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Simulation of Interaction of Colliding Nanoclusters Beam with Solid Surface

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One of the effective methods changing surface physical and chemical properties of a material is high energy impact of nanoclusters with solid surface. Molecular dynamic simulation is one of the most popular approach to study this process. It is very important for material science and nanotechnology to know as much as possible about conditions for control of getting given properties of the deposited layer. This work is devoted to the simulation of an angular impact for Cu_n ($n = 13, 55, 147$) nanoclusters with the substrate, consisting of 54000 atoms of copper. As contrast to our previous paper [Batgerel B., Nikonov E.G., Puzynin I.V. Simulation of Impact Intereaction of Uncharged Metallic Nanoclusters with Metallic Surface // Bulletin of Peoples' Friendship University of Russia. Series "Mathematics. Information Sciences. Physics". — 2013. — No 4. — Pp. 42–56.] we have studied properties of deposited layer on the surface particularly a penetration depth of the cluster atoms and a thickness in angular impact conditions. It is found that these parameters depend on the energy and size of nanoclusters, a number of clusters in the beam, a frequency of irradiation and a value of impact angle.

Key words and phrases: molecular dynamics, simulation, Verlet method, impact interaction.

1. Introduction

One of the effective methods changing surface physical and chemical properties of a material is high energy impact of nanoclusters with solid [1, 2]. Molecular dynamic simulation is one of the most popular approach to study this process. Many researchers are working on this subject [1–5]. 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 the 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. We have used LPMD software package [6].

2. Simulation Procedure

One of a essential point in atomic scale modelling method is the choice of interatomic potential. It is widely recognized that empirical many-body potentials can reproduce with good accuracy the thermodynamic and structural properties of most transition metals. In our simulations we have used the Sutton-Chen potential [7]. The parameters of the potential for a copper are $a = 3.61(\text{Å})$, $c = 39.755$, $\epsilon = 0.0124(\text{eV})$, $m = 6$, $n = 9$.

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.

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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 a face centred cubic (fcc) and has a (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 experiment, generally, cluster is produced 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 1 and compared with the icosahedron structure. From this analysis we can see that the last configuration's structure is close to it.

Table 1

The CNA analysis of cluster configuration

Pairs				Configuration			Pairs				Configuration		
i	j	k	l	Init.	Last	Icos.	i	j	k	l	Init.	Last	Icos.
1	0	0	0		1.03		1	4	1	1		0.29	
1	1	0	0	0.15	1.47		1	4	2	1	62.00	28.01	18.02
1	2	0	0	7.22	6.45		1	4	2	2		27.27	31.53
1	2	1	1	7.22	6.30		1	4	3	3		1.47	
1	3	0	0		2.79		1	5	4	4		1.17	
1	3	1	1	23.42	18.48	36.04	1	5	5	5		0.15	5.4
1	3	2	2		5.13	9.01							

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. Then the whole system was thermalized for 1000 time steps.

3. 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.

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

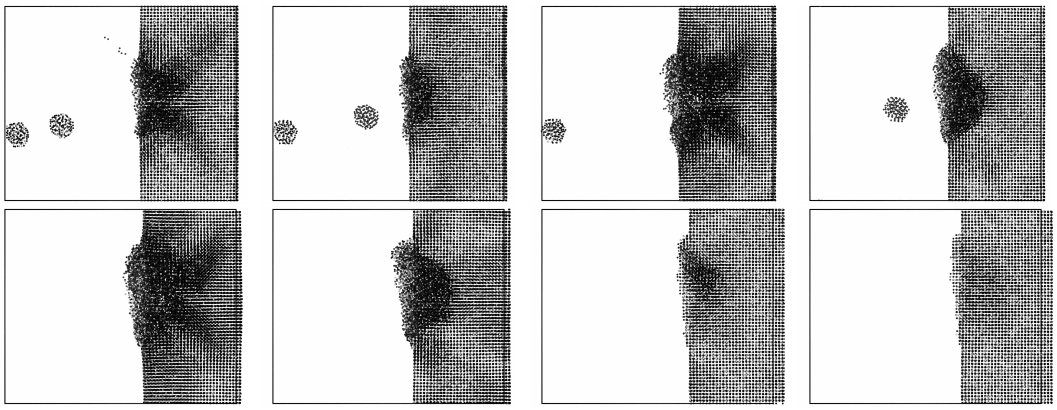

Figure 1. Snapshots of the impact at time $t =$ 2.3, 5, 6.5, 9,10.5, 13, 30, 40 ps. The clusters' size are $N = 147$, impact energy is $E = 10.0$ eV/atom and the impact period is $T = 5$ ps

We have studied the penetration depth of clusters atoms inside solid substrate and the thickness of deposited layer on surface. In Figure 2 shows 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 penetrates deeply inside solid substrate and then it reflects back. So, penetration of next cluster depends on the impact periods. Figure 3 shows the impact energy dependence on penetration depth h and also the thickness of surface layer d for different impact periods.

