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Simulation of Fabrication toward High Quality Thin Films for Robotic Applications by Ionized Cluster Beam Deposition

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Abstract

The most commonly used method for the production of thin films is based on deposition of atoms or molecules onto a solid surface. One of the suitable method is to produce high quality metallic, semiconductor and organic thin film is Ionized cluster beam deposition (ICBD), which are used in electronic, robotic, optical, optoelectronic devices. Many important factors such as cluster size, cluster energy, impact angle and substrate temperature have important effects on the quality of final thin film such as cluster implanted atoms, substrate sputtering atoms and surface roughness. In this paper, molecular dynamics (MD) simulation of nano-Si cluster impact on Si(100) substrate surface has been carried out for energies of 1-5 eV/atom. The 3-body Stillinger-Weber potential (SW) was used in this simulation. Si cluster sizes of 30, 70, and 160 atoms were deposited on a Si (100) substrate whose temperatures were set around 300 K. Our results illustrate that the maximum substrate temperature, heat transferred time, the cluster implantation and sputtering atoms from the surface increase with increasing the cluster size and energy of the clusters. We found that small nano-clusters with high kinetic energy can produce flatter surface.

Keywords: *Molecular Dynamics Simulation, Ionized Cluster Beam Deposition, Thin Films.*

1. Introduction

There are many different methods for production of thin films and electronic devices. In some of these methods, to produce activation energy, substrate temperature is increased to several hundred Kelvin above room temperature. Many materials, however, are not resistant to such high temperature. Therefore, instead of heating the substrate, sometimes the incoming particles are accelerated to high kinetic energies. Today, this method is known as ionized cluster beam deposition (ICBD). This method is received much attention because of various applications, such as semiconductors, metal films and dielectric for micro-electronic devices, robotic devices, optical coatings, optoelectronic devices, magnetic materials and organic materials [1-5].

In ICBD, first, clusters earn very high kinetic energy and then they impact by surface. Many factors such as cluster size, cluster energy, impact angle and substrate temperature have important effects on the quality of final thin film such as cluster implanted atoms, substrate sputtering atoms and surface roughness. To study these

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factors, there are experimental and theoretical methods. Experimental methods are very difficult because the impact time is very short (about several ps) and the impact region is very small (about several nano-meter), thus theoretical methods such as ab initio quantum mechanics and molecular dynamics (MD) are suitable in these investigations. It is technically impossible to study a system consisting of thousands of atoms from quantum mechanics, thus molecular dynamics simulation method has an important role. Many groups used MD to study the ICBD process [6-13]. For example, Hong et al. [14] used MD to study the impact between Cobalt cluster and Copper surface. They reported that Co30 cluster with incident energy of 1eV/atom and a deposition rate of 30 atoms/ps does not penetrate into the surface of the substrate. Their results show that the surface becomes smoother with increasing deposition rate, cluster energy and substrate temperature.

Yang et al.[15] studied the burrowing of Nickel nano-cluster deposited onto the Copper surface. They show that the burrowing process goes extremely slow as temperature is at or under 900 K. They found that the kinetic energy will play a key role in the acceleration of the burrowing process. Gong et al.[16] investigated deposition of Cu clusters on a Si (001) substrate. Their results indicated that the degree of epitaxy and film flatness generally increased with the deposition velocity. They found that Cu13 cluster at 1500 m/s, Cu55 at 1000 m/s and Cu147 at 500 m/s produced more flat epitaxial layers that matched well with the substrate surface.

In our previous papers, we studied the impact between metallic nano-clusters and metallic surfaces [17-18]. In this paper, we studied the impact between Si nano-cluster and Si(100) surface. We used MD to study the effect of cluster size and kinetic energy on the cluster implantation, sputtering atoms, maximum substrate temperature, heat transfer time and root-mean-square roughness of surface.

