Molecular Dynamics Simulation of Al Energetic Nano Cluster Impact (ECI) onto the Surface

K. Mirabbaszadeh[i *], P. Nayebi[ii], S. Saramad and E. Zaminpayma

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ABSTRACT

On the atomic scale, Molecular Dynamic (MD) Simulation of Nano Al cluster impact on Al (100) substrate surface has been carried out for energies of 1-20 *eV/atom* to understand quantitatively the interaction mechanisms between the cluster atoms and the substrate atoms. The many body Embedded Atom Method (EAM) was used in this simulation. We investigated the maximum substrate temperature T_{max} and the time t_{max} within which this temperature is reached as a function of cluster sizes. The temperature T_{max} is linearly proportional to both energy per atom and total cluster energy. For the constant energy per atom and the cluster size increase, the correlated collisions rapidly transferred energy to the substrate, and the time t_{max} approached a constant value. We investigated the temperature T_{max} dependence on the total energy E_T and the cluster size. We showed that the cluster implantation and sputtering atoms from the surface are affected by the cluster size and kinetic energy of the clusters. Finally, time dependence of the number N_{dis} of disordered atoms in the substrate was observed.

KEYWORDS

Molecular Dynamic Simulation, Embedded Atom Method potential, Nanocluster, Al, Thin Film, Disordered Atoms, Implantation Atoms, Sputtering Atoms

1. INTRODUCTION

A widely used method for the production of thin films is the deposition of atoms or molecules onto a solid surface. In conventional deposition techniques, the most common method for supplying this activation energy consists of heating the substrate to several hundred Kelvin above room temperature.

Many materials, however, are not resistant to such high temperatures. Therefore, instead of heating the substrate, sometimes the incoming particles are accelerated to high kinetic energies, in order to activate other kinds of lateral mass transport. Unfortunately, these energetic ions can penetrate the solid, thus causing radiation damage or sputtering. In contrast, energetic clusters can deposit a large amount of energy at the surface without penetrating the substrate. This is due to the fact that the energy per atom is fairly low, even if the cluster is accelerated to a very high kinetic energy. Therefore, Energetic Cluster Impact (ECI) has been introduced as a method for producing high quality thin films of a great variety of materials [1].

Cluster deposition is softer than the atom deposition and has been regarded as a method for growing high quality film at low substrate temperatures [2-4] This method has received much attention because of various applications, such as semiconductors, metals film and dielectric for micro electronic devices, optical coatings, optoelectronic devices, magnetic materials and organic materials [5-9].

Molecular Dynamic (MD) simulations have been widely used in order to study interactions between atoms and solid surfaces [10-11]. MD studies of energetic clusters with surfaces give us a picture of the mechanism of ECI method [12-19].

2. THE SIMULATION METHOD

It is technically impossible to simulate a system consisting of thousands of atoms from first principles, i.e., by quantum mechanics. The approach of modeling the interactions on atomic scale is based on the approximation of quantum interactions by classical ones. Instead of solving the Schrödinger equation, a semi empirical model of classical interaction between atoms is constructed and then the Newton equations are solved [20]. For MD simulations we use an effective code LAMMPS stands for

i * Corresponding Author, K.Mirabbaszadeh is with the Department of Physics and Nano Technology Center, Amirkabir University of Technology, Tehran, Iran (e-mail: mirabbas@aut.ac.ir).

ii P.Nayebi is with the Department of Physics, Islamic Azad University Saveh branch, Saveh, Iran

Large-scale Atomic/Molecular Massively Parallel Simulator, written by Sandia National Laboratories. LAMMPS integrates Newton's equations of motion for collections of atoms, molecules, or macroscopic particles that interact via short- or long-range forces with a variety of initial and/or boundary conditions.

The MD simulations in this work are fully dynamical, three-dimensional calculations. The Embedded Atom Method (EAM) potential [20] was employed for the interaction between an Al cluster and an Al substrate, which is an empirical many- body potential energy function used primarily for the description of metals, e.g., Au, Cu. Ag, Pt and their alloys. Style EAM computes pair wise interactions for metals and metal [21]. The total energy E_i of an atom I is given by

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\alpha\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}\left(r_{ij}\right) \quad (1)$$

where F is the embedding energy which is a function of the atomic electron density ρ, φ is a pair potential interaction, and α and β are the element types of atoms I and J. The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbors J of atom I within the cutoff distance.

