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Molecular dynamics simulation of atomic beam bombardment on a solid surface

Koichiro Ezato [a,*], Tomoaki Kunugi [b]

[a] Department of Fusion Engineering, Japan Atomic Energy Research Institute, 801-1, Mukohyama, Naka-machi, Naka-gun, Ibaraki, 311-01, Japan

[b] Department of Reactor Engineering, Japan Atomic Energy Research Institute, Tokai-mura, Naka, Ibaraki 319-11, Japan

Abstract

Molecular dynamics simulations regarding the life-time assessment of the fusion reactor materials are carried out. In this study, the high energy impacts of a mono-atom and clusters of atoms on a solid surface are treated as sputtering and re-deposition processes. In case of the 3.2 KeV mono-atom impact, the projectile penetrates deeply into the target material and creates a high temperature region similar to volumetric heating. A phase change from liquid to solid accompanies this heating. In case of the 256 atom, 12 eV per atom cluster impact, the energies are transferred to the surface atoms of the target. The high temperature region propagates into the target like a thermal shock wave. The energy dependency of the target wearing due to the cluster impact is discussed.

1. Introduction

Collisional processes between solid surfaces and the high energy particles, especially sputtering and re-deposition, have an important role to determine the life-time of the plasma-facing material. A continuum approach to this non-equilibrium impact process occurring in very short times (∼ps) and very short lengths (∼nm) may not be appropriate. To grasp these non-equilibrium microscale phenomena, a molecular dynamics (MD) approach could be one of the more promising methods. The MD method has been widely used to study the interaction between the high energetic atoms and the surface of materials[1–3].

In this paper, the energy and momentum transfer and the dynamic behavior of atoms of the solid material during the energetic mono-atom and cluster impacts are investigated by means of the MD method. We attempt to estimate the loss of the target material so that we can make a life-time assessment for fusion reactor materials.

2. Simulation model

We chose copper as the target thin film and the projectile atom, so that we are considering self-sputtering. The projectile is considered to be neutral because of the charge exchange with the other atoms. Assuming that a classical system consists of N atoms and that the interatomic force $\mathbf{F}_i$ acting on the i-th atom is expressed by using the N-body potential function E_c, the motion of the i-th atom is expressed as follows:

$$m\frac{d^2\mathbf{r}_i(t)}{dt^2} = \mathbf{F}_i(t) = -\sum_i \frac{\partial E_c^i}{\partial r_i} \quad \text{and} \quad \mathbf{v}_i(t) = \frac{d\boldsymbol{r}_i(t)}{dt}, \quad i = 1, 2, \ldots, N, \tag{1}$$

where m, $\mathbf{r}_i$ and $\mathbf{v}_i$ are mass, position and velocity vectors of i-th atom. We apply the N-body potential function proposed by Rosato et al. [4], which can describe the bulk and defect properties of a transition metal.

$$E_c^i = E_b^i + E_r^i, \tag{2}$$

$$E_b^i = -\left\{\sum_j \xi^2 \exp\left[-2q(r_{ij}/r_0 - 1)\right]\right\}^{1/2},$$

$$E_r^i = \sum_j A \exp\left[-p(r_{ij}/r_0 - 1)\right], \tag{3}$$

* Corresponding author. Tel.: +81 029 270 7552; fax: +81 029 270 7558; e-mail: ezato@nbisun10.naka.jaeri.go.jp.

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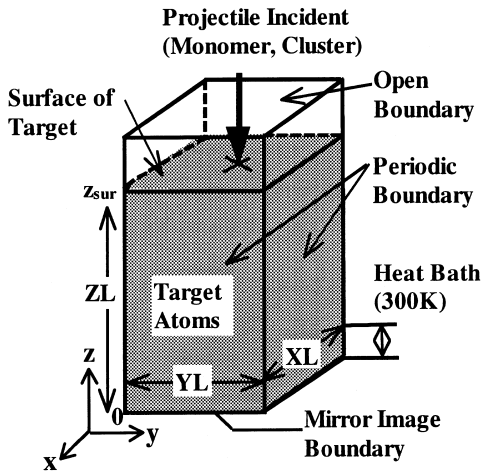

Fig. 1. Configuration of the atomic system and boundary conditions (Z_{sur} is the height of the surface, $Z_{sur} = 160\sigma$, where σ is the atomic diameter).

where E_c^i, E_b^i and E_r^i are the cohesive, the binding and repulsive energy of the i-th atom. r_{ij} $(= |\boldsymbol{r}_{ij}| = |r_i - r_j| = |r_i - r_j|)$ is the distance between i-th and j-th atoms. There is as yet no reliable potential to describe the non-equilibrium state for the particle-solid collisions being considered. So we apply the empirical equilibrium function in the present study for the first step.

