Molecular Dynamic Simulation of Impact Nanoclusters Beam with Solid Surface

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Introduction

One of the effective methods for changing physical and chemical properties of material surface is high energy impact of nanoclusters with solid surface [1, 2]. Molecular dynamic simulation is one of the most popular approach to study this process. Many researchers are working on this subject [1, 2, 3, 4, 5]. The thin-film growth by energetic cluster impact normal to the surface is studied in work [3]. Simulation of the solid surface modification by high energy normal impact studied in work [4]. The structural response of the target is described in work [5] for different velocities of projectile, ranging from 6.0 to 16 km/s in conditions of normal impact.

The main goal of our investigation here is to study dynamics of penetration depth of cluster's atoms inside solid material and the thickness of deposited layer depending on clusters size, energy and impact's periods for normal and angular impacts. We have used LPMD software package [6].

Simulation procedure

One of the essential point in atomic scale modelling method is a choice of interatomic potential. It is widely recognized that empirical many-body potentials can reproduce with good accuracy the thermodynamic and structural properties of the most transition metals. In our simulations we have used the Sutton-Chen potential [7]. Parameters of the potential for a copper are shown in Table 1.

Table 1: Parameters of the Sutton-Chen potential

Metal	a(Å)	c	ϵ(eV)	m	n
Cu	3.61	39.755	0.0124	6	9

The simulating system consisted of the fixed solid substrate and 3 similar impacting clusters. Before simulating the impact, the substrate and clusters are separately equilibrated.

The metallic substrate has a size $54.15 \times 108.3 \times 108.3$ (Å) and consists of 54000 atoms of copper. The structure is face centred cubic (fcc) and has (1 0 0)-surface. The substrate is thermalized separately at $T = 300K$ using Berendsen thermostat for 10000 time steps. Boundary conditions are periodic in y- and z-directions only.

Most stable clusters have an icosahedral structure and number of atoms are calculated by formula $n = (10k^3 + 15k^2 + 11k + 3)/3,\ k = 1, 2, \ldots$ [8]. The first 3 number of atoms in cluster with icosahedral structure are 13, 55, and 147. So, we tried to simulate clusters with these sizes, consisting of copper atoms. The initial configuration of the cluster was prepared from a face centred cubic crystal of size 14.44 Å by choosing required number of atoms, closest to the center. In real experiments, generally, cluster is produces by following method: firstly the material is brought into the gas phases and then undergoes cooling and expansion in stream of inert gases. So, to be realistic, we followed by this manner. The cluster was heated up to 1800 K, much higher than melting temperature of copper. Then, it was cooled down to the room temperature and equilibrated. Each heating, cooling and equilibrating stages are done for 100000 time steps.

After that we have analyzed the structure of the clusters using the Common Neighbor Analysis (CNA) method [9]. This method is a technique used in atomistic simulations to determine the local ordering in a given structure. In this method every pair of atoms is labeled according to four indices (i, j, k, l).

The different structures have the following distribution of pairs: fcc has only (1 4 2 1) pairs; hcp has pairs distributed equally between (1 4 2 1) and (1 4 2 2); bcc has (1 4 4 4) and (1 6 6 6) presented in ratios 3/7 and 4/7, respectively. The distribution of pairs in a icosahedron structure depends on a number of atoms. The results of our analysis of the cluster with 147 atoms are shown in Table 2 and compared with the icosahedron structure. From this analysis we can see that the last configuration's structure is close to it.

The total simulation time for cluster-surface interaction shown in Figure 1 was 40 ps, with a time step $\Delta t = 1$ fs.

After separate equilibrating, the solid substrate and clusters were joined to evolve together. The clusters were placed in equal distances, so that they do not interact to each other and to solid substrate.

