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Large-scale molecular dynamics simulations of highly accelerated cluster impact on diamond surface

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Abstract Large-scale molecular dynamics simulations with high acceleration energy cluster impact on a diamond surface are performed in order to investigate the surface erosion process. A CO_2 cluster of 960 atoms with different acceleration energy (10, 50 and 100 keV/cluster) impacts on the (1 1 1) surface of diamond that consists of more than one million carbon atoms. A typical transient crater and two or three-layered shockwaves are formed for 50 and 100 keV impacts while only small elastic deformation can be seen for 10 keV. The kinetic energy and the volume of the crater are almost linear functions of the acceleration energy, but the erosion is only enhanced by the 100 keV impact. A strong peak of CO appears in the size distribution of the evaporating clusters in that case.

1
Introduction

Various possibilities have been reported on the applications of atomic or molecular cluster beams for surface modification including deposition, ion implantation, polishing, and chemical and physical erosion [1, 2]. The authors' group has applied highly accelerated ionized cluster beams as the erosion source of nano- and micro-scale surface structuring [3, 4]. In this technique, clusters consisting of about 1000 CO_2 molecules are accelerated up to 100 keV. The impact-induced high energy density creates reactive plasma of cluster and surface material, and therefore, the technique is called reactive accelerated cluster erosion (RACE). Very smooth eroded surfaces were obtained with continuous impacts for various materials ranging from teflon, silicon, glass, and diamond. Especially for artificial diamond, the erosion resulted in a much smoother surface than the original one. Considering also the results by single impacts, the surface smoothing seemed to be ascribed to the fluidization of the surface material. In addition, non-reactive argon cluster impacts resulted in a smoother surface compared to CO_2 impacts although the erosion rate was about 4 times lower. The technique has a potential as a direct micro-machining tool.

We have performed molecular dynamics (MD) simulations of cluster impacts on a diamond surface [5] in order to investigate the surface erosion process, and single impacts of argon and CO_2 with the acceleration energy of 100 keV have already been carried out. In that case, a hemispherical crater was once created after the impact and two or three-layered shockwaves were formed, but the crater was immediately filled up with the fluidized hot carbon atoms due to elastic recovery. In addition, compared to the argon cluster impact, the CO_2 cluster impact induced significant evaporation of the surface material with the activated carbon and oxygen atoms from the cluster, and that corresponded well to the experimental result.

In this paper, the crater formation and erosion effect by CO_2 cluster impact is studied further with different acceleration energies by using the molecular dynamics simulations in order to examine the physical phenomena on the surface in detail.

2
Method

The detail of the calculation is described in our previous report [5]. The empirical potential function proposed by Brenner [6] is applied for the interaction among carbon atoms, and the interaction potential of C-O and O-O were constructed based on Brenner's formula.

The diamond (1 1 1) impact target consists of a hexagonal internal full-simulated surface region and a surrounding external region. Only 1/6 of the external region is simulated, and its symmetric images are connected with the internal region to reduce the calculation time. The internal and external regions contain 758,440 and 308,240 carbon atoms, respectively (2,584,741 carbon atoms including virtual images). The vertical depth and the length of the diagonal line of the internal region are about 115 and 122 Å, respectively, and the external region extends by another 50% of the symmetric region. The outer boundary of the external region is fixed and the temperature is controlled at 300 K near the outer boundary with the Langevin method.

The impact cluster contains 960 CO_2 molecules in accordance with our experimental data [3]. Verlet's method was adopted to integrate the equation of motion with the time step Δt of 0.2 fs for the first 2 ps and 0.5 fs afterwards.

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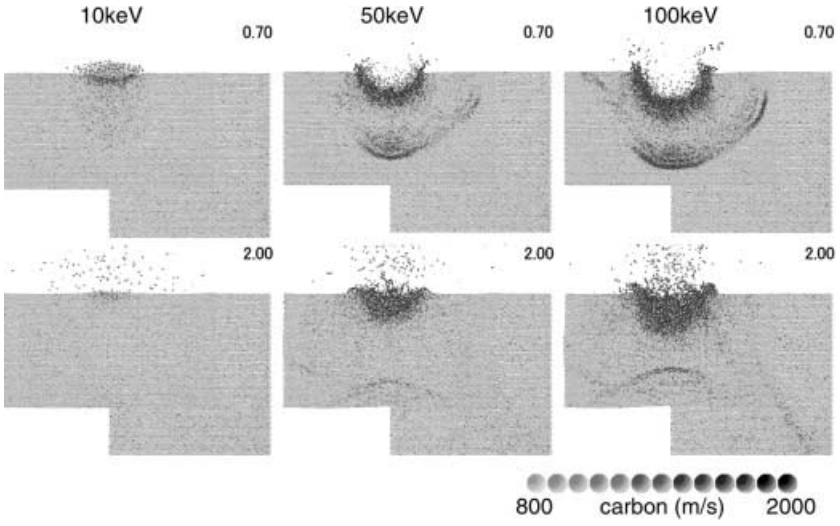

Fig. 1. Snapshots of impact induced surface structures at 0.7 and 2 ps after the impact for different impact energies

