알루미늄 덩어리를 사용한 알루미늄 성장에 관한 분자동력학 연구

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Molecular Dynamics study of Aluminum growth using Aluminum Cluster Deposition

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Abstract - In this work, we investigated Al cluster deposition on Al (100) surface using molecular dynamics simulation. A result of simulations showed that large cluster with low energy was proper for good surfaced-films without craters at the low temperatures. We investigated the maximum substrate temperature and the time taken for substrate temperature to reach its maximum as a function of cluster size in the case of the same total energy and in the case of the same energy per atom. The correlated collisions play an important role in interaction between energetic cluster and surface, and as cluster size and cluster energy increases, the correlated collisions effect affects interaction between energetic cluster and surface.

1. Introduction

Cluster deposition is softer than atom deposition and has been regarded as a method for growing high-quality films at low substrate temperatures[1,2,3]. Metal cluster deposition can make the fine metal thin films and can help to fabricate the upgraded semiconductor devices. Molecular dynamics (MD) simulations have been widely applied to the investigation of interactions between ions and surfaces. Hesieh and Averback[4] found out that the interaction between an energetic cluster and a substrate is far different from that between a single particle and a sold since the correlated collisions of the cluster play an important role. They also obtained the important results that no point defects were created. In our previous work[5], we found the reason that, in the case of cluster deposition, faced-center cubic (FCC) structural rearrangement occurs easily on the surface. Since the collision time between clusters and the substrate is longer than that of single atom and the surface collisions, the substrate receives thermal energy from energetic clusters during a long period and the thermal energy dissipates slowly. Therefore, the thermal energy of cluster deposition maintains a higher temperature longer than that of atom deposition, which leads to the self-annealing effect. In the case of cluster deposition, the soft impacts allow the thermal energy to remain for a long time in the substrate, and the self-annealing, which is induced by this energy, plays a very important role in the structural rearrangement of the surface. Topics to study interaction between an energetic cluster and surface are crater generation on surface, sputtering, properties of deposited film by cluster structure etc.

2. Simulation Method

In this work, we investigated the interaction between an energetic cluster and surface using a classical molecular dynamics simulation. The code for molecular dynamics simulation in this work is that of our previous work[5], which used the second-moment approximation of the tight-binding scheme (TB-SMA) as proposed by Tomanek, Aligia and Balseiro[6], the Verlet algorithm, a periodic boundary condition, the neighbor lists to improve performance, and the constraint dynamics. We used parameters for aluminum in the TB-SMA potential fitted by Clei and Rosato.[7] Table I shows values of physical properties calculated by the TB-SMA, long-range FS model, and EAM model and experimental values for the FCC aluminum. The TB-SMA potential is a good agreement with other methods and experiment. To investigate interaction

between an energetic cluster and surface, we used the FCC structured clusters, such as Al_{13}, Al_{19}, Al_{43}, Al_{55}, Al_{78}, Al_{87}, Al_{177}. Energetic aluminum cluster starts upper 4 Å from surface, the simulated time is 15 ps, and the time step is 0.5 fs.

3. Results and Discussions

We investigated the impact effects and structural rearrangement using Al_{13} and Al_{43} clusters. Figure 1 shows the maximum substrate temperature as a function of total cluster energy in the cases of Al_{13} and Al_{43} cluster impacts. For the both cases, as total cluster energy increased, the maximum substrate temperature increased. However, the slope of Al_{43} is less than that of Al_{13}. Figure 2 shows the variations of the number of disordered atoms in the substrate (N_{dis}) using the Kang-Choi-Byun-Hwang (KCBH) method[5] as a function of time. Figure 2(a) is the cases of Al_{13} cluster impacts and Fig. 2(b) the cases of Al_{43} cluster impacts. In both Al_{13} and Al_{43} cluster deposition, the number of disordered atoms increases after cluster impact on surface and reduces as time pass, and finally there is no point defect like as previous works.

In both Al_{13} and Al_{43} cluster depositions, structural rearrangement occurred easy. Table II shows that the number of vacancy in crater on the surface increased with cluster energy and that of the cases of Al_{13} is larger than that of the cases of Al_{43}. Figure 3(a) and 3(b) show the cut-side-views of Al_{13} with 20 eV energy per atom and Al_{43} with 5 eV energy per atom at 15 ps, respectively. Therefore, we expect that large cluster be proper for good surfaced-films without craters at the low temperatures.

Figure 4 shows the maximum substrate temperature (T_{Max}) and the time taken for substrate temperature to reach its maximum (t_{Max}) as a function of cluster size (n) in the case of the same total energy (E_T), 195 eV. Since the total cluster energy is constant, energy per atom (E_a) is E_T/n. In Fig. 4, T_{Max} is linearly proportional with E_a. In the case of the same total energy, when cluster size increases, energy per atom and cluster velocity decrease, impact area increases, and cluster momentum has linear proportional with $\sqrt{n}$. As cluster size increases, since cluster velocity decrease and total time of collisions between cluster and surface increase, t_{Max} increases and the fitting function of t_{Max} in Fig. 3 is $0.2101 \times \log(n) - 0.201357$.