Table 2: The CNA analysis of cluster configuration

Pairs				Configuration		
i	j	k	l	Initial	Last	Icosahedron
1	0	0	0		1.03	
1	1	0	0	0.15	1.47	
1	2	0	0	7.22	6.45	
1	2	1	1	7.22	6.30	
1	3	0	0		2.79	
1	3	1	1	23.42	18.48	25.86
1	3	2	2		5.13	12.93
1	4	1	1		0.29	
1	4	2	1	62.00	28.01	17.24
1	4	2	2		27.27	38.79
1	4	3	3		1.47	
1	5	4	4		1.17	
1	5	5	5		0.15	5.17

Then the whole system was thermalized for 1000 time steps.

Results

We have simulated collisions of three different impact energy values, E=0.1, 1.0, 10.0 eV/atom, according to the modes soft landing, droplet spreading and implantations. The beam's frequency is defined by period T, which is the time between impact to impact. We also simulated three different time periods, T=4, 5, 6 ps. After giving an impact energy to the clusters, we have only used Berendsen thermostat for the solid substrate.

We have studied the penetration depth of clusters atoms inside solid substrate and the thickness of deposited layer on surface. In Figure 2 it is shown the time dependence of the penetration depth for single impact and different impact periods $T = 4, 5, 6$ ps. The impact energy is $E = 10$ eV/atom and cluster size is $N = 147$. The impact angle is $\alpha = 15°$. After each impact the cluster's atoms penetrates deeply inside solid substrate and then it reflects back. So, penetration of next cluster depends on the impact periods. In Figure 3 is shown the impact energy dependence of penetration depth h and the thickness of surface layer d for different impact periods. We have simulated an impact of nanoclusters beam with solid surface and following summary were obtained:

1. Soft landing: For the energy of the incident $E < 0.1$ eV/atom target surface is not destroyed and the structure of the cluster is very close to that of the original state. The atoms of cluster does not penetrate inside the surface. The thickness of the deposited layer d is increased with the size of cluster and the time of irradiation. As evident from Figure 4 cross-

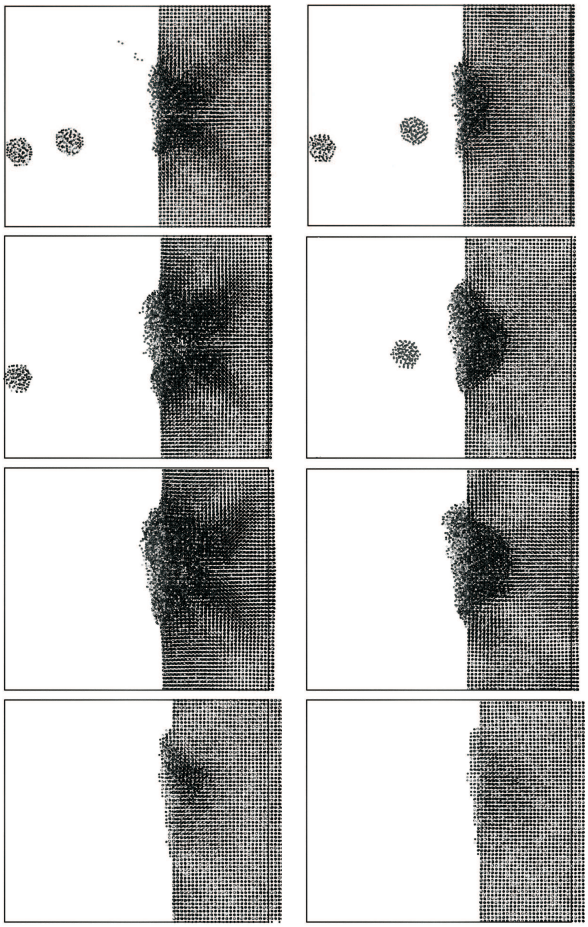

Figure 1: Snapshots of the impact at time $t = 2.3$, 5, 6.5, 9,10.5, 13, 30, 40 ps. The clusters' size are $N = 147$, impact energy is $E = 10.0$ eV/atom, and impact period is $T = 5$ ps. The impact angle is $\alpha = 15°$.

