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Molecular dynamics simulations of interactions of Ar and Xe ions with surface Cu clusters at low impact energies

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Abstract

Molecular dynamics simulations of sputtering of copper cluster, consisting of 27 Cu atoms, on a (0001) graphite substrate were performed. Ar and Xe bombardment was calculated with ion energies from 100 to 400 eV. Ion energy losses in the target, angular and energy distributions of back scattered ions as well as sputtered Cu atoms and their sputtering yields were examined.

1. Introduction

Investigations of nanodimensional atomic objects, their creation and modification are of interest in electronics, chemistry and biotechnology. Metal clusters are intensively studied nano-objects during the last decade [1–10]. However some aspects of the nature of metal cluster are still outside of researchers' activity. Sputtering of large spherical Au clusters by high energy Au ions was simulated in [11]. On the other hand, low energy sputtering of and scattering from metal nanoclusters, consisting of a few tens of atoms, on different substrates are still poorly available in literature [12].

The present work is devoted to molecular dynamics (MD) simulations of low energy sputtering of copper nanocluster consisting of 27 Cu atoms (Cu_27 cluster) on a (0001) graphite substrate by Ar and Xe ions at 100, 200 and 400 eV. This work is a continuation of previous work [13], in which sputtering of clusters, consisting from 13 to 195 Cu atoms, by 200 eV Ar ions was investigated. Calculations [13] showed that for Cu cluster consisting between 27 and 200 atoms similar sputtering and scattering results were obtained. So, a Cu_27 cluster was chosen for more detailed investigations of its sputtering behaviour at different impact energies. Angular distributions and yields of sputtered cluster atoms were examined. Polar distributions and the mean energies of back scattered bombarding ions as well as ion energy losses in the target were obtained.

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2. Model

The graphite substrate for the Cu_27 cluster included 1920 carbon atoms in two layers. A tight binding many body potential, directly connected to the Born–Mayer potential [14,15] with a cut-off radius of $R_{cf}^{(Cu)} = 5.5\,\text{Å}$, was used for the Cu–Cu interactions. The Tersoff potential [16] with $R_{cf}^{(C)} = 2.1\,\text{Å}$, splined to the Ziegler–Biersack–Littmark (ZBL) potential [17], was applied to the C–C interactions. C–Cu interactions were simulated using a Lennard–Jones potential [18] with $R_{cf}^{(Cu-C)} = 3.75\,\text{Å}$ and also splined to the ZBL potential. The binding energy of the Lennard–Jones potential for Cu–C was 0.11 eV. The ZBL potential was also used for the ion–Cu and ion–C interactions. Every ion impact was calculated during 2 ps for impinging Ar and 3 ps for Xe ions.

The initial copper cluster was obtained from MD calculations. A Cu lattice fragment of the appropriate size was heated to 1700 K and afterwards cooled to 0 K in accordance to a previously used algorithm [8] and put on the surface. Relaxation of the cluster/substrate system was calculated for 40 ps. More details are presented in [13].

Previous simulations [12] for copper clusters on graphite substrates have shown, that more than 99% of all randomly over the whole surface chosen impacts, which will lead to sputtering of a Cu cluster atom fulfill the following 37 eV criterion. Thus in each case 2000 ion impacts normally to the graphite substrate were randomly selected, for which the maximum potential energy of, at least, one ion–Cu pair interaction was larger than 37 eV. In accordance to this criterion the border of ion impact area repeats the form of the external border of the normal projection of the cluster onto substrate surface. For all other impact points the probability of sputtering a Cu atom can be neglected.

