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The influence of landing points on the sputtering of mono-crystal solids due to cluster impacting

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ABSTRACT

The mechanism of sputtering due to cluster impacting which has been widely studied is an important but unsolved problem. In present research, we discuss the effect of the landing point on the sputtering with the method of molecular dynamics. The results show that the landing points play significant roles on sputter yield when the temperature of target is low. Specific landing points can cause particular sputtering patterns which lead to different sputtering yield and moving directions of sputtered atoms. The mechanism of this phenomenon is that specific landing keeps symmetries and anisotropies of target lattice, which influence the sputtering yield.

1. Introduction

The sputtering phenomenon due to the bombardment of single-particle or cluster is a process of both practical and fundamental importances in many fields [1]. A series of application fields develops very fast such as self-organized periodic erosion patterns at nano-scale induced by ion bombardment [2,3], nano-structured surface growing due to cluster impacting [4], surface smoothing [5,6], sputter enhancing related to the explosive ejection of large clusters [7], steep surface treatment[8] etc. The hyper-velocity impact of interstellar nano-grains is also a potential field of sputtering theory for the erosion features of the surface of spacecraft [9], thrusters [10] and other astronomical objects [11]. The plasma contamination owning to the sputtering of plasma-facing materials is a focused problem for fusion science[12].

Although both experiments [13–15] and simulations [16–19] have been performed for the interactions between various clusters and solids [20–22], the understanding of cluster sputtering process is still not clear enough comparing to the well-developed mono-atomic sputtering theory. The reason of the lack of clearness mostly is caused by the complexities of the cluster-surface interaction process. According to the current knowledge, atom mass, incident energy [23,24] and angle [25,26], cluster charge [27] and the properties of target solid (surface binding energy and components [28], for example) play important roles in cluster sputtering which is similar to mono-atomic sputtering [1]. But owning to characteristics of the cluster, external complexities are induced in sputtering process. On one hand, more factors affecting the sputtering yield are involved. For example, the size effect of the cluster can enhance the sputtering yield [29,30]. Also, the distribution of different components of the cluster is a factor affecting sputtering yield. Higher temperature which is mostly ignored in mono-atomic sputtering contributes to sputtering yield [31]. On the other hand, the collision process is different from and more complicated than that of mono-atomic impacting, as Samartsev pointed out in the reference [32]. The non-linear and non-additive effect of cluster sputtering reported by Belykh [33,34] is an example of this complexity. And C. Szakal illustrated the surface sensitivity in cluster sputtering from the experiments of Au_mimpacting in reference [35]. Discussions on experimental observation of velocity-correlated cluster emission are published in [36]. Chernysh reported a new mechanism of sputtering in Ref. [37]. However, the study of the mechanism of cluster sputtering is still far from satisfying.

In present research, we discussed the effects of the cluster landing location on target with the method of molecular dynamics simulation. In the following sections, we will firstly introduce the simulation and describe methods in Section 22 and in Section 3, discussions of the simulation results are performed. A conclusion is given in Section 4.

2. Methods

A classical molecular dynamics (MD) simulation is carried out to trace the temporal evolution of the sputtering process with

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the aid of an open source MD code LAMMPS [38]. Both the materials of cluster and target are tungsten (W). The lattice of W is body-centered cubic (BCC) and the lattice constant is 3.165 Å [39]. The binding energy is 8.9 eV[40]. The size of the cluster is 12 Å, containing 524 atoms. The exactly impact velocities of Stardust around low Earth orbit is not clear, but the average value is around 16 km/s [9]. In fusion devices, hyper-velocity dusts move at a speed beyond 10 km/s [41]. Based these facts, the incident speed of the cluster in present research is 20 km/s. The geometry of the simulation system is described by Cartesian coordinates. The x- , y- and z-directions correspond to the [100], [010] and [001] crystallographic orientations, respectively. The solid block is in the range of $[-x_{length}/2, x_{length}/2], [-y_{length}/2, y_{length}/2], [-z_{length}, 0]$, where $x_{length} = 760$ Å, $y_{length} = 760$ Å and $z_{length} = 633$ Å are the dimensions in x- , y- and z-directions, respectively. The size has been tested to make sure it is big enough for present simulation, namely, no significant movements in the entire simulation process. Periodical conditions are applied in x- and y-directions. Before the impacting of cluster, a five-femtosecond(fs) relaxation of the solid is performed to minimize the total energy of it. Different kinds of landing points are selected which will be stated in the following parts. The temperature of the solid is 0 K or 300 K. An automatically adapted time step is used and the minimum and maximum time step is 10^{-2} and 1 fs, respectively. To be close to reality, we set a thermal bath layer around the solid. The thickness of thermal bath is two atom layers. Embedded atom method (EAM) potentials are applied to describe the forces between W atoms which is developed by Finnis and Sinclair [42]. The potential is combined with the ZBL [43] potential to improve the accuracy of forces when two atoms are close.

