maximum of 1.97 atoms/ion at the energy of 70 eV for the 26-atom cluster and 3.01 atoms/ion at the energy of 400 eV for the 78-atom cluster. Reaching the maximum temperature of the larger clusters at the higher energies of bombarding ions was demonstrated.

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