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Molecular dynamic simulations of the high-speed copper nanoparticles collision with the aluminum surface

V V Pogorelko and A E Mayer

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

E-mail: vik_ko83@mail.ru

Abstract. With the use of the molecular dynamic simulations, we investigated the effect of the high-speed (500 m/s, 1000 m/s) copper nanoparticle impact on the mechanical properties of an aluminum surface. Dislocation analysis shows that a large number of dislocations are formed in the impact area; the total length of dislocations is determined not only by the speed and size of the incoming copper nanoparticle (kinetic energy of the nanoparticle), but by a temperature of the system as well. The dislocations occupy the whole area of the aluminum single crystal at high kinetic energy of the nanoparticle. With the decrease of the nanoparticle kinetic energy, the dislocation structures are formed in the near-surface layer; formation of the dislocation loops takes place. Temperature rise of the system (aluminum substrate + nanoparticle) reduces the total dislocation length in the single crystal of aluminum; there is deeper penetration of the copper atoms in the aluminum at high temperatures. Average energy of the nanoparticles and room temperature of the system are optimal for production of high-quality layers of copper on the aluminum surface.

1. Introduction

In recent years the high-speed interaction of the atomic clusters, nano- and microparticles with the solid surface was actively investigated [1]. Actuality of this topic is due to the possibility of using such particles to modify the surface of a solid and for improvement of its physical and chemical properties. The magnetron sputtering is the most perspective method of the surface treatment of such materials, because it allows a high speed sputtering of nanoparticles at low operating voltages (600–800 V), provides high purity of the film formed without overheating of the substrate and provides the uniformity of the film thickness at deposition on a large area of the substrate surface. Variations of the deposition parameters (speed, size and material of the nanoparticles, temperatures of the substrate and nanoparticles) can form various properties of the modified layer. Therefore, the simulation of high-speed collision of the metal nanoparticles with the surface may allow determining the optimum parameters for producing a modified deposition layer with desired properties.

One of the effective investigation methods of the high-speed collision of nanoparticles with a solid surface is a molecular dynamics (MD) simulation. There are a number of works devoted to the MD simulation of the high-speed collision of nanoparticles with a solid surface [2-7]. Collision of the copper, iron and cobalt atomic clusters with a copper surface, and the aluminum clusters with the aluminum surface were investigated in these works.

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With the use of MD simulations, we have investigated the effect of the high-speed copper nanoparticles impacts on the mechanical properties of an aluminum surface. This investigation may allow one to determine the optimal parameters for producing a modified deposition layer with desired properties.

2. MD setup

Molecular dynamic simulations were carried out with using of the LAMMPS package [8] and the interatomic potential [9], which is an angular dependent potential (ADP)—generalization of the embedded atom method (EAM) potential [10].

We considered sample of monocrystalline aluminum with size $100 \times 150 \times 150$ lattice periods of aluminum $(40.5 \times 60.75 \times 60.75 \text{ m}^3)$ which corresponds to 9 000 000 atoms. Lattice directions [100], [010], [001] coincide with the monocrystalline aluminum faces (with the coordinate axes x, y and z). Near by the monocrystalline aluminum surface, at a distance of 3 lattice periods, we placed the copper nanoparticles with the radius $R/a_{\text{Cu}} = 10$ –30, where a_{Cu} is the lattice period of copper (R = 3.6–10.8 nm). Thereafter, the whole system was kept at a constant temperature T_0 , which was initial temperature of impact, and at the pressure of 1 bar during the time interval of 10 ps. Then atoms of copper nanoparticles got an initial velocity V_0 of 500 or 1000 m/s directed along the x axis towards of the aluminum surface. Thus, direct impact of the copper nanoparticles on the aluminum surface was simulated. Periodic boundary conditions were set for lateral surfaces, which were perpendicular to y and z axes. The bombarded and back surfaces (perpendicular to the x axis) were free. Software package OVITO [11] was used for visualization of simulation results and for dislocation analysis.

3. Results and discussion

Figure 1 shows the pressure fields in the system (aluminum substrate + copper nanoparticle) at different time during high-speed collision with velocity of $V_0 = 1000$ m/s for particle radius $R = 30 a_{\rm Cu} = 10.8$ nm.

At impact, a high pressure area is formed near the contact spot between the nanoparticle and target (figure 1). The pressure reaches up to 16 GPa and decreases rapidly with time. High stresses lead to intensive plastic deformations of nanoparticle and the bombarded target during first tens of picoseconds after impact.

At the times of about 15 ps, after impact beginning, the system reaches the stationary state. Residual stresses do not exceed 8 GPa. The area of maximum stress observed inside the copper nanoparticle. Reducing of the kinetic energy of the nanoparticle (decrease of its speed or size) does not change the picture principally.

Figures 2–8 show the distribution of dislocations in the system (aluminum substrate + nanoparticle) at the different speeds and sizes of the incoming copper nanoparticle and different temperatures of the system.