Figure 5 shows T_{Max} and t_{Max} as a function of cluster size (n) in the case of the same energy per atom (E_a), 5 eV. Since the energy per atoms is constant, total cluster energy (E_T) is $n \times E_a$ and cluster velocity is constant. In Fig. 5, T_{Max} is linearly proportional with E_T. Therefore, T_{Max} is linearly proportional with cluster size n. In the case of the same energy per atom, when cluster size increases, total cluster energy and impact area increase and cluster momentum has linearly proportional with n. Since cluster velocity is constant, we expect that total time of collisions between cluster and surface be related with cluster size. However, in Fig. 5, we cannot find any relationship between t_{Max} and cluster size (n). As cluster size increases, t_{Max} is approximated to constant value in Fig. 5. Since the correlated collisions made energy rapidly transfer to substrate, t_{Max} was approximated to a constant value. Therefore, the correlated collisions play an important role in interaction between energetic cluster and surface. Especially, as cluster size and cluster energy increase, the correlated collisions effect affects interaction between energetic cluster and surface.

Figure 6 shows the variation of the number of disordered atoms in the substrate (N_{dis}) as functions of cluster size and time using the KCBH method. Figure 6(a) is the case of Fig. 4 and Fig. 6(b) the case of Fig. 5. In the both cases of Figs. 6(a) and 6(b), N_{dis} increases with cluster size. In the Fig. 6(a), as cluster increases, N_{dis} increases, since the force applied to surface from cluster do not increase but interaction area between surface and cluster increases and atoms in cluster interacting with substrate increases. However, in the Fig. 6(b), since the force applied to surface from cluster, interaction area between surface and cluster, and atoms in cluster interacting with substrate increase, N_{dis} rapidly increases with cluster size. The force applied to surface mainly affects most of them.

4. Summary

In this work, we investigated the interaction between energetic Al cluster and Al (100) surface using molecular dynamics simulation. A result of simulations showed that large cluster with low energy was proper for good surfaced-films without craters at the low temperatures. We investigated the maximum substrate temperature and the time taken for substrate temperature to reach its maximum as a function of cluster size in the case of the same total energy and in the case of the same energy per atom. Maximum

substrate temperature was linearly proportional with both energy per atom and total cluster energy. In the cases of the same energy per atom, since the correlated collisions made energy transfer to substrate, the time taken for substrate temperature to reach its maximum was approximated to a constant value. The correlated collisions play an important role in interaction between energetic cluster and surface, and as cluster size and cluster energy increases, the correlated collisions effect affects interaction between energetic cluster and surface. In the cases of the same total cluster energy, as cluster increases, N_{dis} increases, since the force applied to surface from cluster do not increase but interaction area between surface and cluster increases and atoms in cluster interacting with substrate increases. However, in the cases of the same energy per atom, since the force applied to surface from cluster, interaction area between surface and cluster, and atoms in cluster interacting with substrate increase, N_{dis} rapidly increases with cluster size. The force applied to surface mainly affects most of them. For film growth with low impact and without craters, controls of cluster size and cluster energy are very important and must be investigated. Impact dynamics by cluster structure also is important to understand interaction between energetic cluster and surface.

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Table I. Values of physical properties calculated by the TB-SMA, long-range FS model, and EAM model and experimental values for the FCC aluminum

Method	E_C (eV)	a_0 (Å)	C_{11}	C_{22}	C_{44}	$\langle B \rangle$
TB model[a]	-4.05	3.339	0.950	0.7400	0.3700	0.81
FS model[b]		3.340	0.820	0.7200	0.1600	0.75
EAM[c]	-4.03	3.340	1.143	0.6192	0.3162	
Experiment[d]	-4.03	3.340	1.070	0.6100	0.2900	0.76

Table II. In the cases of Al_{13} and Al_{43} impacts, the number of vacancies in the carter on surface.