The initial target atomic layer uses an FCC lattice consisting of $N = 360{,}000$ atoms at the thermal equilibrium at 300 K and the simulation cell size is $XL \times YL \times ZL = 108 \times 108 \times 364$ [Å^3]. The boundary conditions are as same as in our previous study [5]. Two kinds of the projectiles are chosen: a copper mono-atom with an energy of 3.2 KeV; and copper clusters consisting of 256 atoms with an energy of 12 eV per atom. The projectile is ejected normally at 5σ (σ, atomic diameter) from the center of target surface as shown in Fig. 1. The variable time step is used to prevent the fastest particle from moving further than 5% of the lattice constant of copper and the maximum time-step size is 0.1 fs. The MD simulation is performed for a period of 2 ps and one projectile impact is assumed to occur in this period.

3. Results and discussion

3.1. Mono-atom impact

Fig. 2 shows three snapshots of the target material with the thickness of 3 σ at (a) 0.2 ps, (b) 0.4 ps and (c) 0.8 ps after a Cu mono-atom impact. The gray-scale of the atoms indicates the atomic kinetic energy in terms of their temperature. It is shown that a high temperature region with the temperature above the melting point of the copper, is generated along the projectile's penetration path. This high temperature region is localized near the projectile in the early stage of the projectile penetration (<0.2 ps) because the projectile's energy is high and the interaction time is very short. Thereafter, the projectile energy is transferred to the atoms by atomic collisions. Thus, the high energy mono-atom impact deposits its energy inside the target material and causes a volumetric heat generation.

In order to investigate the dynamic behavior of the microscopic structure of the target material, we estimate the radial distribution function g_r defined in a sliced cylindrical region which is centered on the projectile with the thickness of 4σ in Fig. 3. The values of T_{av} and z/σ in Fig. 3 represent the mean temperature in the sliced cylindrical region and the penetration depth of the projectile from the surface. Immediately after the impact (at 0.2 ps), Fig. 3(b) and (c) show a loss of sharpness of the peaks, which is a determination of a solid phase materials (see Fig. 3(a)). This suggests that the material is damaging to a liquid-like phase due to the mono-atom impact.

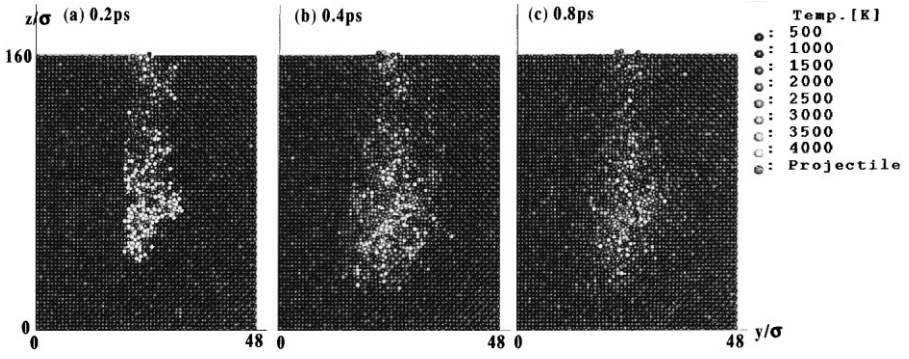

Fig. 2. Cross section view of the atomic configuration with temperature gray-scale in case of mono-atom impact with energy of 3.2 KeV at (a) 0.2 ps, (b) 0.4 ps and (c) 0.8 ps.