3. Results and discussion

3.1. Ion energy losses and depth distributions of bombarding ions

Qualitatively similar distributions for Ar and Xe ions with impact energies between 200 and 400 eV were obtained for the Cu_27 cluster/graphite target. For 100 eV and Xe bombardment no ion penetration into the graphite substrate was found and the backscattering coefficient was close to one. Essentially all the impinging ions are reflected. The backscattering coefficient has a strong energy dependency for both Ar (0.9 (100 eV), 0.66 (200 eV), 0.43 (400 eV)) and Xe (0.98 (100 eV), 0.61 (200 eV), 0.4 (400 eV)) ions. The probability for an impinging ion to come to rest in the Cu_27 cluster is in all cases insignificant. In the Xe–Cu interaction the many-body mechanism of backscattering must be dominant as backscattering during one binary Xe–Cu interaction is impossible due to the larger Xe atomic mass.

Energy losses for Ar and Xe ions in the different layers as well as energy reflection are presented in Fig. 1. The dominant energy loss is in all cases to the cluster. On the other hand, energy reflection is 3–6 times larger for Ar than for Xe ions at the same impact energy. For Ar and Xe energy reflection from and energy deposition to the Cu cluster decrease with increasing ion energy, i.e. the amount of energy deposited to the substrate increases.

3.2. Polar angular distributions and mean energy of backscattered ions

The polar angular distributions of the backscattering probability for Ar and Xe ions have maxima in the range of 60–80° for all cases excluding the case of 400 eV Xe, where the maximum is not clearly visible. All distributions show a uniform low probability part in the polar range below 45°. In addition a small fraction of backscattered ions has polar angles larger than 90°, which is connected with the limited sizes of our model graphite substrate. Thus some backscattered particles will miss the substrate. The observed maximum in the range between 60° and 80° is due to the contribution of particles scattered directly from the cluster and particles reflected from the substrate after being scattered from the cluster, as was discussed in detail in [13]. Generally the backscattering probability decreases with increasing particle energy for all polar angles. The minimum probability occurs at 0° (normally to the substrate surface) in all cases.

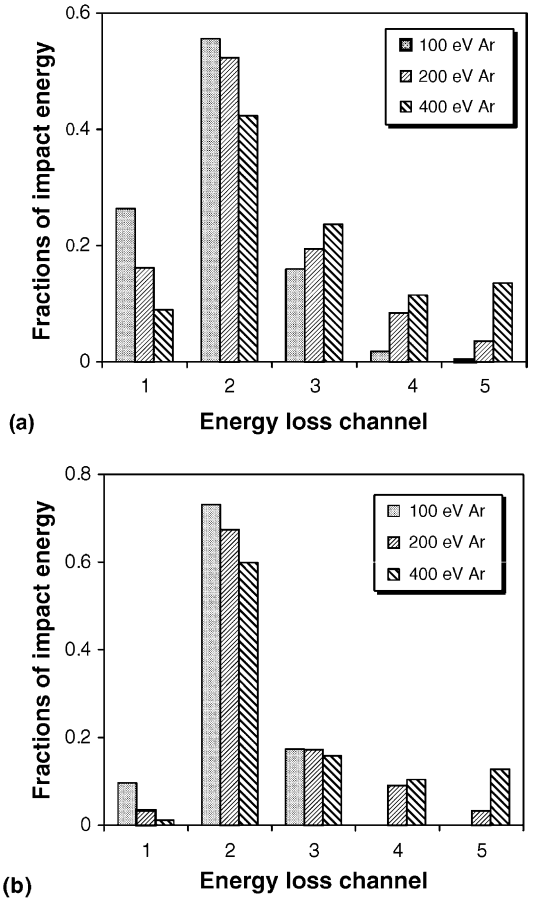

Fig. 1. Depth distribution of the elastic energy loss for 100, 200 and 400 eV Ar (a) and Xe (b) ion bombardment of a Cu_27 cluster on C. Ranges: 1 – backscattered ions; 2 – Cu_27 cluster; 3 – the 1st atomic layer of the graphite substrate; 4 – the 2nd atomic layer of the graphite substrate; 5 – ions penetrating below the bottom of the substrate.

