Depth Profiles Due to Big Cluster Impacts

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The depth profiles of big cluster impacts on amorphous targets have been investigated by using the time-evolution Monte Carlo simulation code DYACAT, where $(Ag)_n$ clusters of 200 eV/atom are bombarded on an Al target (n being 1 to 500). It is found that the recoiling Al atom clears the way for the following cluster and that the projected range of the $(Ag)_{500}$ cluster is about 4 times larger than that of the monoatomic ion.

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A cluster impact deposits a lot of energy and particles in a localized region. It produces a very active transient state in a small impact region of the target material. In 1982, Yamamura [1] developed the time-evolution Monte Carlo simulation code (DYACAT) based on the binary collision approximation, in order to investigate nonlinear sputtering due to high-energy heavy ions. The concept of time-evolution Monte Carlo simulation has been successfully applied to the investigation of relativistic nuclear collisions [2]. In 1988, using this DYACAT code, Yamamura [3] investigated the sputtering by 100 eV/atom $(Ar)_n$ cluster impacts on carbon targets, and found some very interesting effects, e.g., the front-runner effect and the acceleration effect. The front-runner effect, which is often called the "clearing-the-way effect," is that the front runners clear away target atoms for atoms coming afterward, which results in a larger projected range than that of the monoatomic ion with the same energy. When the cluster impacts and is trapped in the solid, there are a lot of energy-enhanced multiple collisions in the solid. As a result, some of the constituent atoms are accelerated to larger energies than the incident energy. These two cluster effects were studied by Shulga and Sigmund using molecular-dynamics calculations [4].

Up to now there is no experimental or theoretical work which has investigated the depth profiles of constituent atoms and recoiled atoms due to impacts of large clusters with energies more than 100 eV/atom. The clearing-the-way effect and the acceleration effect depend strongly on the atomic mass ratio of the mass of the cluster atom (M_1) and that of target atom (M_2). In this paper, the present DYACAT [5] code is applied to calculations of the depth profiles of constituent atoms for $(Ag)_n$ cluster impacts on Al (n being 1 to 500), and a cluster energy of 200 eV/atom. The depth profiles for 400 eV/atom $(Al)_n \rightarrow$ Ag are also calculated for comparison.

The DYACAT program was developed for the dynamical simulation of atomic collisions in amorphous targets within the framework of the binary collision approximation. It is the dynamical mode of the ACAT code [6]. The details of the DYACAT code were described elsewhere [5]; thus only a brief introduction of the DYACAT code is presented here. The DYACAT code can treat the collision between two moving particles. At each collision event, we calculate the distances in time between a moving atom and neighboring atoms, and pick up a real collision partner which has the minimum distance in time. The time-dependent information about the target is stored and used for the next-step calculation. The incident particle and the recoil atom are followed until their energies fall below cutoff energies E_{c1} and E_{c2}, which are the cutoff energies of the cluster atom and the target atom, respectively. The cluster shape is assumed to be spherical, and the binding energy of the spherical cluster is neglected, because the cluster kinetic energy of present interest is larger than the cohesive energy of the cluster atom.

In this paper the Moliere potential [7] is used as an interatomic potential. The electronic energy loss is estimated by using the path-dependent nonlocal model [8]. The interatomic spacing of constituent atoms is assumed to be the average value in the solid state. The numbers of the primary cluster ions used in the present calculations are 2000, 200, 40, 20, and 4 for $n=1$, 10, 50, 100, and 500, respectively, E_B is set to be 1.0 eV for all cases, and the cutoff energies E_{c1} and E_{c2} are set to be 10 eV for all elements.

The projected range is inversely proportional to the stopping power which is a function of the scattering cross section between the constituent atom and the target atom. So long as the cluster energy is the same, the stopping power of an n-atom cluster will be n times that of the monoatomic ion, and so the projected range of an n-atom cluster will be the same as that of the corresponding monoatomic ion provided the linear approximation holds. However, the cluster impact phenomenon cannot be described simply as the superposition of monoatomic ion bombardment because of several special effects associated with the cluster impact, such as the clearing-the-way effect, the acceleration effect, enhanced sputtering, and enhanced reflection [3].