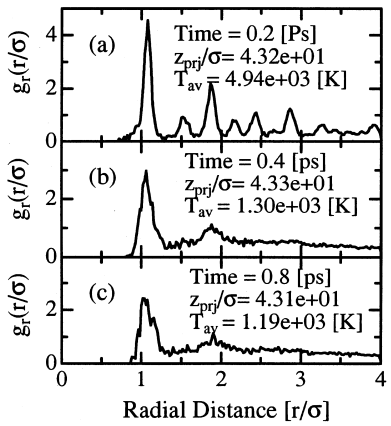

Fig. 3. Radial distribution function, g_r, of the target material in a cylindrical region centered in the projectile with the radius of 5 s at (a) 0.2 ps, (b) 0.4 ps, (c) 0.8 ps after the projectile impact (σ: atomic diameter, Z_{prj}: height of the projectile, T_{av}: mean temperature in the spherical region).

3.2. Cluster impact

Fig. 4 shows three snapshots of the target atomic layer at (a) 0.4 ps, (b) 0.8 ps and (c) 1.6 ps after the Cu_{256} cluster impact with an energy of 12 eV per atom. The thickness of the sliced region and the gray-scale are as same as Fig. 2. In the early stage of the impact (Fig. 4(a) at 0.4 ps), a high energy region appears in the boundary region between the cluster and the target material. Thereafter, this high energy region expands into the target material. At 0.8 ps (Fig. 4(b)), the cluster atoms are recoiled from the target surface as small fragments. The atoms in the boundary region near the impact point move to the surface because of the impact recoil force. The surface structure near the impact point appears like a crater. At 1.6 ps (Fig. 4(c)), mixing of atoms in the boundary region is enhanced and the kinetic energy of the atoms is reduced due to the cooling at the base of the system configuration where the temperature is controlled to be at 300 K.

Fig. 5 shows three dynamic behavior effects in the target material: (a) the mean kinetic energy, expressed in term of the temperature T, (b) number density, and (c) pressure. These values are estimated from the atoms in the spherical region centered in the impact point ($r/\sigma = 0$). As shown in Fig. 5(a), the high temperature peak occurs at $r/\sigma = 0$ and then expands into the target material as a function of time, similar to a thermal shock wave.

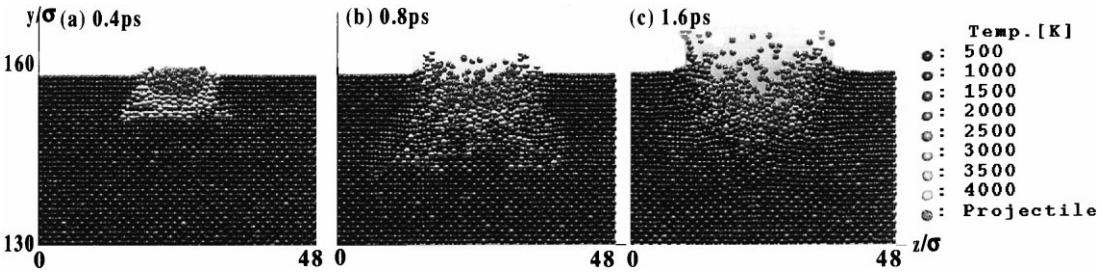

Fig. 4. Cross section view of the atomic configuration with temperature gray-scale in case of Cu_{256} cluster impact with the energy of 12 eV/atom at (a) 0.4 ps, (b) 0.8 ps and (c) 1.6 ps.

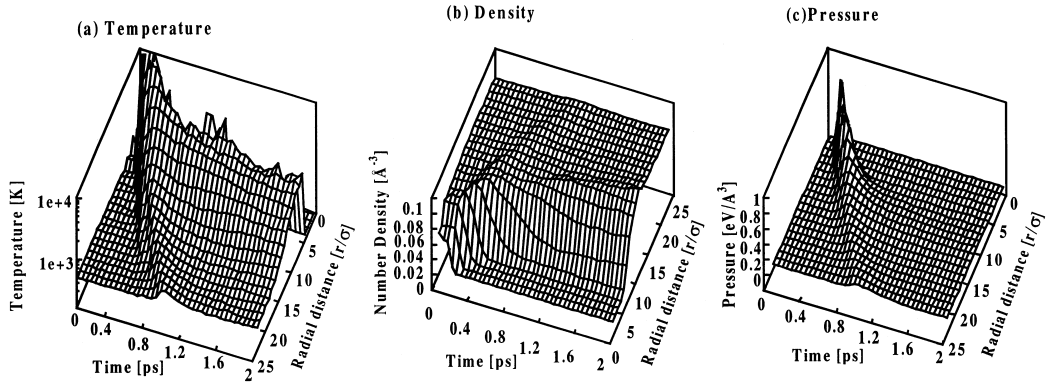

Fig. 5. Time history of the profiles of (a) mean temperature, (b) number density and (c) pressure inside the target material in a hemispherical region centered on the impact point of Cu_{256} cluster. (1 eV/Å^3 $\approx 1.62 \times 10^2$GPa.)