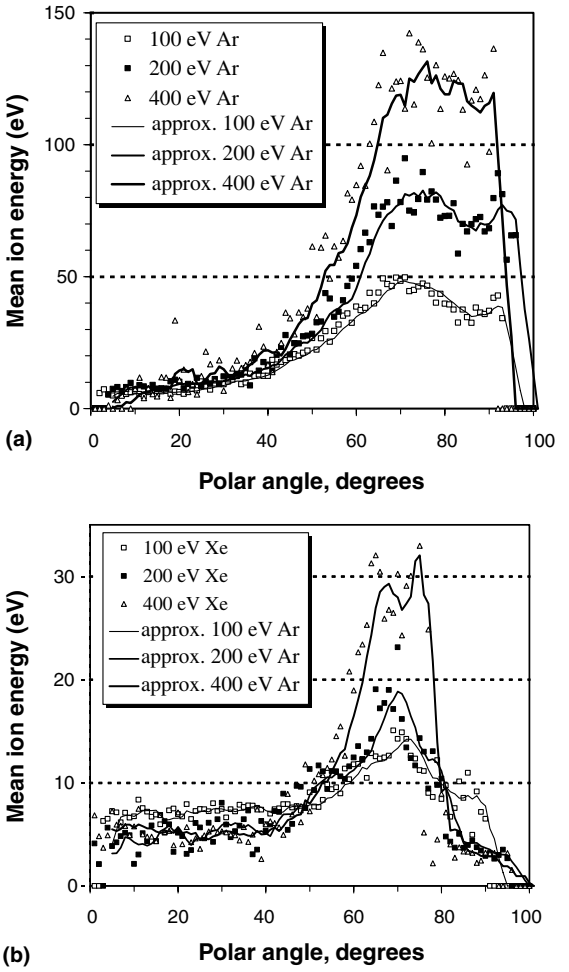

Fig. 2. Polar angular distributions of the mean energy of backscattered Ar (a) and Xe (b) ions, impinging with 100–400 eV on a Cu_27 cluster on graphite substrate. The smoothing curves are drawn to guide the eye.

The polar dependency of the mean energy of backscattered Ar and Xe ions are presented in Figs. 2(a) and (b). For polar angles below 45° the backscattered ions exhibit a low mean backscattering energy, which is similar for all impact energies, but is specific for Ar and Xe ions. In the case of Ar ions there is a slow increase of the mean energy with polar angle, while in the case of Xe ions it is more or less constant. In the case of Ar ions, the polar range below 45° is determined by binary Ar–Cu interactions, as was shown in [13]. In the case of Xe ions the low energy part of the polar distribution is due to many-body collisions or a sequence of two or more collisions, because of the larger mass of Xe.

Two maxima of the mean energy of backscattered Ar ions can be seen in the ranges from 70° to 90°. Only one maximum exists for Xe. The maximum in the mean energy distribution of Ar ions around 90° has the same binary nature as the energy distribution in the range of polar angles less than 45° and cannot exist for reflected Xe ions. The maximum around 70°, which is observed both

for Ar and Xe bombardment, is a result of the superposition of contributions from ions backscattered directly from the cluster and ions, which are scattered from the cluster towards the substrate and then reflected from it (see above).

3.3. Angular distributions and yields of sputtered cluster atoms

The azimuthal angular distributions of Cu cluster atoms sputtered by Xe ions are presented in Fig. 3. Qualitatively both Ar and Xe ions give the same quasi-periodical azimuthal dependency, which consists of six maxima with a periodicity of 60°. It was found that the atomic structure of the Cu surface cluster is strongly determined by the substrate and therefore the cluster exhibits a hexagonal structure corresponding to the (0001) surface structure of the graphite substrate [13]. The maxima of sputtering intensity are connected with the most transparent ⟨1100⟩ directions in the atomic structure of the surface cluster. At 100 eV the six maxima structure is not clearly resolved, partly due to insufficient statistics.