In Fig. 1, we show the snapshots of the depth profiles of Ag atoms and recoil Al atoms at various instants for 200 eV/atom $(Ag)_{500} \rightarrow$ Al, where the broad solid line and the thin solid line correspond to the Ag atom and the recoil Al atom, respectively. For comparison, we also plot the depth profiles of monoatomic Ag ions, which are drawn in broken lines. There is a big difference between

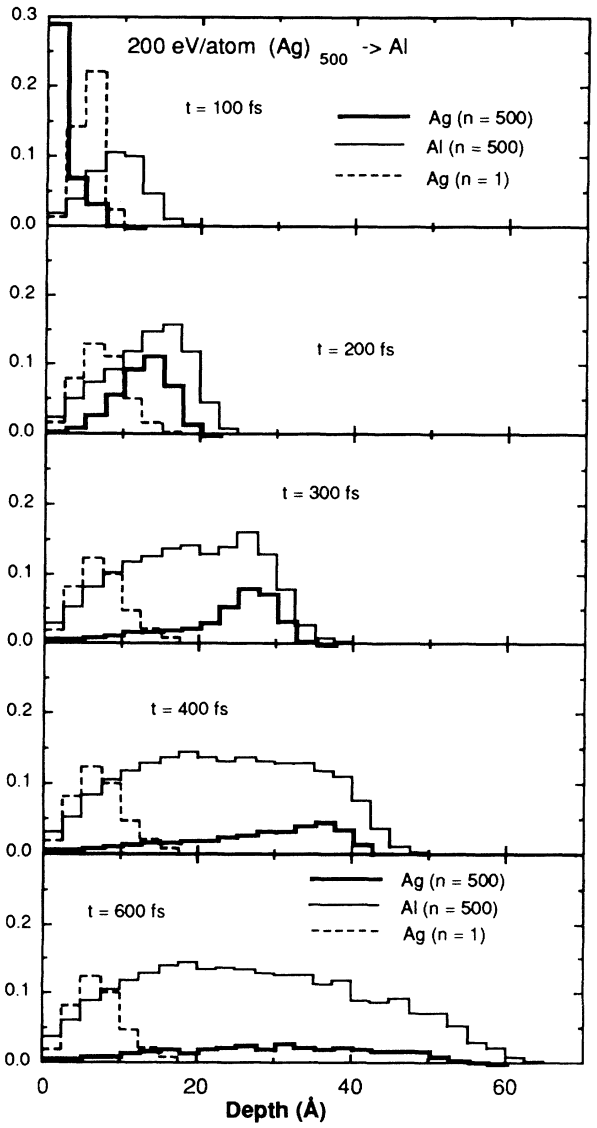

FIG. 1. The depth profiles of Ag atoms and recoil Al atoms due to 200 eV/atom $(Ag)_{500}$ cluster bombardment on an amorphous Al target at $t=100$, 200, 300, 400, and 600 fs. For comparison the depth profiles of Ag atoms from monoatomic Ag ion bombardment with the same energy are also plotted in broken lines.

the depth profile of the monoatomic ion and that of big cluster impact. The projected range and the straggling of the $(Ag)_{500}$ cluster impact are much larger than those of the monoatomic ion. At the early stage the recoil Al atoms go ahead of the cluster, and they clear the way for the following Ag cluster atom, because the maximum velocity of a recoil Al atom is faster than the initial velocity of a cluster Ag atom. Here the maximum recoil velocity v_{max} is given as $2M_1v_0/(M_1+M_2)$, where $v_0=2E_0/M_1$ is the initial cluster velocity, and E_0 is the cluster energy. For $(Ag)_n \rightarrow$ Al, $v_{max}=1.6v_0$. In this case, the main contributor of the clearing-the-way effect is the recoil atom, not the cluster atom.