Al_{13}		Al_{43}	
Energy/ Atom (eV)	# of vacancy in crater	Energy/ Atom (eV)	# of vacancy in crater
1	-	1	-
5	-	2	-
10	3	3	-
15	17	4	1
20	26	5	10

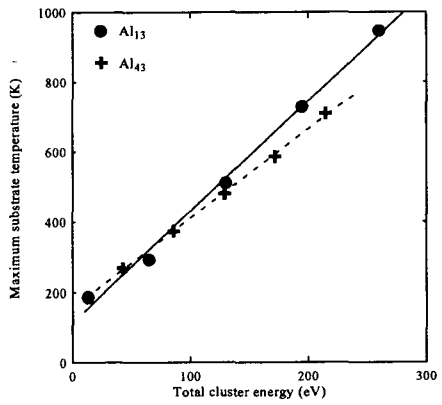
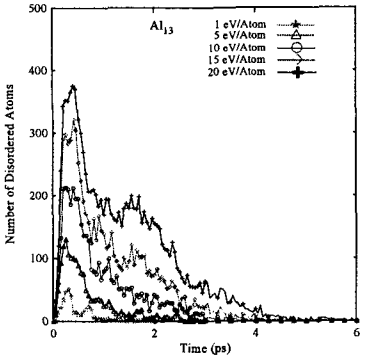
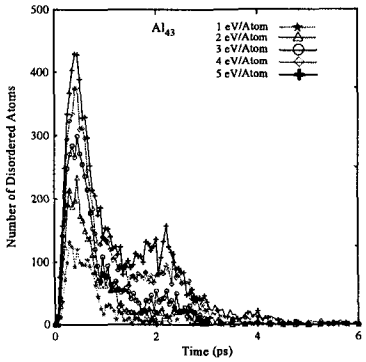


Figure 1. The maximum substrate temperature as a function of total cluster energy in the cases of Al_{13} and Al_{43} cluster impacts.

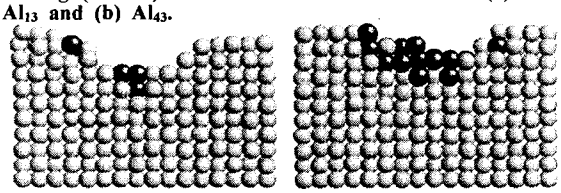


(a)



(b)

Figure 2. The variations of the number of disordered atoms using the Kang-Choi-Byun-Hwang (KCBH) method as a function of time. (a) Al_{13} and (b) Al_{43}.



(a) (b)

Figure 3. The cut-side-views of Al_{13} with 20 eV energy per atom (a) and Al_{43} with 5 eV energy per atom (b) at 15 ps.

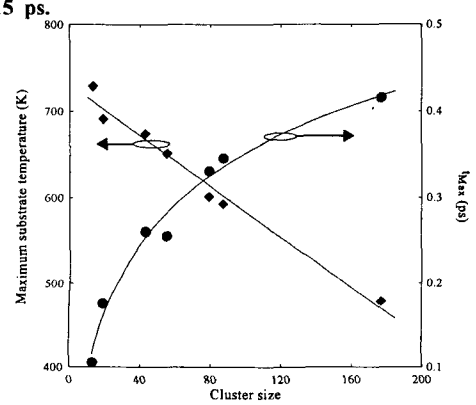


Figure 4. The maximum substrate temperature and the time taken for substrate temperature to reach its maximum (t_{Max}) as a function of cluster size (n) in the case of the same total energy (E_T), 195 eV.

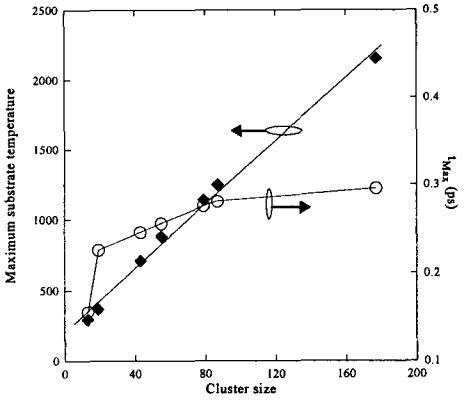
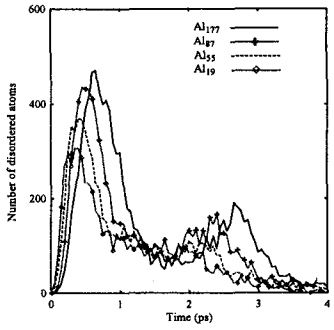
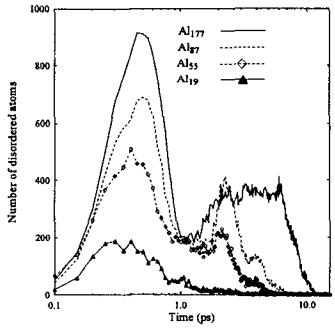


Figure 5. The maximum substrate temperature and the time taken for substrate temperature to reach its maximum (t_{Max}) as a function of cluster size (n) in the case of the same energy per atom (E_a), 5 eV.



(a)



(b)

Figure 6. The variation of the number of disordered atoms (N_{dis}) in the substrate as functions of cluster size and time using the Kang-Choi-Byun-Hwang (KCBH) method. (a) in the case of the same total energy (E_T), 195 eV and (b) in the case of the same energy per atom (E_a), 5 eV.