Polar distributions of sputtered Cu cluster atoms at all impact energies for both Ar and Xe ions show an increase of the sputtering probability with increasing polar angle and a maximum in the range of 85–95°. From these angular distributions

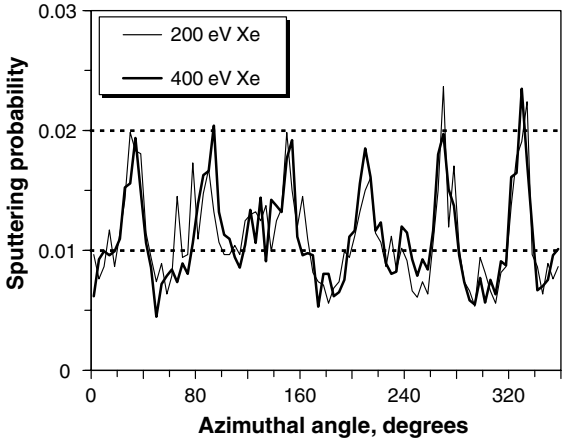

Fig. 3. Azimuthal distributions of the sputtering probability for Cu atoms from a Cu_27 cluster on graphite under 200 and 400 eV Xe ion bombardment.

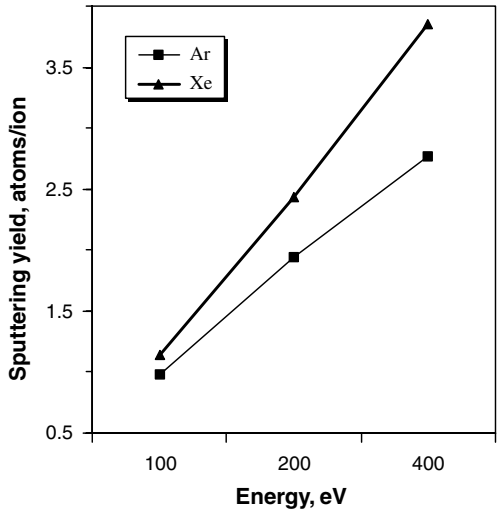

Fig. 4. Sputtering yields for a Cu_27 cluster on graphite for 100–400 eV Ar and Xe ion bombardment.

we can conclude that the largest part of sputtered cluster atoms move into directions nearly parallel to the graphite substrate surface.

Values of the Cu sputtering yield are presented in Fig. 4. Yield values for Xe are larger at all energies, than for Ar bombardment. Moreover, the difference increases with increasing impact energy. We consider that this peculiarity of the sputtering yield energy dependency is determined essentially by the energy deposited in the cluster, which can be estimated using Fig. 1. In addition we found, that for Xe bombardment the contribution of sputtered dimers and trimers was about twice as large as for Ar bombardment at all bombarding energies. For Ar the values for Cu atoms sputtered in the form of many-atomic Cu particles were 4.0% (100 eV), 9.0% (200 eV) and 11.0% (400 eV). For 400 eV Xe ions fragmentation of the whole cluster followed by the emission of large chunks (up to 19 atoms) was observed.

4. Conclusion

MD simulations of sputtering of a Cu_27 cluster on (0001) graphite substrate at bombarding energies from 100 to 400 eV for Ar and Xe ions have been performed. The backscattering coefficients for Ar and Xe ions are similar, while the

mean energy of backscattered Xe ions is 3–6 times smaller than for Ar ions, which is connected with a different mechanisms of back scattering of Ar and Xe ions, i.e. binary versus many body interactions. This difference is also visible in the polar distributions of the mean energy of backscattered Xe and Ar ions, where one or two maxima are observed, respectively. Sputtering is mostly into directions parallel to the substrate surface. For the azimuthal distribution of sputtered particles a periodical structure with six maxima was observed in all cases. Sputtering yield values for the Cu_27 cluster are larger for Xe ions as compared to Ar ions for the whole energy range.

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