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Sputtering and reflection of self-bombardment of tungsten material

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ABSTRACT

In present research, the sputtering and reflection yield of self-bombardment of tungsten are investigated with the aid of molecular dynamics simulations. The source of sputtered and reflected atoms is detected by traced the original locations of sputtered and reflected atoms. Results show that for the reflected atoms no specific region exists which means cluster atoms are randomly reflected. But almost all of sputtered atoms are from a conical region under the landing point of cluster. So we can determine the sputtering yield by study the dimension of the sputtering region. Molecular dynamics shows the depth and radius of the conical are power functions of impacting energy. The effects of cluster size and temperature of target on sputtering and reflection rate are also preformed in present study. Both sputtering and reflection yield are proportion to cluster size in present cluster size, i.e. 66–2647 atoms. Higher target temperature can increase sputtering yield and deduce sputtering threshold energy, but little effect on reflection rate.

1. Introduction

Studies on the interactions between energetic cluster and solids can be applied in a series of fields such as cluster deposition [1,2], implantation [3,4], surface smoothing [5–7] and modifications [8–10], thin-film growth [11,12], secondary ion mass spectrometry (SIMS) [13,14], etc. The landing process of dust particles in planets and comets is also a further application of cluster impacting studies [15]. The cluster impacting process involves complicated physical process. For example, cluster can generate high-density and high-energy region under land point which is different from monatomic bombardment[12,4]. According to the impacting energy, clusters can soft land or implant on target, with different effects on target surface [3,16]. Soft landing clusters may form thin-film on the surface without damage it [17–19]. Implantation, however, can generate crater and produce sputtering atoms [20,21]. Sputtering yield of energetic clusters have been studied both experimentally and theoretically [22,23]. With the aid of molecular dynamics (MD) simulations, fruitful results have been obtained [24–27]. The angle dependence on sputtering has been discussed in Ref. [28] and other relative references. The effect of binding energy and mass in cluster-induced sputtering has been published in Ref. [29]. Anders et al. used rational function to fit sputtering and reflection yield versus impacting energy [22,30].

In present research, we investigate the sputtering and reflection yield using molecular dynamics method. In particular, we want to learn about the relation between impacting energy and sputtering and reflection rate. The source of sputtered atoms is another question of our concern. The size of cluster and temperature of target are also taken into account in present study. Our results may be helpful to understand the mechanism of cluster sputtering.

2. Method

Molecular dynamics (MD) is applied to study the interaction between cluster and target. Both the materials of cluster and target are tungsten (W). An open code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code is used to perform MD simulation [31]. The model used to describe the interactions between W atoms is embedded atom method (EAM), namely, Finnis–Sinclair potential [32]. A repulsive pair potential named Ziegler–Biersack–Littmark (ZBL) is used when distance of two atoms is smaller than 1.6 Å to improve the compressibility at high pressures [33]. The structures of W clusters and W material are body-center-cubic (BCC) and the lattice constant for tungsten is 3.1652 Å. The (001) plane is normal to cluster impacting direction. Automatically adapted time step is used, the minimum and

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maximum time step are 0.0001 fp and 1 fp, respectively. The system sizes are selected based on both energy and size of cluster and the maximum size of target is 2,894,400 atoms. For each collision case two different sizes are selected to exclude size dependence. Periodic boundary condition is for the directions perpendicular to the normal direction of W material surface and non-periodic boundary condition for the parallel direction. Three temperature of the system are selected, viz. 0 K, 300 K and 650 K. The shape of tungsten clusters is spherical and broken sphere in order to exclude shape dependence. The size of clusters ranges from 66 to 2647 atoms/cluster and the energy is 2–500 eV/atom.

3. Results and discussion

3.1. Source of reflection and sputtering

The total sputtering yield of cluster impacting can be divided into two contributions, i.e. sputtered atoms from target and reflected atoms from cluster, $Y_{\text{total}} = Y + R$. Fig. 1 investigates the original locations of sputtered and reflected atoms in order to study the source of sputtering and reflections. The slash shadow part is the profile of final state of cluster–target interactions, where a significant crater forms. The points stand for the original location of sputtered and reflected atoms. There is no significant place tendency of reflection in cluster, which means cluster atoms are uniform randomly reflected. We also used broken and half spherical clusters to perform the same simulation and still no significant place tendency is found. So we reasonably conclude that the distribution of reflected atoms is independent on the shape of cluster.

But for target material, most of the sputtered atoms concentrate in the conical region just under the landing point of cluster, which is the region 1 in Fig. 1. The dimension of region 1 is determined by the impacting energy of clusters. Region 2 is the space between sputtering region and crater surface. The atoms in this place are not sputtered out of target but to form interstitial atoms and penetrate into deeper part of the material. The place labeled region 3 is not significantly influenced by cluster impacting. It is obvious that the volume of region 1 is the key factor which determines the sputtering yield Y.