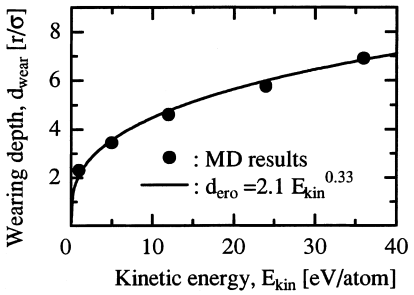

Fig. 6. Energy dependency of the wear depth for Cu_{256} cluster impact with the energies of 1, 5, 12, 24 and 36 eV per atom.

The cluster takes about 0.01 ps to hit the target after it is ejected at 5σ away from the surface. However, the time when the maximum value of temperature and pressure appear inside the target in Fig. 5(a) and (c) is about 0.2 ps. These results show that the energy transfer from the cluster to the atoms after the cluster impact requires a finite time, i.e., a relaxation time.

In Fig. 5(b) and (c), the peak values of number density and pressure move into the target material at the same rate as the kinetic energy peak shown in Fig. 5(a). The number density in the boundary region between the cluster and the target material is larger than the bulk value due to the cluster impact. From Fig. 5(c), we can estimate the propagation velocity of the pressure peak is about 5.23×10^3 m/s, which is very close to the longitudinal wave velocity in bulk copper, 5.10×10^3 m/s. This result shows that the pressure peak caused by the cluster impact is transferred with the velocity close to the speed of sound in the solid.

Fig. 6 shows the clusters incident energy dependency on wear of the target material. We define the wear depth d_{wear} as the radial distance from the center of surface to the point where the number density is less than 10^{-3} Å^{-3} at 2 ps. The solid line in Fig. 6 indicates the experimental prediction of crater depth of a solid surface due to the high velocity impact with a macroscopic body in range of the 1–10 times the speed of sound, c [6],

$$\frac{d_{wear}}{d_p} = K\left(\frac{\rho_p}{\rho_t}\right)^{2/3}\left(\frac{v_p}{c}\right)^{\kappa}, \quad (4)$$

where, v_p and d_p are the velocity and the diameter of the projectile, ρ_p and ρ_t are the density of the projectile and the target material, and K is an empirical constant. The value of κ ranges between 2/3 and 1/3, depending on the assumption whether the crater volume is proportional to the energy or momentum of the projectile. As shown in Fig. 6, the wear depth, d_{wear}, depends on the incident energy of cluster, E_{kin}, that is, d_{wear} is proportional to the cluster incident energy, $E_{kin}^{0.33}$. From this result, the value of κ is estimated to be about 0.66. Since this result is estimated at 2 ps after the cluster impact, the target atomic layer cannot reach the steady state. Therefore, much longer MD simulation will be necessary to confirm this result.

4. Summary

Molecular dynamics simulations are carried out to investigate the behavior of a thin film subjected to the impact of the high energy mono-atom and clusters. The results show clearly the differences in the thermal and structural responses of the target material. In case of the mono-atom impact with high kinetic energy, the projectile penetrates into the target material and causes a volumetric heating inside the material. In this region, the atomic structure changes from a solid to liquid phase. In case of the cluster impact with relatively low kinetic energy per atom, the energy deposits on the target surface and generates a high energy region at the material surface. This region propagates into the target at almost the speed of sound of the target material. The target surface takes on the shape of a crater and its wear depth is proportional to the incident energy of the cluster. This relation is very similar to the crater depth of a high velocity projectile impact with a macroscopic body. This shows that the wear processes of the microscopic cluster impact can be estimated by means of a macroscopic correlation like Eq. (4).

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