The main idea of our method is that only a rather small region surrounding the point of impact of the cluster will suffer substantial displacements of the atoms. In this region, the trajectories of all atoms have to be calculated explicitly. Contrary to this, in the surrounding of this primary zone only slight displacements of atoms occur, which can be described by assuming harmonic interactions. We apply in our simulations the model sketched in Fig.1: We consider the substrate as three parts and one cluster. One part of the substrate is impact zone containing 5819 atoms under cluster collision. Around this region is surrounded by periodic boundary walls with 62832 atoms attached to a Longevin thermostat with the temperature of 70K. At the bottom of the substrate, a fixed layer is placed with 9362 atoms. The boundary conditions in x, y axis are periodic but in z direction is not periodic, so that particles interact across the boundary, and they can exit one end of the box and re−enter the other end. The cluster is generated by cutting a sphere from fcc bulk crystals in its equilibrium state.

In order to investigate the interactions between an energetic cluster and the surface, we used fcc structured clusters, such as Al_{14}, Al_{18} , Al_{47} , Al_{55} , Al_{87} ,and Al_{177}.

A simulation run of such an energetic Al cluster was 4 A° away from surface. The initial temperature was 70K and it followed the evolution of the system during 6 ps, with time steps of 0.001ps. Before it we run the program for 50000 run in order to prepare the system.

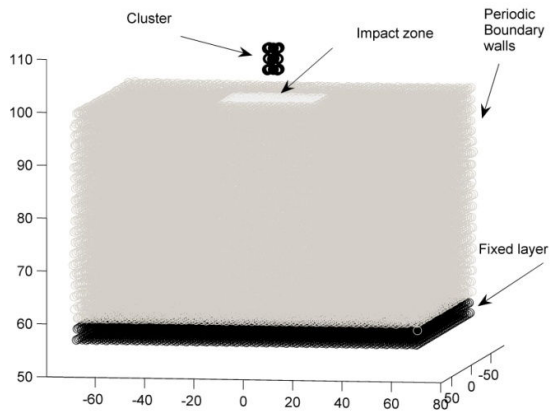


Figure1. The simulation system: Cluster; Impact zone; crystalline zone; fix zone.

3. RESULTS AND DISCUSSION

Appendixes, As a sample, the interaction between an Al (100) substrate and Al cluster of 47 atoms with a kinetic energy of 1 eV/atom is shown as function of time in Fig. 2.

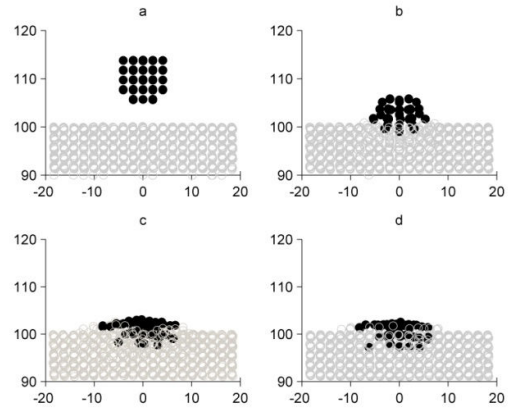


Figure2. Collision dynamics between an Al_{47} cluster with 1 eV/atom and an Al (100) substrate after 0 ps (a), 0.3 ps (b), 3 ps (c), 9 ps (d).

The snapshots of the atom positions are at various instants of time. As the impact begins, the atoms in the cluster begin to compress the substrate interface, at the same time the cluster and the substrate lose their crystalline structures. As the time elapses, cluster atoms are broken up and penetrate into the substrate, which is intermixing layer formed. Although the energetic clusters penetrate into the surface, at equilibrium the initial damage is repaired.

Fig. 3 shows the number of implantation of atoms for all clusters with kinetic energy of 5eV/atoms. With increasing the cluster size (increasing in total energy) the number of implantation atoms is increased.