In the case of $M_1 < M_2$, the maximum recoil velocity is less than the initial cluster velocity. In Fig. 2, we plot the depth profiles of the constituent Al atoms (broad solid line) and recoil Ag atoms (thin solid line) at some typical instants for 400 eV/atom $(Al)_{500} \rightarrow$ Ag. As a comparison, we also plot the depth profiles of Al atoms (broken line) due to the monoatomic ion bombardment. At the early stage the recoil Ag atoms do not go ahead of the Al cluster, because the maximum recoil velocity v_{max} is $0.4v_0$. But, after 100 fs the clearing-the-way effect is observed. In this case front runners of cluster Al atoms clear the way for following Al atoms, and so the

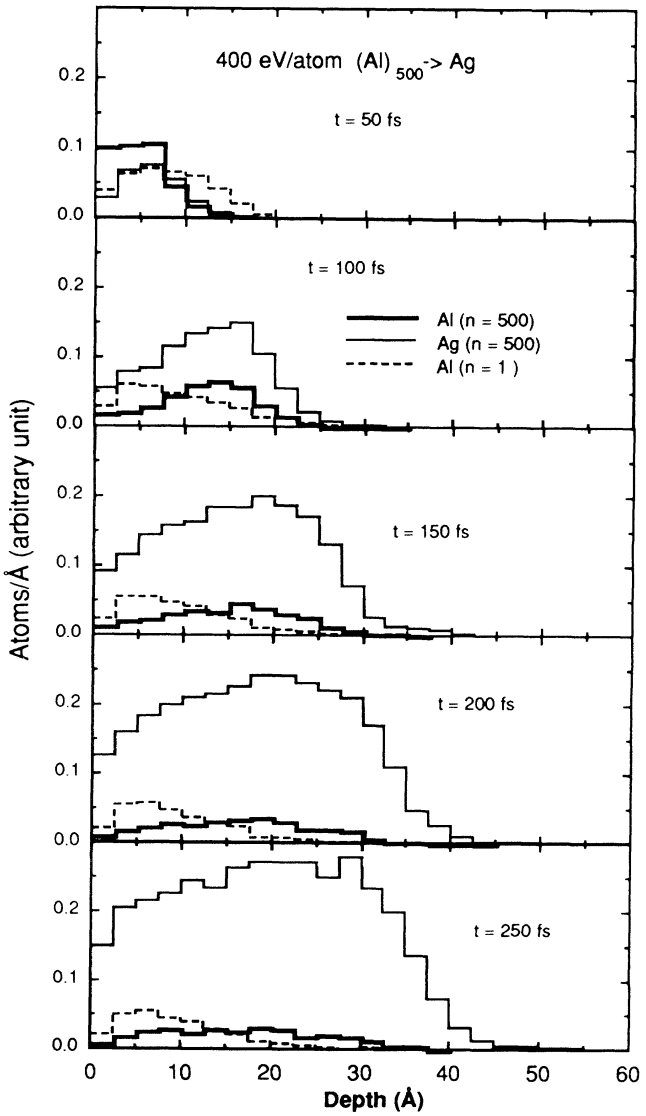

FIG. 2. The depth profiles of cluster Al atoms and recoil Ag atoms due to 400 eV/atom $(Al)_{500}$ cluster bombardment on an amorphous Ag target at $t=50$, 100, 150, 200, and 250 fs. For comparison the depth profiles of Al atoms due to monoatomic ion bombardment with the same energy are also plotted in broken lines.