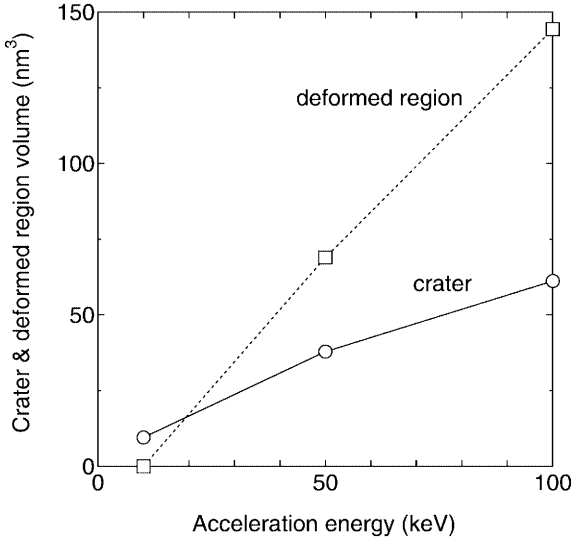

Fig. 2. Volumes of the crater and the deformed region as a function of the cluster acceleration energy

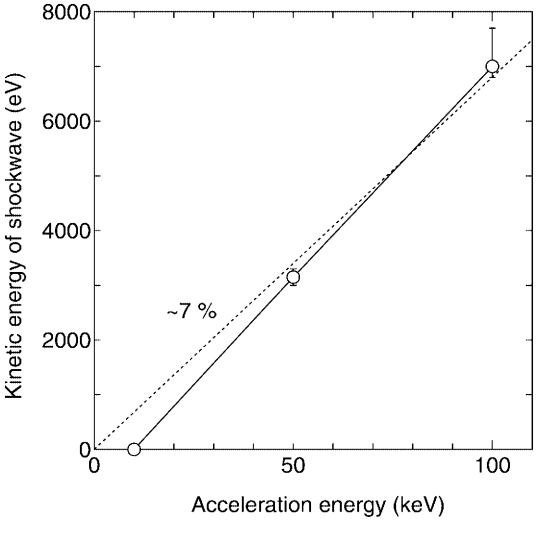

Fig. 3. Kinetic energy transferred to the outer-region by the shockwave as a function of the cluster acceleration energy. The dashed line corresponds to 7% of the cluster acceleration energy

3 Results and discussions

Figure 1 shows snapshots of the simulations for acceleration energies of 10, 50 and 100 keV, where a 10 Å sliced view parallel to the impact direction is shown, and atoms with larger velocity have darker color. A typical transient hemispherical crater appears in cases of 50 and 100 keV about 0.7 ps after the impact, and two or three layered shockwaves can also clearly be seen. The propagation direction and the velocity of the shockwave are almost the same for these two energies. On the other hand, only a simple elastic surface deformation can be seen for 10 keV impact, and the shockwave structure is also difficult to determine.

All of the impact-induced craters are immediately filled up with the fluidized carbon materials due to the elastic recovery before 2.0 ps without an effect of the reflected shockwave.

Figure 2 shows the volumes of the crater and the deformed region calculated as a hemispheroid, where almost no plastic deformation can be seen in the case of the 10 keV impact as shown in Fig. 1, and the volume of the deformed region is considered as zero. Both crater and deformed region volumes are almost linear functions of the acceleration energy, and that corresponds well to macroscopic projectile impacts [7].

Figure 3 shows the kinetic energy transferred from the inner region to the outer symmetric region with the shockwave. The kinetic energy transfer with the shockwave is also too small to measure for 10 keV, but those for 50 and 100 keV are again almost linear functions of the acceleration energy with the ratio of about 7%. Considering that the kinetic energy of the reflected cluster was about 6% [5], more than 85% of the cluster acceleration energy is transferred to the inner surface region. Thereby, a very high energy density condition in obtained on the surface allowing erosion or modification.

Figure 4 shows the number of evaporating carbon atoms N_C^{out} and the ratio of activated CO_2 molecules F_a in the impact cluster, i.e. the fraction of CO_2 molecules not keeping their original composition. For the 10 keV impact,

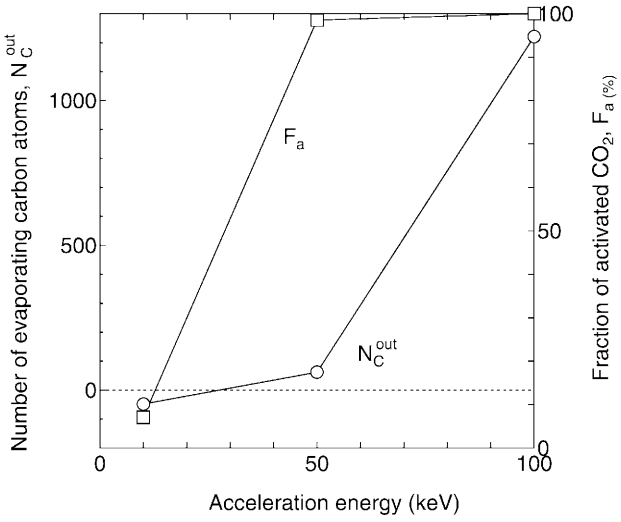

Fig. 4. Number of evaporating carbon atoms and fraction of activated CO_2

only less than 10% of the CO_2 molecules are activated and some of the CO_2 molecules simply stick on the surface, therefore, N_C^{out} is below zero. Almost all CO_2 molecules are dissociated and activated by the impact already at the acceleration energy of 50 keV. However, the N_C^{out} is still very small at this impact energy. The evaporation can only be enhanced with higher acceleration energy of 100 keV when surface material reacts with the dissociated CO_2 species.