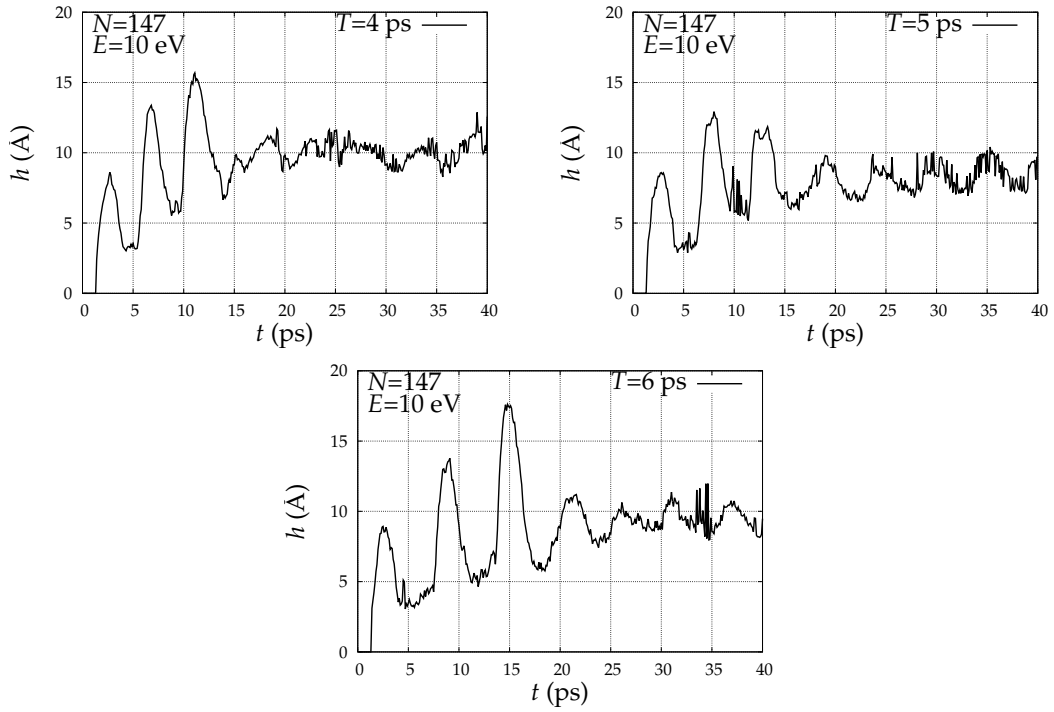

Figure 2. The dependence of penetration depth h

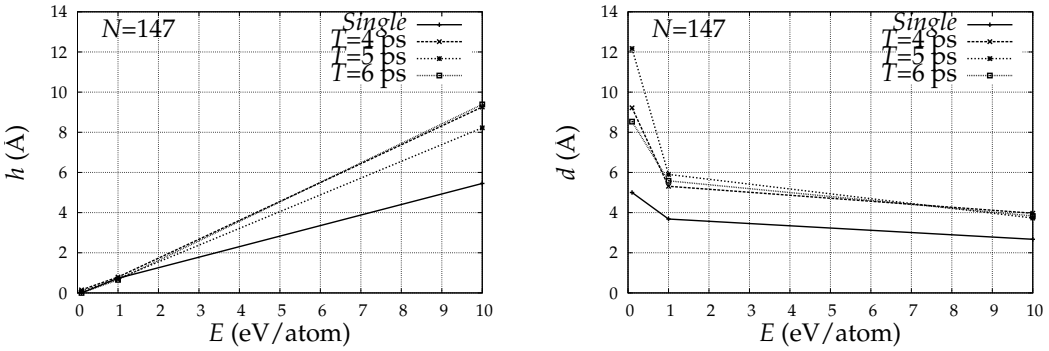

Figure 3. The thickness of deposited layer d from impact energy E and impact periods T. The impact angle is $\alpha = 15^\circ$

4. Summary

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 are not penetrated inside the surface. The thickness of the deposited layer d is increased with the size of cluster and the time of irradiation.
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.
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.

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Моделирование взаимодействия нейтральных металлических нанокластеров при соударении с металлической поверхностью

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Одним из самых эффективных методов изменения поверхностных физических и химических свойств материала является облучение нанокластерами твёрдой поверхности. Моделирование методами молекулярной динамики представляет собой наиболее популярный подход к изучению такого типа процессов. Очень важно для материаловедения и нанотехнологий знать как можно больше об условиях, при которых можно управлять процессом получения заданных свойств осаждённого на поверхность материала. Работа посвящена моделированию процессов углового ударного взаимодействия нанокластеров Cu_n ($n = 13, 55, 147$) с поверхностью образца, состоящего из 54000 атомов меди. В отличие от нашей предыдущей работы мы исследовали свойства образованного в результате соударения поверхностного слоя, в частности, глубину проникновения атомов налетающих нанокластеров и толщину осаждённого слоя в условиях углового удара. Было обнаружено, что данные параметры зависят от размера, энергии налетающих нанокластеров, количества кластеров в пучке, частоты импульсного источника и величины угла пучка налетающих нанокластеров.

Ключевые слова: молекулярная динамика, нанокластеры, моделирование, метод Верле, ударное взаимодействие.