ENERGY DISTRIBUTIONS OF SPUTTERED ATOMS OF SURFACE METAL NANOCLUSTERS BY LOW-ENERGY IONS

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We have performed the molecular dynamics (MD) simulations of the sputtering of single copper clusters, which consisted of 13 and 75 Cu atoms on (0001) graphite surface, by 100- and 400-eV Ar and Xe ions. Energy effects of the ion sputtering of atoms of isolated surface clusters are discussed.

1. Introduction

An increase of the activity of experimental and model researches of the physical processes running in nanodimensional clusters on different surfaces occurred during the last decade [1–3]. Ion sputtering of and backscattering from Cu clusters consisting of 13-195 atoms on (0001) graphite plane at the bombardment by 100–400-eV Ar and Xe ions were simulated previously [4–7], by using the MD technique. On the other hand, the results discussed in [4–7] do not allow the concise conclusions about peculiarities of the energy distributions of sputtered cluster Cu atoms for both the Ar and Xe bombardments. The energy distributions of sputtered particles from surface nanoclusters were qualitatively compared here with the energy distributions of the linear cascade theory [8–11] for the flat surface of semiinfinite targets. The results of such a calculation for an isolated surface cluster can be compared with the experimental results of sputtering a substrate with a low coverage of clusters. For example, the sputtering yields from an array of well-separated clusters on a substrate can be deduced from these MD results as discussed in [5]. Moreover, the technologically reliable arrays of practically monodisperse surface clusters [12] on single crystals at low coverages can intensify the sputtering regularities of cluster atoms as found for isolated clusters in the MD calculations and allow the comparison with the corresponding experimental data.

2. Model

The analysis was performed for single clusters consisting of 13 and 75 Cu atoms on the (0001) graphite two-layer substrate which consisted of 1584 and 3000 carbon atoms, respectively. Such a substrate is optimal, because it allows keeping the computer time at minimum without falsifying the model results of sputtering from the cluster. The sputtering of the graphite substrate will need a target with more layers, but this question was not addressed in this paper, because only the sputtering of surface clusters was investigated here. The bombardment was simulated for Ar and Xe ions at impact energies of 100 and 400 eV, as well as under the normal incidence. The Tersoff potential [13] with the cut-off radius $R_{(\mathrm{C})\mathrm{cf}} = 0.21$ nm, splined to the Ziegler–Biersack–Littmark potential [14], was applied to the C–C interactions. A tight binding many-body potential directly connected to the Born–Mayer potential [15,16] with a cut-off radius $R_{(\mathrm{Cu})\mathrm{cf}} = 0.55$ nm was used for the Cu–Cu interatomic interactions. The C–Cu interactions were simulated using the Lennard-Jones potential [17] with $R_{(\mathrm{Cu-C})\mathrm{cf}} = 0.375$ nm. The C–Cu potential was splined to the Ziegler–Biersack–Littmark potential.

The ion–Cu and ion–C interactions were simulated, by using only the purely repulsive Ziegler–Biersack–Littmark potential with $R_{(\mathrm{ion-target})\mathrm{cf}} = 0.5$ nm. The trajectories of particles were calculated in accordance to the Newton's equations of motion using the Verlet numerical algorithm [18]. Periodic boundary conditions [18] and a dissipation layer (the Berendsen bath at zero temperature [19]) were applied only to the substrate lateral border atoms. Every ion impact was calculated for 2 ps (Ar) or 3 ps (Xe). For each energy and each cluster size, 2000 impacts were performed with random ion impact points [4]. Every ion impact was chosen randomly in accordance to a criterion [4], which defines impact regions for which the sputtering can occur. The law of energy conservation was executed with accuracy no worse than 1% in all cases. Details of the preparation of the substrate–Cu cluster system are presented in [5].

3. Results and Discussion

The energy distributions of sputtered Cu atoms under the bombardment of 13 Cu atom and 75 Cu atom clusters by 100- and 400-eV Xe and Ar ions are presented in Figs. 1 and 2. The theoretical consideration [8–11] of the energy distribution at keV bombarding energies, within the validity of linear cascade theory, predicts both a maximum at $U_B/2$, where U_B is the surface binding energy, and the E^{-2} dependence at higher energies.

We found from the simulations that the maxima of the energy distributions were for both cluster sizes under the Ar ion bombardment and for a larger cluster under the Xe ion bombardment (shown in Figs. 1 and 2) Only in the case of the Xe ion bombardment for small clusters (shown in Fig. 1 for a 13 Cu atom cluster), there is the strong indication that the maximum of the energy distribution has shifted close to 0 eV. We assume that this deviation of the energy distribution from the theoretical distribution [8] is due to the small cluster size and low bombarding energies and indicates, therefore, a break down of the linear cascade theory. Another reason for the deviation from the linear cascade theory is given by the graphite substrate which acts as a sink for the ion impact energy.