3.2. Reflection and sputtering yield

Fig. 2 shows the reflection rate as a function of normalized incident energy $\epsilon = E/(NU)$. E is the total kinetic energy of cluster, U is the cohesive energy of target material, $U = 8.9$ eV for tungsten. N is the number of atoms in cluster, in Fig. 2, $N = 1036$. The reflection

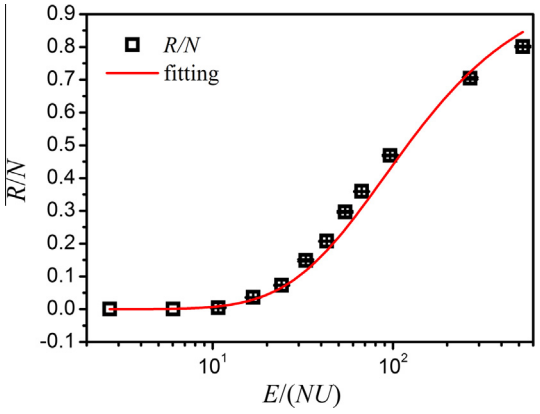

Fig. 2. Reflecting rate R/N as a function of impacting energy.

yield R is normalized by N. We find that when $\epsilon < 6$, the number of reflected atom R/N is zero. When $\epsilon > 6$, $R > 0$ but the increasing speed of R/N is slow. In such case, most of the cluster atoms are deposited on the target surface. When $\epsilon > 16$, more cluster atoms are sputtered so the increasing speed grows until $\epsilon \sim 250$. When $\epsilon > 250$, the increasing speed become slow again. This is because the reflection rate R/N cannot be over 1. The solid line in Fig. 2 is the fitting line using the following equation [30]:

$$\frac{R}{N} = \frac{\epsilon^f}{(\epsilon_c + \epsilon)^f} \tag{1}$$

where ϵ_c and f are fitting parameters, the values of them are 18 and 4.5, respectively. When $\epsilon \to 0$, $\frac{R}{N} \to 0$ and $\epsilon \to \infty$, $\frac{R}{N} \to 1$.

Anders and Urbassek simulated the reflection rate R/N of self-bombardment of Cu material [30]. The fitting parameters of Cu_{1000} is $\epsilon_c = 33$ and $f = 2.76$. The cohesive energy of copper U is selected 3.54 eV. R/N becomes quite close when $E/(NU) > 17$. But when impacting energy is less than this value, R/N of Cu cluster is greater than that of W. For example, when $E/(NU) = 6$, $R(Cu)/N = 0.02$ while $R(W)/N = 0$. This may be lead by different cohesive energy of cluster. The cohesive energy of Cu is 3.54 eV and 8.9 eV for W. In low energy case, Cu clusters are more easier to be reflected because Cu cluster is easier to be broken into atoms. The reflection rate of Ar_{1000} cluster in the same paper is greater than that of Cu, which supports the idea. The cohesive energy of Ar cluster is 0.082 eV.

Fig. 3 shows the comparison of sputtering yield and the number of atoms in sputtering region as a function of normalized incident

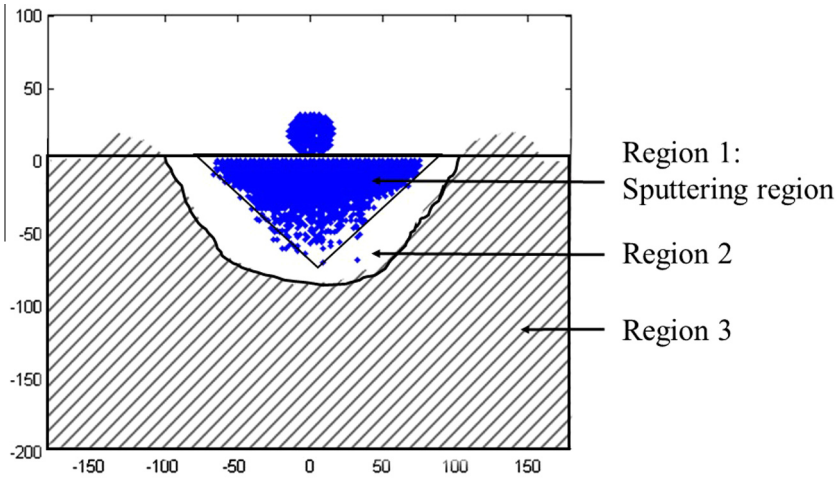

Fig. 1. Original location of sputtered atoms.