2. Simulation Method

We used the MD software called LAMMPS, which stands for Large-scale Atomic/Molecular Massively Parallel Simulator [19]. This software has many different force fields which are suitable for metallic, semiconductor and organic materials. Fig. 1 shows our model that illustrates cluster, free, thermal control and fix layers. Three Si clusters with 30, 70 and 160 atoms are generated by cutting a sphere from bulk crystals in its equilibrium state and their initial distance of surface is about 10 Å. Dimensions of free layers are 54.3*54.3*16.6 Å and it has 2476 atoms. An NVE ensemble is used for free layers, which means that the number of particles (atoms), volume and energy of the ensemble are maintained constant. Thickness of thermal control layers is about 13 Å with 1780 atoms. We fixed temperature of thermal control layers at 300 K with a Nose-Hoover thermostat. At the bottom of the substrate, a fix layer is placed with 1144 atoms which it does not move during simulation. The boundary conditions in x, y axis are periodic but in z direction is not periodic. Before deposition of the clusters, the simulation system was equilibrated for 5 ps at 300 K then the clusters were deposited normal to the surface. The equations of motion were integrated using the Verlet algorithm with the time step of 1fs.

We used 3-body SW potential developed by Stillinger and Weber [20]. This force field is suitable for semiconductors and it can reproduce mechanical and thermodynamical properties. The terms of SW potential are as follows:

$$E = \sum_i \sum_{j>i} \Phi_2(r_{ij}) + \sum_i \sum_{j\neq i} \sum_{k>j} \Phi_3(r_{ij}, r_{ik}, \theta_{ijk}) \quad (1)$$

$$\Phi_2(r_{ij}) = A_{ij}\varepsilon_{ij}\left[B_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{p_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{q_{ij}}\right] \exp\left(\frac{\sigma^{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right)$$

$$\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk}\varepsilon_{ijk}[\cos(\theta_{ijk}) - \cos(\theta_{0ijk})]^2 \exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right) \exp\left(\frac{\gamma_{il}\,\sigma_{ik}}{r_{ik} - a_{ik}\sigma_{ik}}\right)$$

Where φ_2 is a two-body interaction and φ_3 is a three-body interaction. The B, A, p, and p parameters are used only for φ_2. λ and θ_{0ijk} parameters are used only for three-body interactions. The ε, σ and a parameters are used for both two-body and three-body interactions. These parameters are extracted from ether experimental data or quantum computational data. We consider these parameters as follows: ε=2.1683 eV, σ=2.0951 Å, a=1.8, λ=21, γ=1.2, $\cos(\theta_{0ijk})$= -0.3333, A=7.0495, B=0.6024, p=4 and q=0 [20]. We exported the coordinates of cluster and free layers and counted the number of atoms of cluster under the surface (implanted) and the number of atoms of free layers on the surface (sputtering).

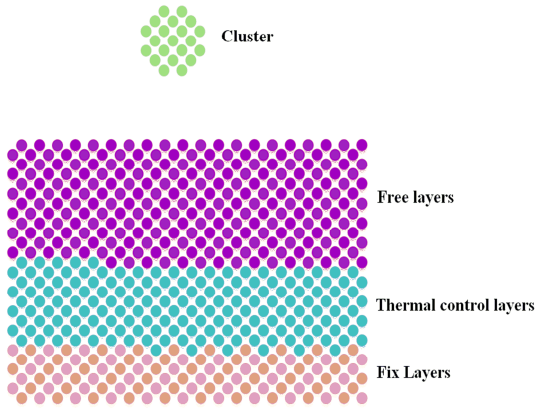

Fig. 1. The simulation system: Cluster, Free, Thermal control, Fix layers

3. Results and Discussion

The most effective region for the cluster impact with the surface is the free layers, therefore we performed all the calculation in this area. Fig. 2 shows the impact between surface and Si cluster of 30 atoms with a kinetic energy of 1eV/atom as a function of time at 300K.