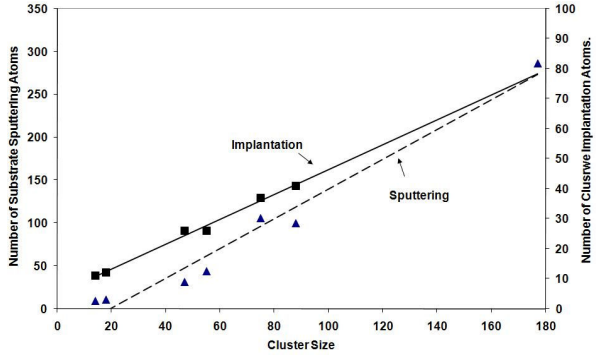


Figure 3. Number of implantation of atoms for all clusters in 5eV/atoms.

Fig.4 shows the temperature T_{max} as a function of the total energy of the cluster. As the total energy increases, the temperature T_{max} increase, but this increase is steeper for Al_{14} than for Al_{47}.

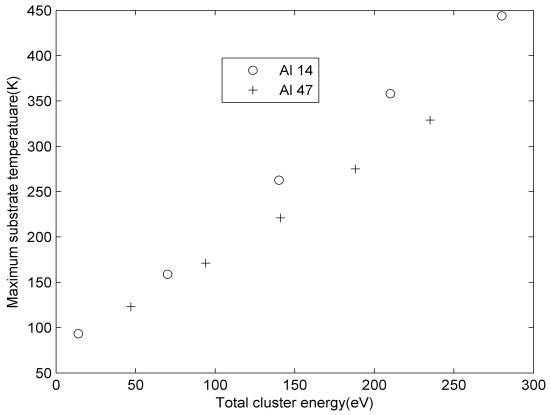
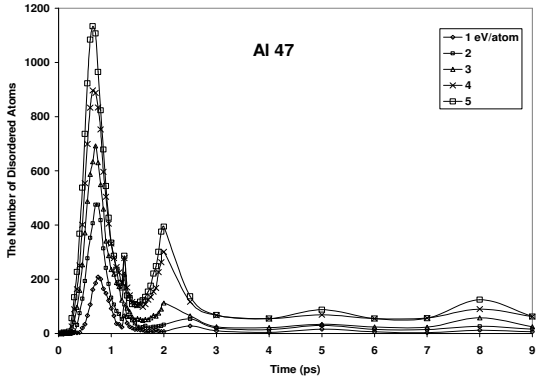


Figure 4. The maximum substrate temperature as a function of total energy.

Figure 5 shows time dependence of the number N_{dis} of disordered atoms in the substrate for Al_{47} and Al_{14}. N_{dis} increases after the impact and decreases later on. We found that as the total energy increases, N_{dis} increases.



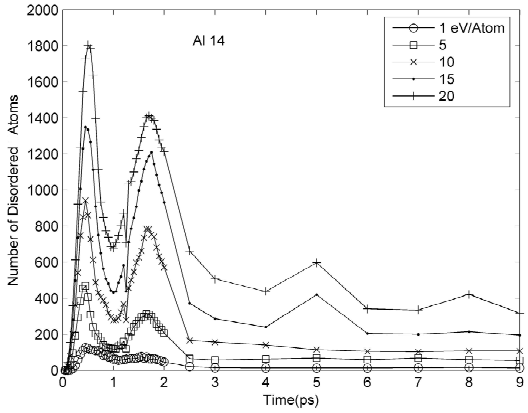


Figure 5. Time dependence of the number N_{dis} of disordered atoms in the substrate for Al_{47} and Al_{14}.

Fig. 6 shows the temperature T_{max} as a function of cluster size and the time t_{max} for $E_T = 195eV$. Since the collision time between clusters and the substrate is longer than that for single atom collisions, the substrate receives thermal energy from energetic clusters during a longer period and the thermal energy dissipates more slowly. Thus, high temperature is maintained longer (about 3 ps), which leads to self-annealing. This self-annealing plays a key role in the structural rearrangement of the surface.