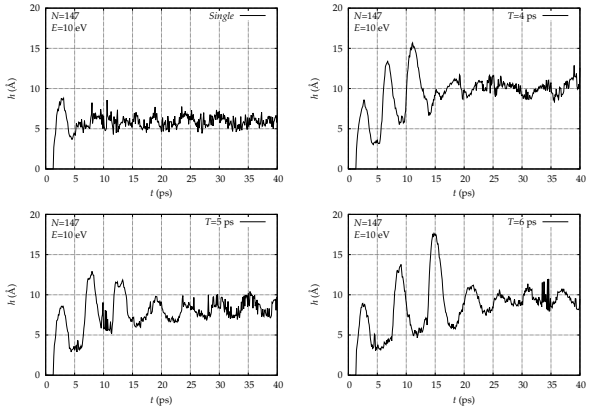

Figure 2: Dynamics of penetration depth h for single and for different impact periods.

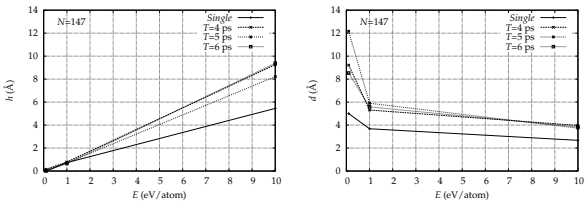

Figure 3: Dependence of penetration depth h and the thickness of deposited layer from impact energy E and impact periods T.

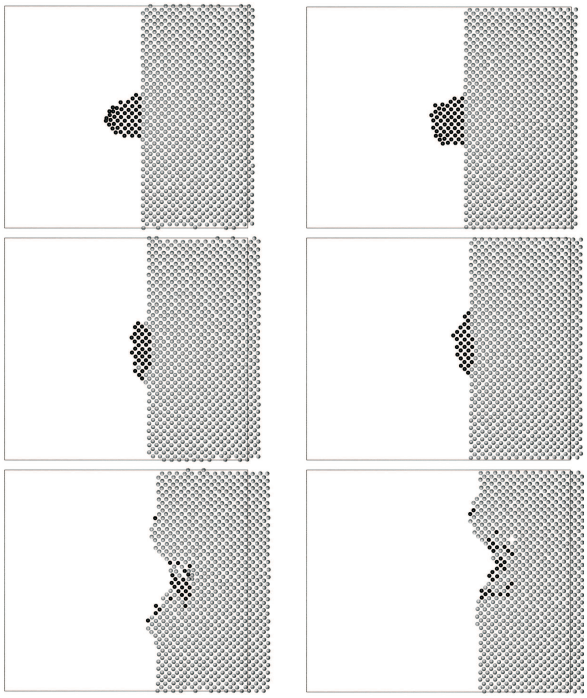

Figure 4: The cross section of the direct and angular ($\alpha = 15°$) impacts for different impact energies: top E =0.1 eV/atom, middle E =1.0 eV/atom, bottom E =10.0 eV/atom.

section profile in reaction plane of clusters adhering is more flat for angular impact then for normal one. It means that impact angle adjustment is possible to use for geometrical configuration of deposited layer grains.

2. Droplet spreading: In the case of energy of the incident $E \approx 1$ eV/atom, the structure of cluster greatly deformed and the penetration depth h is increased. The thickness of the deposited layer d is decreased, but it increases with increasing the size of clusters. Figure 4 shows, pictures at the middle line, that qualitatively, results of impact for this regime is almost the same like in previous case of soft landing. But for droplet spreading we can see that because of penetration process presence, asymmetrical deformation of deposited layer grains is a little bit less then in the case of soft landing.

3. Implantation: At energies $E > 10$ eV/atom, the structures of clusters and target are greatly deformed and the crater is created on the surface. It has been found that the penetration depth h increases gradually with raising the energy and it depends on the size of clusters and the time of the irradiation. The beam's frequency is affected by increasing size of cluster. As can be seen from Figure 4 in this regime result of cluster impact is funnel-shaped deformation of target surface. And in the case of angular impact we can observe an asymmetry in the formed funnel and decreasing of the penetration depth value in compare with normal impact correspondingly.

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