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Molecular dynamics simulation study of damage formation and sputtering with huge fluorine cluster impact on silicon

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ABSTRACT

Damage formation and sputtering processes by large reactive cluster impact on solid target were studied by molecular dynamics (MD) simulation. A $(F_2)_{500,000}$ cluster was accelerated at 1 MeV (1 eV/atom, 3.2 km/s) and projected toward a Si(100) target which consisted of more than 130,000,000 atoms. The MD simulation result showed that wide and shallow crater is formed due to the impingement of the bottom part of the incident cluster. The target atoms in a large area surrounding the impact point were largely displaced and some of them remained as a point defect or as a stacking fault, which reached more than 10 nm deep into the target surface. By the single impact of the cluster, about 12,000 silicon atoms were desorbed into the vacuum. The desorbed products were in the form of not only mono-silicon fluoride but also in larger silicon-fluoride composite clusters. The distribution of initial position of desorbed silicon atoms showed that most of desorbed products were generated in the region close to the crater edge corresponding to the radius of incident cluster.

1. Introduction

The gas cluster beam process, which generates an aggregate of molecules/atoms and is radiated on solid target material in the form of energetic beam, has been demonstrated as a promising method for surface modification such as high yield sputtering and surface smoothing [1]. Various experiments [2,3] and simulations [4,5] have been performed over the last decade to understand these characteristic radiation effects of gas clusters, in terms of cluster size, incident energy and material properties of both cluster and target. In these previous works, the typical cluster being studied contained several hundred to several ten thousand in size and had several to several tens of keV energy. These fundamental and application studies raised the potential of the larger cluster impact for a material modification process. For example, it has been reported that energetic nano droplets used in the electro-spray method, which consists of more than ten thousand molecules, is available for the etching of hard materials such as SiC and B_4C [6]. Another example is the supersonic injection of clusters of ClF_3 to a Si target, which has demonstrated high speed and directional etching [7,8]. The latter example is of interest from the view point that huge and reactive cluster can etch a target at a much lower velocity of impact compared with previous works. The impact processes of reactive clusters with the size up to 100,000 and energy up to 1 eV/atom have been studied by our group, which suggests that enhancement of surface reactions and chemical reactions occur in the near surface region without much surface damage [9], but the collisional process for larger cluster is not clear. In this paper, we performed large scale molecular dynamics simulation of fluorine cluster with 1,000,000 atoms impacting on a silicon target. The collisional process of damage formation and sputtering mechanism of surface atoms are discussed.

2. Simulation model

In this work, the collisional process of fluorine clusters is analyzed by means of molecular dynamics simulations. In order to describe the interactions between Si–Si, Si–F and F–F, the Stillinger and Weber (SW) type potential model was applied. The SW type potentials were developed by Stillinger et al. [10,11] and modified by Weakliem et al. [12]. A F_2 cluster consists of 500,000 molecules (1,000,000 F atoms totally) was prepared as the projectile. This cluster was annealed in the simulation at 10 K before impact using the Langevin dynamics method, and then impacted normally onto a solid target. A Si(100) substrate was prepared as a target material. The target consists of about 130,000,000 atoms and its dimensions were 173 × 173 × 86.5 nm (320 × 320 × 160 unit-cells). The Si atoms which reside within 1 unit cell length from the bottom or sides of the target were fixed in diamond structure. A thermal bath

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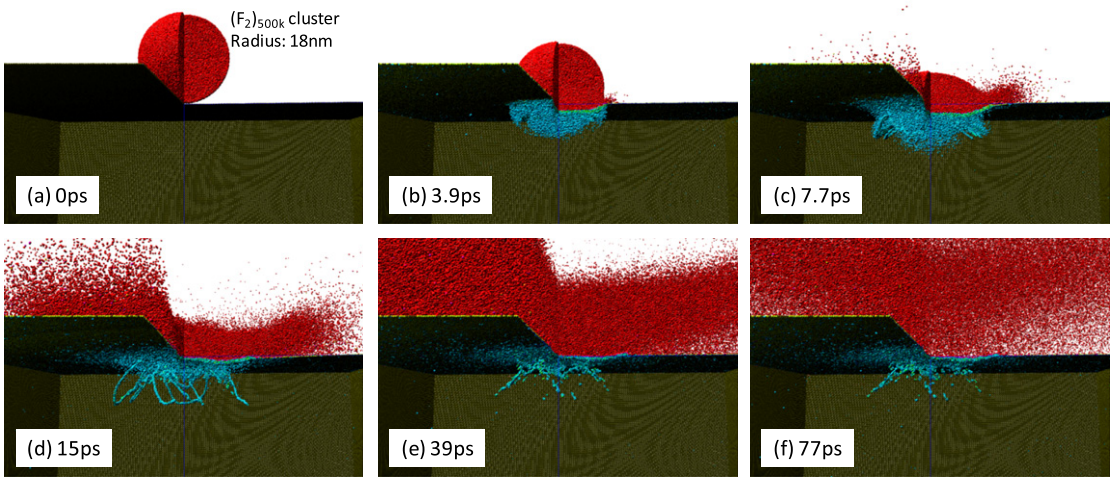

Fig. 1. Snapshots of $(F_2)_{500,000}$ cluster impacting on Si(100) target. Only fluorine atoms and silicon atoms belonging to surface planes and displacement are drawn. A quarter part of the target is removed.