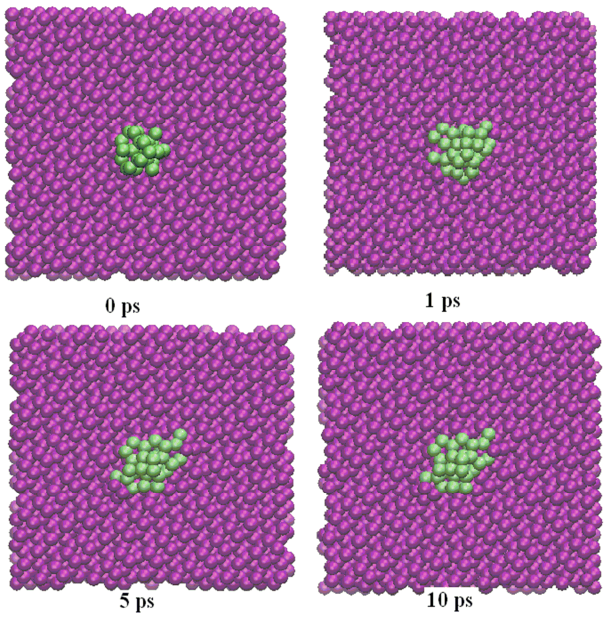

Fig. 2. Collision dynamics between a Si30 nano-cluster with 1 eV/atom and Si(100) substrate

As the figure shows, when the impact on the surface begins, the crystalline natures of the surface are destroyed. As the time elapses, cluster atoms are broken up and penetrate into the substrate. This figure shows that after 5 ps, cluster atoms only oscillate on the surface and they reached to an equilibrium state. Fig. 3 shows the simulation results of 160-atom cluster with a kinetic energy of 1eV/atom for deposition up to 30 ps at 300 K.

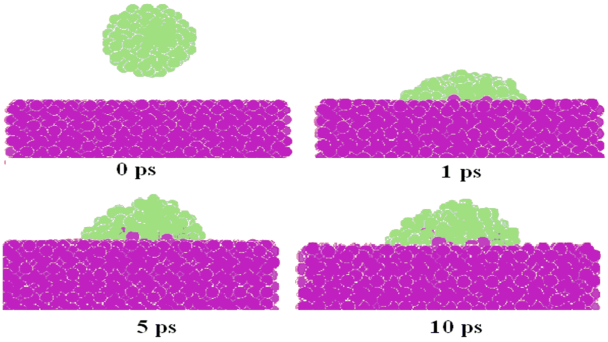

Fig. 3. Collision dynamics between a Si160 nano-cluster with 1 eV/atom and Si (100) substrate.

Fig. 4 shows temperature of free and thermal control layers as a function of time when a Si cluster of 30 atoms with a kinetic energy of 1eV/atom impacted to the surface. When a cluster impacted to the surface, much energy

transferred from cluster to free layer, thus its temperature increased. This figure shows that maximum temperature of free layers is about 370K. As the time elapses, heat transferred from free to thermal control layers, so the temperature of free layers decreased until it reached to the temperature of thermal control layers. As the figure shows, after 10 ps, temperature of free and thermal layers closed together.

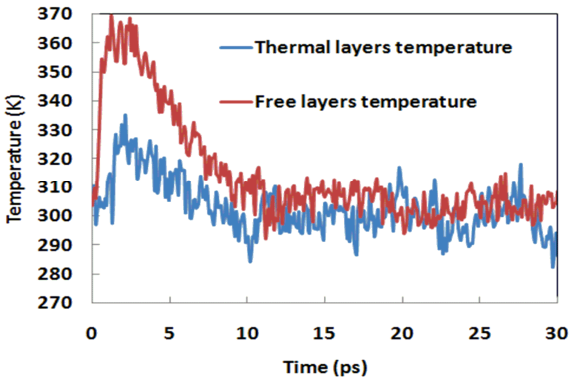

Fig. 4. Temperature of free and thermal control layers as a function of time.