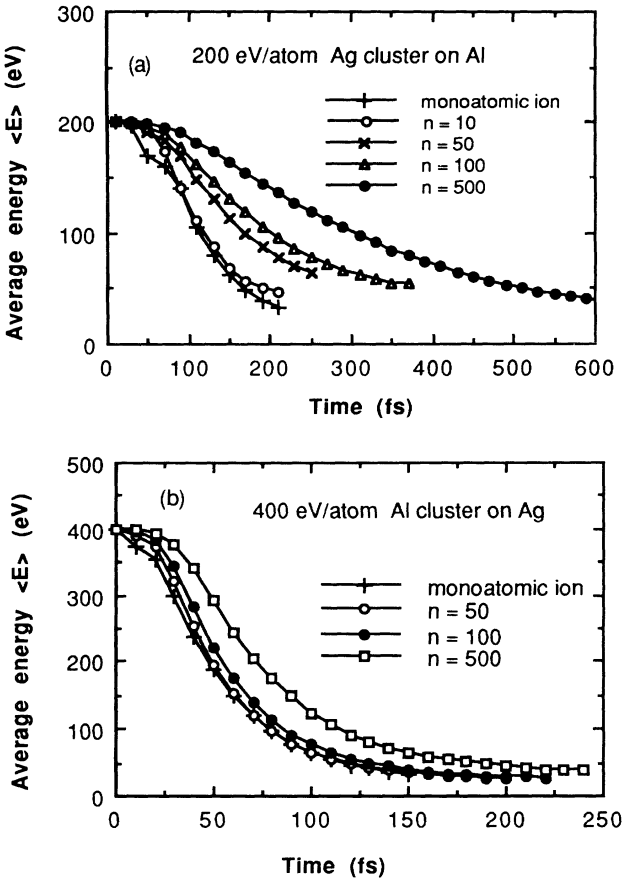

FIG. 3. The plots of the average energy $\langle E \rangle$ of cluster atoms for 200 eV/atom $(Ag)_n \rightarrow$ Al and for 400 eV/atom $(Al)_n \rightarrow$ Ag vs the slowing-down time for various sizes of clusters. (a) Average energy of Ag atoms and (b) average energy of Al atoms.

clearing-the-way effect is smaller than the case of $M_1 > M_2$. The projected range of the $(Al)_{500}$ cluster is about 1.5 times larger than that of the monoatomic ion. After 100 fs the mean depth of the constituent Al atoms does not change appreciably, because Al atoms and the Ag atoms are already randomized.

The cluster size is a very important factor for cluster impact phenomena. We show the size dependences of the slowing-down time in Fig. 3, where we plot the average energies $\langle E \rangle$ of constituent atoms for 200 eV/atom $(Ag)_n \rightarrow$ Al [Fig. 3(a)] and 400 eV/atom $(Al)_n \rightarrow$ Ag [Fig. 3(b)], respectively, as a function of time. The larger the cluster size, the longer the slowing-down time we have, especially for $(Ag)_n \rightarrow$ Al, where the recoil Al atom clears the way for cluster Ag atoms. In the case of $(Ag)_n \rightarrow$ Al, due to the clearing-the-way effect of recoil Al atoms it is unlikely that Ag atoms lose their energies by elastic collisions with Al target atoms at rest. Figure 3(b) says that the slowing-down time of $(Al)_n$ with $n < 100$ is nearly equal to that of the monoatomic ion because of the smaller clearing-the-way effect, but the cluster size effect of $(Al)_{500}$ is significant.

Table I presents the size dependences of various parameters at the final stage such as the projected range R_p, the straggling $(\Delta x^2)^{1/2}$ of constituent atoms, the deposition energy E_{dep} near the projected range, the particle reflection coefficient per cluster R_N, and the energy reflection coefficient per cluster R_E, where the present reflection coefficient R_N corresponds to the number of reflected cluster atoms whose energies are larger than 10 eV. The size effect of $(Ag)_n \rightarrow$ Al on the projected range is very strong as compared with the case of $(Al)_n \rightarrow$ Ag. In the former case, recoil Al atoms are front runners, while front runners of $(Al)_n \rightarrow$ Ag are the constituent atoms. Both the projected range and the straggling of $(Ag)_{500}$ cluster impact are about 4 times larger than those of the monoatomic ion bombardment. As is suggested from E_{dep} values of Table I, due to the strong clearing-the-way effect of $(Ag)_{500} \rightarrow$ Al, the stopping power of each constituent Ag atom is much less than that of the monoatomic Ag ion. A similar tendency is observed for $(Al)_{500} \rightarrow$ Ag.