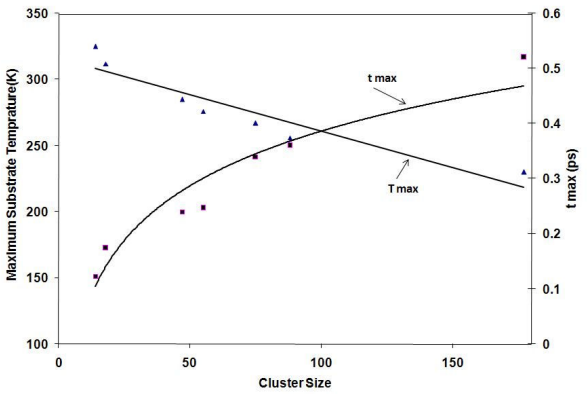


Figure 6. The temperature T_{max} and the time t_{max} for 195eV total energy as a function of cluster size.

For constant E_T, when the cluster size increases, the energy per atom and the cluster velocity decrease, the impact area increases. Since the cluster velocity decreases and the time of the collision with the surface increases, the time t_{max} increases. The dependence of the time t_{max} on n in Fig.7 can be approximated by

$$t_{\max} = 0.143\ln(n) - 0.272 \qquad (2)$$

Fig.7 shows the temperature T_{max} as a function of cluster size and the time t_{max} for 5 eV/atom. T_{max} is proportional to E_T , hence it is proportional to n the number of atoms in the cluster.

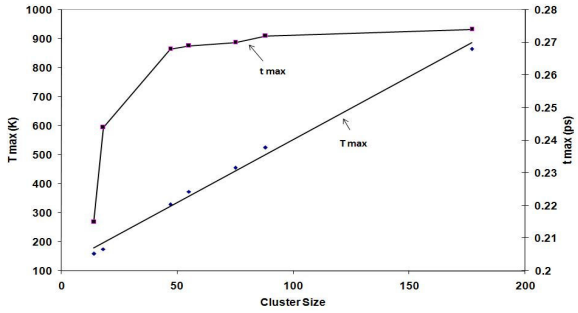


Figure 7. The temperature T_{max} and t_{max} as a function of cluster size in 5 eV/atom.

Fig.8 illustrate how the number N_{dis} of displacement atoms in the substrate depends on the cluster size n and the elapsed time t for Al_{18} ,Al_{55} and Al_{177} clusters. We consider total constant cluster energy ($E_T = 195eV$).

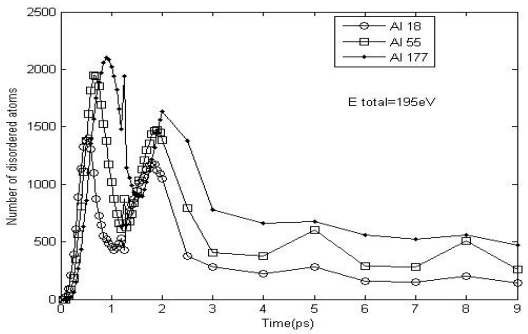


Figure 8. Time dependence of the number N_{dis} of disordered atoms in the substrate for $E_T = 195eV$.

The figure shows that after cluster impact to the surface, atoms of the surface disorder and destroys the crystalline structure. After 4 ps disorder atoms become stable.

4. SUMMARY AND CONCLUSION

In this work, we investigated interactions of Al clusters and an Al (100) substrate using MD simulation. With different impact energy and different cluster sizes the energy dependence of the Al cluster interaction with Al substrate are studied. These clusters are implanted into the substrate. The results of MD simulation show that the substrate atoms disordering, the cluster implantation and sputtering atoms from the surface are affected by the cluster size and energy of the clusters.

Our results show that for the constant total energy the temperature T_{max} depends linearly on the cluster size, while the transient time to reach this temperature varies nonlinearly. When the total energy of the cluster is kept constant, the maximum number of the disordered atoms on the surface increases for larger clusters. For the simulation time of 9ps we show that the system reaches to equilibrium after 4ps. It means that the relaxation time of atoms is 4ps.

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