Obviously, heavy Xe ions are able to penetrate into the copper clusters deeper, and they can even directly transfer some part of the kinetic energy to the substrate in some cases, especially in small clusters. Thus, in the case of Xe bombarding ions, a considerable part of the impact energy does not take part in the development of collision cascades in the surface clusters and, finally, in the sputtering. This explains qualitatively why we observe a maximum of the energy distribution around 2 eV for the Ar ion bombardment of small surface copper clusters, whereas the maximum shift towards 0 eV for the analogous Xe ion bombardment. The high-energy tails in the range of 20–50 eV of the energy distributions for the bombardment of larger clusters (75 Cu atoms) by both 400-eV Ar and Xe ions are close to the E^{-2} dependence, as predicted by the linear cascade theory in the case of a planar surface. We did not estimate analytically the distributions of energies of sputtered Cu atoms for more than 50 eV because of the insignificant statistics of sputtered atoms in this energy range. Obviously, some fragments of a surface of large clusters are closer to a flat semiinfinite surface in the case of low-energy collision cascades with an initial energy of 100–400 eV as compared to the surfaces of small clusters (13 Cu atoms), which are critically different and cannot be estimated as planar even for the case of small linear sizes of low-energy atomic cascades. On the other hand, the impact energy of 100 eV for both Ar and Xe ions, especially in the presence of a substrate, as a sink of the cascade energy, does not allow one to create a well-developed collision cascade in a surface nanocluster. Thus, for small clusters and at low energies like 100 eV, no such dependence, which gives evidences about well-developed collision cascades, can be identified. This indicates again the break down of the linear collision cascade mechanism for the sputtering. Even for the Ar ion bombardment, we always observe the maximum of the energy distribution around 2 eV. The results also show that, with increase in the ion impact energy for the same cluster size, a noticeable decrease of the low-energy part of the energy distributions of sputtered atoms (0–8 eV) and a corresponding increase in the high-energy part in the range of more than 20–30 eV is observed for both Ar and Xe ions. Moreover, the contribution of low-energy sputtered Cu atoms to the energy distribution is more considerable in larger clusters as compared with small ones due to the larger number of atomic collisions and the more efficient redistribution of the cascade energy among cluster atoms. The energy distributions of sputtered Cu atoms for the Xe bombardment have shorter high-energy tails as compared with the case of the Ar bombardment, which is clearly visible in Figs. 1 and 2 at an impact energy of 100 eV. The high-energy tail of the energy distribution of sputtered Cu atoms is practically cut off at 20–25 eV for 100-eV Xe ions and at 25–40 eV for 100-eV Ar ions. This is related to the efficiency of energy transfer in the primary collisions of bombarding ions and Cu atoms, which is higher than that in the case of Ar–Cu interactions.