In the case of $M_1 > M_2$ the acceleration of cluster

TABLE I. The cluster-size dependences of the projected range R_p, the straggling $(\Delta x^2)^{1/2}$ of constituent atoms, the deposition energy E_{dep} near the projected range, the particle reflection coefficient per cluster R_N, and the energy reflection coefficient per cluster R_E for 200 eV/atom $(Ag)_n \rightarrow$ Al and 400 eV/atom $(Al)_n \rightarrow$ Ag.

				Size of cluster				
E_0	Cluster	Target	Parameters	1	10	50	100	500
200	$(Ag)_n$	Al	R_p (Å)	7.3	8.1	12.2	15.7	29.1
			$\langle \Delta x^2 \rangle^{1/2}$ (Å)	3.3	3.5	5.1	7.4	13.4
			E_{dep} (eV/Å)	16	157	616	900	2400
			R_N (atoms/cluster)	< 0.001	< 0.01	< 0.01	0.10	5.7
			R_E (eV/cluster)	...	...	...	8.9	524
400	$(Al)_n$	Ag	R_p (Å)	9.8	9.8	11.5	12.6	16.9
			$\langle \Delta x^2 \rangle^{1/2}$ (Å)	6.4	6.4	6.7	7.2	9.0
			E_{dep} (eV/Å)	20	185	780	1400	5000
			R_N (atoms/cluster)	0.29	3.0	14	26	114
			R_E (eV/cluster)	6.7	69	350	754	4670

atoms is weak, because most of the cluster atoms are oriented inwards at the early stage and follow after fast recoil atoms. The acceleration of recoil atoms is appreciable due to energy-enhanced multiple collisions. As a result, the energetic recoil Al atoms are in a quasiequilibrium state at the early stage [5]. Just after 600 fs when the depth profile of Ag atoms is nearly in the final form, cluster Ag atoms are randomized. Therefore, the acceleration effect of $(Ag)_n \rightarrow Al$ does not influence the projected range.

In the case of $(Al)_n \rightarrow Ag$, cluster Al atoms are accelerated due to many shuttle collisions [9] and they are in the quasiequilibrium state at the early stage [5]. In this case the acceleration of the recoil Ag atoms is also very large, because the recoil Ag atoms are hit several times from the back side by faster cluster Al atoms. The larger slowing-down time of $(Al)_{500}$ atoms in Fig. 3(b) is promoted by both the acceleration effect and the clearing-the-way effect. But, since the fraction of highly accelerated atoms is very low and their angular distribution is nearly isotropic, they do not contribute appreciably to the projected range, but will enlarge the straggling.

The enhanced particle and/or energy reflection, which are often observed for light-element cluster impact, shorten the projected range [10]. The reflection coefficient R_N of $(Ag)_n \rightarrow Al$ is negligible (see Table I), but it is large for $(Al)_n \rightarrow Ag$. Both R_N and R_E of $(Al)_n \rightarrow Ag$ increase as the size increases, but the particle reflection per incident atom R_N/n is a decreasing function of the size, referring to the prolonged projected range, while the energy reflection per incident atom R_E/n increases as the size increases. But the value R_E/n is much less than the cluster energy, and so the present enhanced energy removal does not influence the projected range very much.

The time-evolution Monte Carlo simulation code DYACAT has been used to investigate the depth profiles for large cluster impacts. It is found that the most important effect on the depth profile due to big cluster impact is the clearing-the-way effect. In the case of $(Ag)_n$ cluster impact on the Al target where the recoil atom clears the way for the aftercoming cluster, the projected range of the $(Ag)_{500}$ cluster is about 4 times larger than that of the monoatomic ion.

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