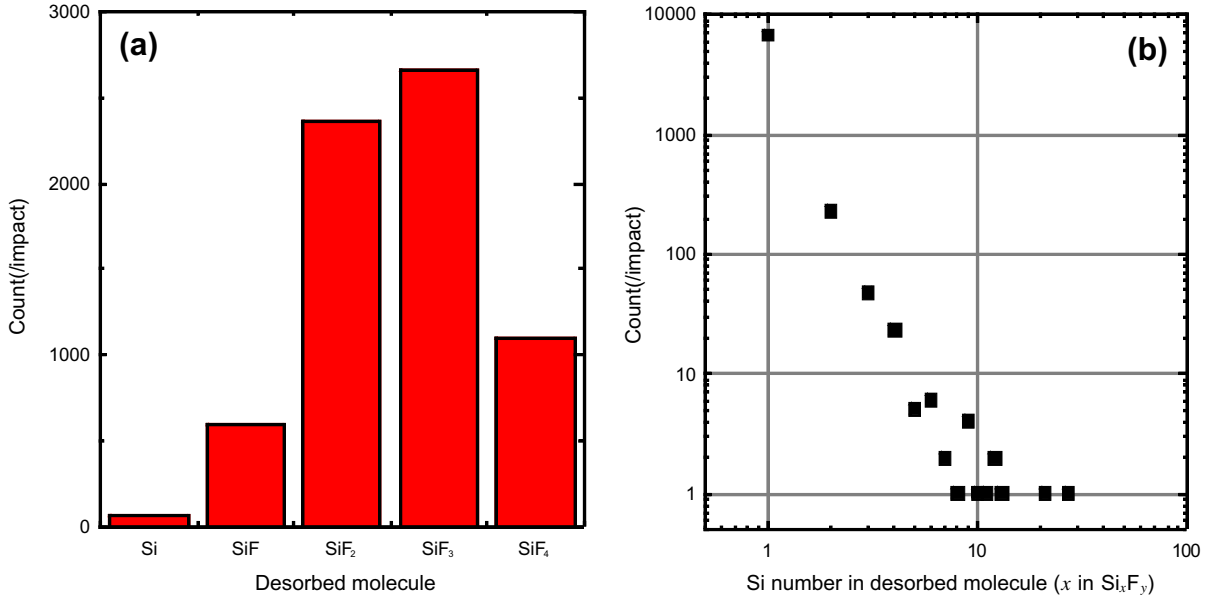

Fig. 2. Number of desorbed molecules by a single cluster impact. (a) Distribution of mono silicon fluorides only. (b) Distribution of all desorbed molecules as a function of the number of silicon atoms in the molecule.

was introduced for a cylindrical region that is more than 73 nm from the surface and 73 nm from the impact point. The thermal bath was governed by the Langevin dynamics method to keep the substrate temperature at 300 K and absorb excess kinetic energy given by cluster impact. Before the impact of the cluster, the target is optimized to construct 2×1 surface structure. The impact simulation was run for 77 ps, which is enough long to observe, the penetration and reflection of the incident cluster, and compression and relaxation of the target. On the other hand, it should be noted that, the starting target material in this work is bare silicon and only single impact was performed, so that the simulation represents the initial stage of huge cluster impact, not the steady state expected for real experiments, where the surface is covered with silicon fluoride compounds.

3. Results and discussion

Fig. 1 shows snapshots of the MD simulation result. A fluorine molecule cluster $(F_2)_{500,000}$ impacts onto a Si(100) target surface. The incident energy is 1 MeV for the whole cluster, which means that each fluorine atom has 1 eV/atom of kinetic energy or 3.2 km/s of velocity along the normal of the target surface. A quarter part of the simulation area is removed to show the cluster-surface interface and displacements which grow and reduce in the target. In Fig. 1, all F atoms and Si atoms belonging to surface planes or displacement are drawn. The displaced Si atom is defined as the atom whose potential energy is 0.2 eV different from the bulk state [13]. As discussed in the previous work [5,9], the threshold where the large cluster penetrates a target surface is mainly dominated by the incident energy per atom, and the threshold energy for fluorine molecule cluster and has been reported as about 0.3 eV/atom. Thus, the collisional process in Fig. 1 also demonstrates that, some atoms penetrate the target surface and generate the crater with a shallow depth and a wide opening radius at the impact point. Fig. 1 also shows that some of fluorine molecules decompose and bind with surface silicon atoms.

As for the displacements in the target, it is shown that, at the initial stage of the collision (Fig. 1(b)), high density displacements

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