Fig. 5 shows the maximum substrate temperature as a function of cluster energy and size. As the energy increases, the maximum temperature of substrate increases, but this increase is faster for larger cluster, because larger cluster has much energy.

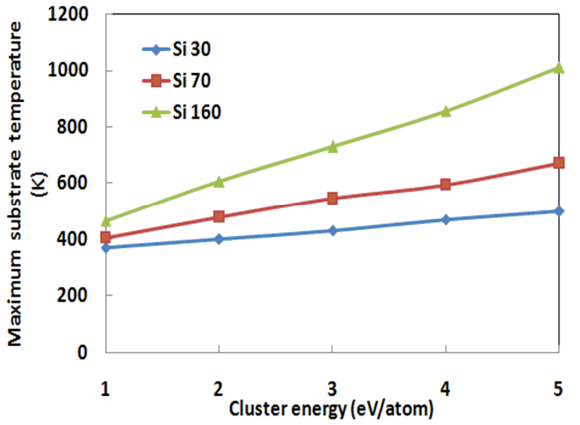

Fig. 5. The maximum substrate temperature as a function of cluster size and energy.

Fig. 6 shows the heat transferred time from free to thermal layers as a function of cluster energy and size. It shows that the heat transferred time increases with increasing cluster energy and size, because impact energy increases.

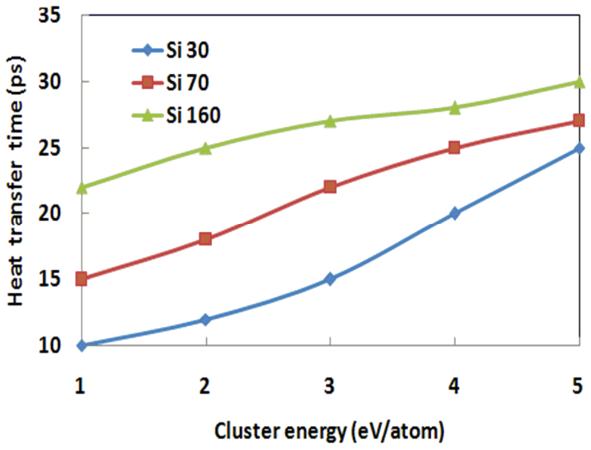

Fig. 6. The heat transferred time as a function of cluster size and energy.

Fig. 7 illustrates number of cluster implanted atoms as a function of cluster size and energy. This figure shows that the cluster implanted atoms increases by increasing cluster size and energy. The number of implanted atoms increases from 1 to 17 for Si30 nano-cluster, from 2 to 38 for Si70 and from 6 to 95 for Si170.

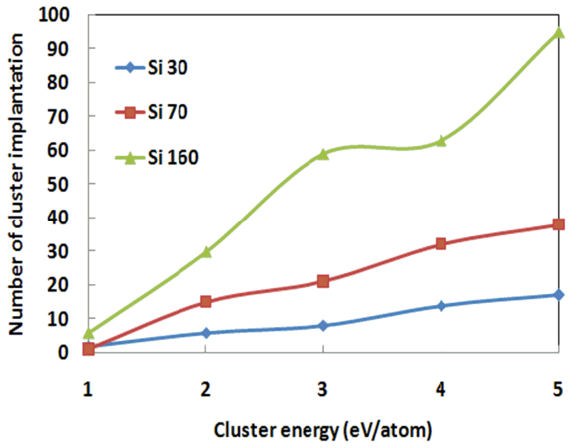

Fig. 7. Number of implantation of atoms as a function of cluster size and energy.

Fig. 8 shows number of substrate sputtering atoms as a function of cluster size and energy. It shows that the number of substrate sputtering atoms increases with increasing cluster energy and size, because large cluster with high energy has a very powerful impact, thus this impact can destroy substrate more. The number of substrate sputtering atoms increases from 5 to 19 for Si30, from 21 to 86 for Si70 and from 50 to 99 for Si170 nano-cluster. Similar behavior was seen for impact between Ni nano-cluster and Ni surface [17].