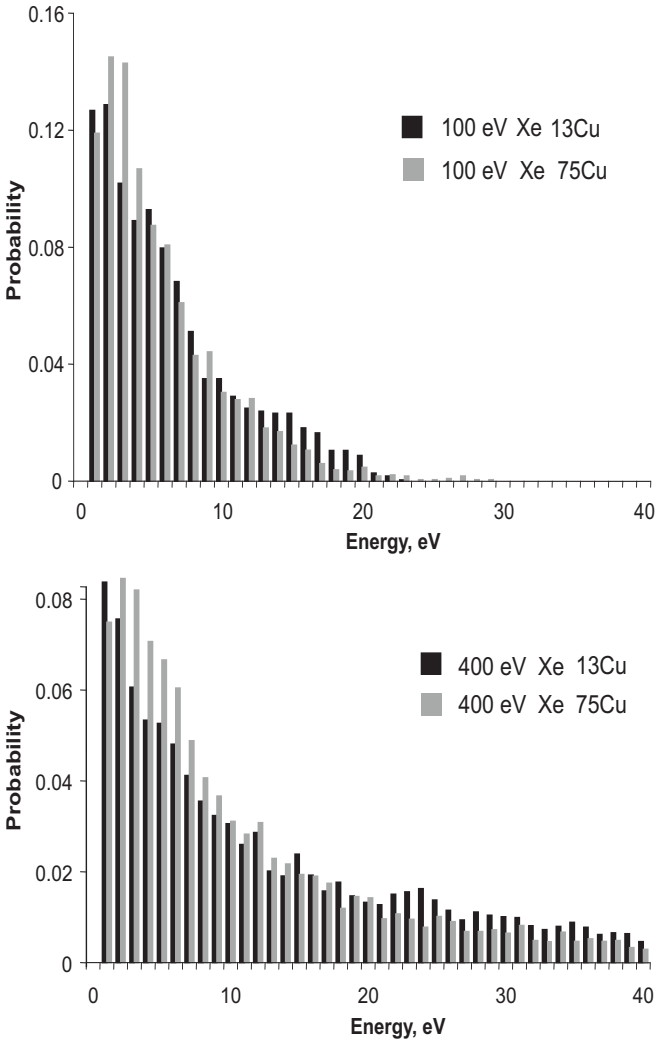

Fig. 1. Energy distributions of sputtered Cu atoms under the bombardment of 13 and 75 Cu atom clusters by 100- and 400-eV Xe ions

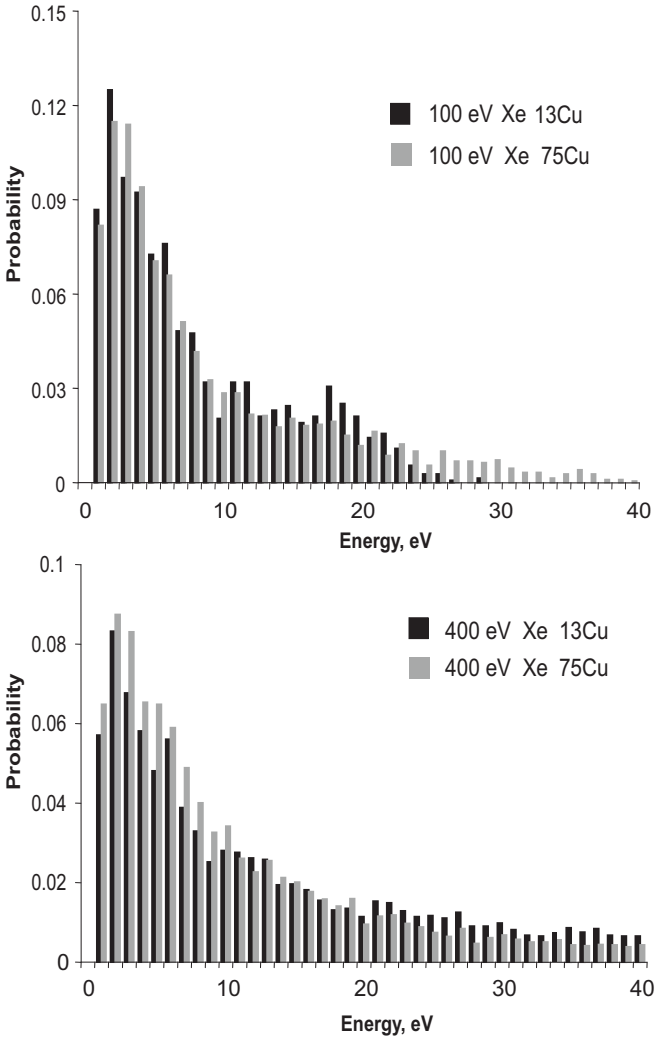

Fig. 2. Energy distributions of sputtered Cu atoms under the bombardment of 13 and 75 Cu atom clusters by 100- and 400-eV Ar ions

4. Conclusion

We have performed the MD simulations of the atomic collisions in surface nanoclusters and the accompanied sputtering of cluster atoms initiated by low-energy bombarding Ar and Xe ions. Except for the smallest cluster, the energy distributions simulated by the MD method show a less deviation from the prediction of the linear cascade theory, as should be expected at these low energies for nonplanar surfaces and in the environment with an energy sink. It is shown that the contribution of low-energy sputtered Cu atoms to the energy distribution is more considerable in larger clusters (75 Cu atoms) as compared with that in small ones (13 Cu atoms).

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ЕНЕРГЕТИЧНИЙ РОЗПОДІЛ АТОМІВ ПОВЕРХНЕВИХ МЕТАЛЕВИХ НАНОКЛАСТЕРІВ, ЯКІ РОЗПИЛЕНІ НИЗЬКОЕНЕРГЕТИЧНИМИ ІОНАМИ

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Р е з ю м е

Виконано молекулярно-динамічне моделювання розпилення поодиноких кластерів міді, що складаються з 13 і 75 атомів, на підкладці (0001) графіту іонами Ar і Xe з енергіями 100 і 400 еВ. Обговорюються особливості розподілу за енергіями атомів, які розпилені з відособлених поверхневих кластерів міді.