Dislocation analysis shows that, a large number of dislocations is generated near the contact spot and then penetrates into the bulk of the bombarded aluminum over time. The total length of generated dislocations is defined by the kinetic energy of the incident nanoparticle (it means, its size and velocity) and temperature of the system. At high velocities and large sizes of nanoparticles, dislocations fill the entire volume of aluminum (figure 1). At lower velocities and sizes of the nanoparticles, dislocation loops are mostly formed (figures 1–7), which penetrate to a limited depth. The main type of generated lattice defects is partial Shockley dislocation. The temperature increase does not affect the total number of generated dislocations, but leads to their deeper penetration into the aluminum (figures 5–6). The temperature increase also leads to a deeper penetration of the copper atoms inside aluminum.

Figure 9 shows the total number of dislocations versus time, which in all calculations reaches a steady-state level 40 ps after the collision beginning.

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Figure 1. Pressure fields in the system. Initial velocity is $V_0 = 1000 \text{ m/s}$, the initial temperature of the system is $T_0 = 300$ K, the nanoparticle radius is $R = 30 a_{\rm Cu} = 10.8$ nm.

<i>T</i> ₀ (K)	$V_0 ({\rm m/s})$	$R~(a_{ m Cu})$	Energy of nanoparticle (keV)	Final thickness of nanoparticle (nm)	Dislocation length (nm)	Dislocation density $(10^{12}/\text{cm})$
300	1000	30	209.73	14.9	7863.76	5.26
300	1000	20	62.43	10.0	2138.25	1.43
300	1000	10	7.62	5.3	255.01	0.17
300	500	30	52.43	18.7	2703.51	1.81
300	500	20	15.61	12.1	942.14	0.63
300	500	10	1.94	5.6	70.90	0.05
500	1000	20	62.43	10.5	2055.36	1.38
700	1000	20	62.43	10.1	1526.77	1.02
900	1000	20	62.43	9.0	1712.60	1.15

Table 1. Results of the molecular dynamic simulations.

Table 1 summarizes the main results of the molecular dynamics calculations. It should be noted that the above dislocation density in the table was defined as the average value in the volume of the aluminum single crystal. According to table 1, the optimal parameters for the structure with a small number of dislocations are the average energies of the nanoparticles and the low (room) initial temperature of the system.



Figure 2. Dynamics of dislocations. Initial velocity is $V_0 = 1000$ m/s, the initial temperature of the system is $T_0 = 300$ K, the nanoparticle radius is $R = 30 a_{\rm Cu} = 10.8$ nm.



Figure 3. Dynamics of dislocations. Initial velocity is $V_0 = 1000$ m/s, the initial temperature of the system is $T_0 = 300$ K, the nanoparticle radius is $R = 20 a_{\rm Cu} = 7.2$ nm.



Figure 4. Dynamics of dislocations. Initial velocity is $V_0 = 500 \text{ m/s}$, the initial temperature of the system is $T_0 = 300 \text{ K}$, the nanoparticle radius is $R = 30 a_{\text{Cu}} = 10.8 \text{ nm}$.



Figure 5. Dynamics of dislocations. Initial velocity is $V_0 = 500$ m/s, the initial temperature of the system is $T_0 = 300$ K, the nanoparticle radius is $R = 20 a_{\rm Cu} = 7.2$ nm.



Figure 6. Dynamics of dislocations. Initial velocity is $V_0 = 1000$ m/s, the initial temperature of the system is $T_0 = 500$ K, the nanoparticle radius is $R = 20 a_{\rm Cu} = 7.2$ nm.



Figure 7. Dynamics of dislocations. Initial velocity is $V_0 = 1000$ m/s, the initial temperature of the system is $T_0 = 700$ K, the nanoparticle radius is $R = 20 a_{\rm Cu} = 7.2$ nm.



Figure 8. Dynamics of dislocations. Initial velocity is $V_0 = 1000$ m/s, the initial temperature of the system is $T_0 = 900$ K, the nanoparticle radius is $R = 20 a_{\rm Cu} = 7.2$ nm.



Figure 9. Total dislocations length versus time at different initial temperatures of the system, velocities and radii (in a_{Cu}) of the incident nanoparticles.

4. Conclusions

In the present work, a molecular dynamics study of a high-speed impact of copper nanoparticles with aluminum surface is carried out. Main attention is given to the nanoparticles impacts leading to either modification (deformation hardening) of the aluminum surface layer or implantation of the nanoparticles material. High stresses lead to intensive plastic deformations of nanoparticle and the bombarded target during first tens of picoseconds after impact. Plastic deformation and attraction between Al and Cu atoms provide an adhesion of nanoparticles to surface.

Dislocation analysis shows that, at high kinetic energy of the nanoparticle, dislocations fill the entire volume of aluminum. At lower velocities and sizes of the nanoparticles, dislocation loops are mostly formed, which penetrate to a limited depth. The temperature increase does not affect the total number of generated dislocations, but leads to deeper their penetration into the aluminum. The temperature increase also leads to a deeper penetration of the copper atoms in aluminum.

Average energy of the nanoparticles ($V_0 < 1000 \text{ m/s}$) and room temperature of the system ($T_0 = 300 \text{ K}$) are optimal for production of high-quality layers of copper on the aluminum surface.

Acknowledgments

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