In order to discover the influence of landing points, four particular locations are selected, namely, center, corner, diagonal and side positions. Three parallel simulations have been performed for each specific landing meanwhile five MD simulations carried out for randomly landing to obtain reliable statistics. Fig. 1 shows one crystal lattice at the very surface of target material. Corner position refers to the location just on one atom. The diagonal position means the locations on the diagonal lines ([110] or [1 −10] directions) and the side refers to location on the edge ([100] and [010] directions). Center position corresponds to the intersecting point of two diagonal lines.

3. Results and discussions

3.1. The influence on sputtering yield

The sputtering yields of cluster impact at different landing points are shown in Fig. 2. The velocity of the cluster is 20 km/s as previously mentioned. It can be seen that sputtering yield depends on the landing point of the clusters. The sputtering yield Y_s is about 3.5, 2.6, 3.3 and 2.5 for center, corner, side and diagonal location, respectively. Here Y_s refers to the number of sputtered atoms divided by the number of atoms in cluster. Because the temperature of target is close to zero, the error bar for the selected locations is so small that it cannot be seen in the figure. If the landing point is not specifically selected (randomly selected), the average sputtering yield is 1.8, which is much less than that of specific landing locations. The error bar is large comparing to that of the specific selected landing points. The standard deviation is about 0.9.

The reason of this phenomenon is illustrated in Fig. 3. The graph shows the top view of sputtering patterns for every kind of impacting landing. Top view refers to the sight along the cluster impacting direction. The graphs labeled from (a) to (e) present the center, corner, diagonal, side and random landing locations sequentially. Each graph contains points presenting the original location of the atoms which are sputtered out of W target. The criteria of determining an atom is sputtered is the distance between the atom and target surface. When the distance is greater than $10c \approx 32$ Å where c is lattice constant, the atom is sputtered. For W, $c = 3.165$ Å. The term "original location" refers to the atom's location before cluster impacting. The purpose of doing this is to investigate the source of sputtered atoms. The 3D views of the original locations of sputtered atoms can be seen in the videos.

It can be seen that the patterns of different landing location have particular characteristics due to the symmetries and anisotropies of target lattice. For the body-centered cubic lattice, four symmetry axes exist (in the surface plane), e.g. the [100], [010], [110] and [1 −10] directions, as shown in figure (f). The diagonal directions ([110] and [1 −10]) are the same essentially while the axis directions ([100] and [010]) are equivalent. Although the sputtering yields are not equal, the sputtering patterns of center and corner landing are quite similar, as shown in Fig. 3(a) and (b). The atoms in both axial and diagonal directions are more likely to be sputtered, especially the ones along diagonal directions. The

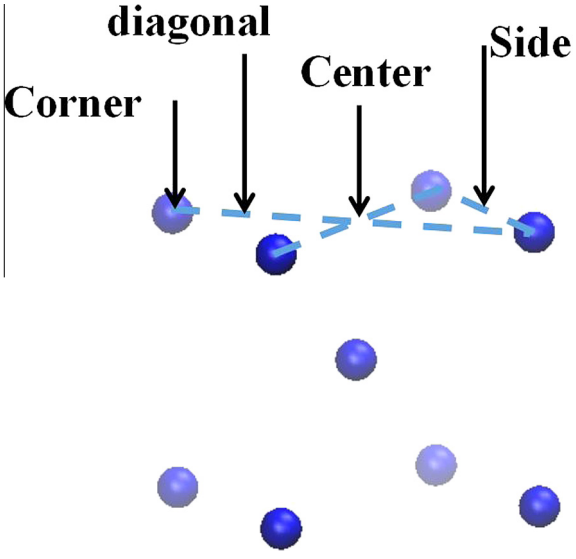

Fig. 1. Locations of four specific landing points.

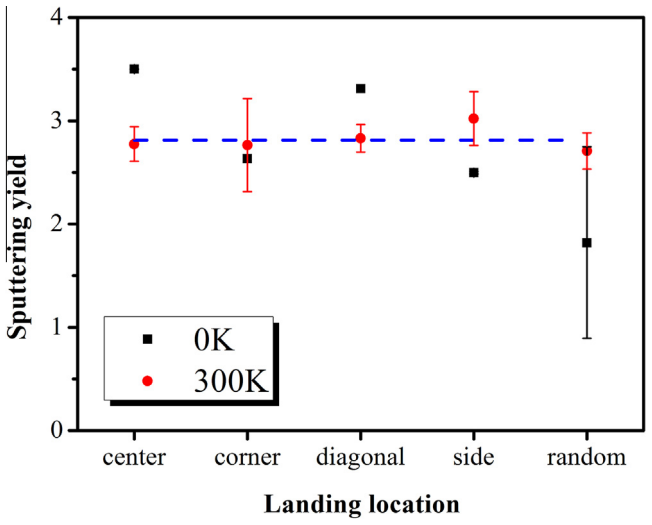

Fig. 2. Sputtering yield of cluster as a function of landing location.

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