Figure 5 shows the size and the angular distributions of the evaporating fragments, respectively. For the 10 keV impact, almost only CO_2 molecules can be seen, which simply impinge onto the surface and reflect without reaction. In that case, the reflection angle is almost glancing to the surface.

Various signals appear for the 50 keV impact due to the activation of the CO_2 molecules, and the intensities of O, CO and CO_2 are especially strong. The CO_2 molecules dissociate once into CO and O during the impact, however, many of these species rearrange again as CO_2 because the impact cannot induce the evaporation of the surface material. The reflection angle is around 30° to the perpendicular impact direction.

For the 100 keV impact, more intense signals of C and CO appear, and that is clearly due to the strong evaporation of the surface material. The reflection angle is also around 30° although it is more distributed compared to the 50 keV impact. These reflected fragment species may eventually stick to vertical surfaces leading to re-deposition.

4
Concluding remarks

By using the molecular dynamics method, CO_2 cluster impacts on a diamond surface with different acceleration energy have been simulated in order to investigate the surface erosion process. A typical transient crater is formed for 50 and 100 keV impacts while only elastic deformation can be seen for 10 keV. The kinetic energy and the volume of the crater are almost linear functions of

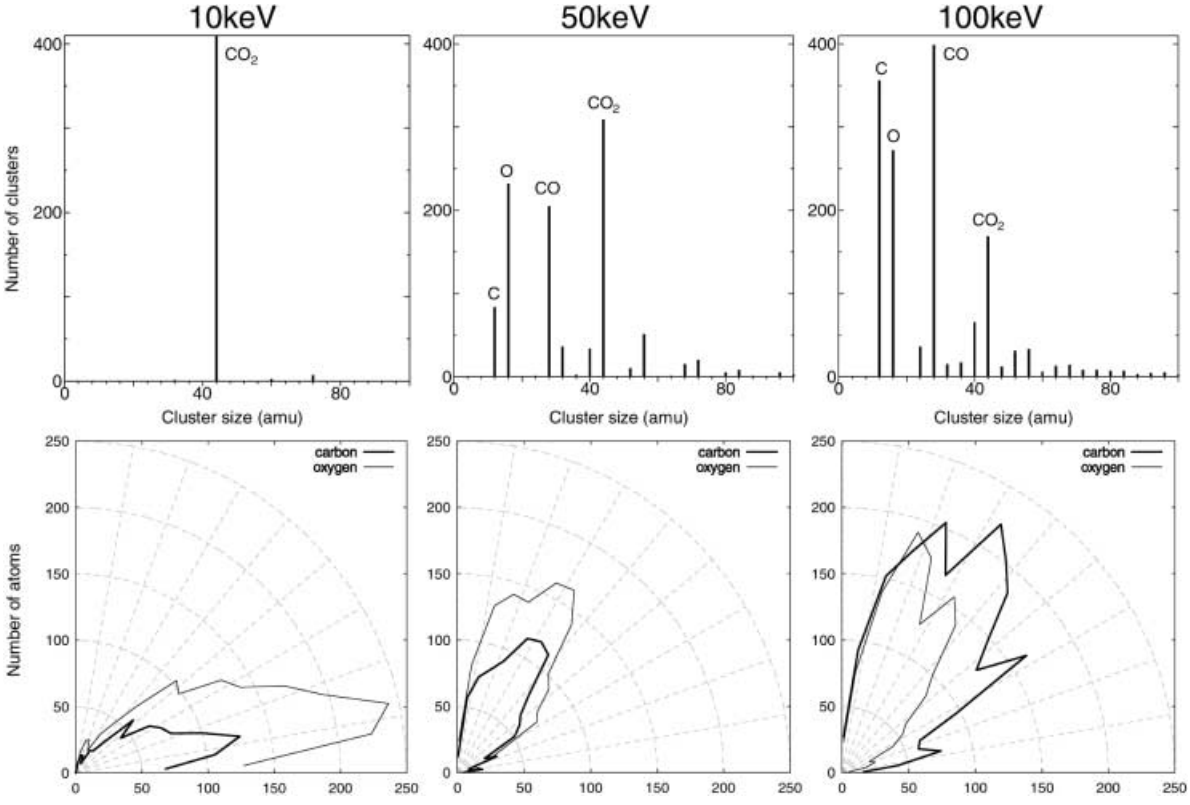

Fig. 5. Fragment size and angular distributions at different cluster acceleration energies

the acceleration energy, but the erosion is enhanced only by the 100 keV impact, where a strong peak of CO appears in the size distribution of the evaporating fragments.

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