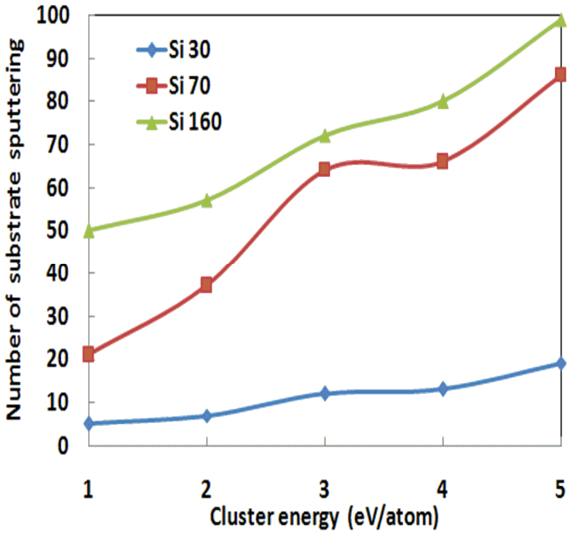

Fig.8. Number of sputtering substrate atoms as a function of cluster size and energy.

To quantify the surface roughness of the grown film, a root-mean-square roughness value is defined as:

$$R = \sqrt{\frac{\sum_{i=1}^{N_{up}} (Z_i - \bar{Z})^2}{N_{up}}} \qquad (2)$$

Where Zi shows the height of the ith atom and Nup shows the number of all of the atoms above the substrate. This parameter is a criterion for flatness and its reduction shows a flatter surface. Fig 8 plots the roughness value as a function of cluster size and energy. It shows that root-mean-square roughness decreases with increasing cluster energy and increases with increasing cluster size. In other words, small size nano-cluster with high kinetic energy can produce a flatter film. This behavior was seen for impact between Al nano cluster on the Cu substrata [21].

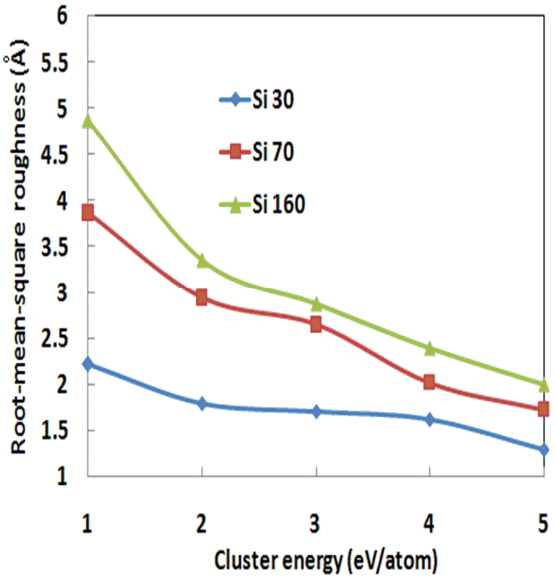

Fig. 9. The root-mean-square roughness as a function of cluster size and energy.

4. Conclusion

By ICBD, we can produce high quality metallic, semiconductor and organic thin film. Many factors such as cluster size and energy have important effects on the final thin film properties. In this paper we used MD to study the effects of these factors on the thin film quality. We studied deposition of Si nano-clusters including Si30, Si70, Si160 on the Si(100) substrate and in our study, nano-clusters have the kinetic energy from 1 to 5 eV/atom. The results of MD simulation show that the maximum substrate temperature, heat transferred time, the cluster implantation and sputtering atoms from the surface increase with increasing the cluster size and energy of the clusters. By increasing the size and energy of nano-clusters, impact energy increases, thus cluster can destroy substrate more. We found that small nano-cluster with high kinetic energy can produce flatter surface.

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