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High-speed collision of copper nanoparticle with aluminum surface: Molecular dynamics simulation

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ABSTRACT

We investigate the effect of the high-speed collision of copper nanoparticles with aluminum surface by means of molecular dynamic simulations. Studied diameter of nanoparticles is varied within the range 7.2–22 nm and the velocity of impact is equal to 500 or 1000 m/s. Dislocation analysis shows that a large quantity of dislocations is formed within the impact area. Overall length of dislocations is determined, first of all, by the impact velocity and by the size of incident copper nanoparticle, in other words, by the kinetic energy of the nanoparticle. Dislocations occupy the total volume of the impacted aluminum single crystal layer (40.5 nm in thickness) in the form of intertwined structure in the case of large kinetic energy of the incident nanoparticle. Decrease in the initial kinetic energy or increase in the layer thickness lead to restriction of the penetration depth of the dislocation net; formation of separate dislocation loops is observed in this case. Increase in the initial system temperature slightly raises the dislocation density inside the bombarded layer and considerably decreases the dislocation density inside the nanoparticle. The temperature increase also leads to a deeper penetration of the copper atoms inside the aluminum. Additional molecular dynamic simulations show that the deposited particles demonstrate a very good adhesion even in the case of the considered relatively large nanoparticles. Medium energy of the nanoparticles corresponding to velocity of about 500 m/s and elevated temperature of the system about 700–900 K are optimal parameters for production of high-quality layers of copper on the aluminum surface. These conditions provide both a good adhesion and a less degree of the plastic deformation. At the same time, higher impact velocities can be used for combined treatment consisting of both the plastic deformation and the coating.

1. Introduction

In recent years the high-speed interaction of the atomic clusters, nano- and microparticles with solid surface was actively investigated [1]. Actuality of this topic is determined by the possibility of using such particles for modification of solid surfaces [2–4] including improvement of their physical and chemical properties and polishing [5,6], as well as formation of various functional nanostructures on them [7]. A number of deposition techniques [8–10] are used including the nanoparticles deposition from suspensions and aerosols [9]. In the last case, a temperature gradient (thermophoretic deposition) [9] or an electrical field (electrophoretic deposition) [11–13] can be used in order to activate the nanoparticles transfer from the aerosol onto surface. The second motivation for investigations in this area is the usage of impacting technique for studying of mechanical properties of matter at nanoscale level, for example in ballistic tests with penetration of projectile in polymer nanocomposites [14] or graphene sheets [15].

Variation of deposition parameters (speed, size and material of the particles, temperature of the substrate and nanoparticles) can lead to various properties of the modified surface layers. Impact velocity for nanoparticles mechanically deposited from an aerosol jet can reach about 100 m/s [16]. Using of the electric field acceleration [2] can substantially increase the impact velocity. A soft landing at low impact velocity [17] is mostly used for deposition in order to avoid the structural damaging of both the deposited particle and the substrate surface. On the other hand, deposition of relatively large nanoparticles at high impact velocities can involve new mechanisms of modification, which can also be useful for some purposes. Therefore, simulation of the high-speed collision of nanoparticles with metal surface may allow determining the optimal parameters

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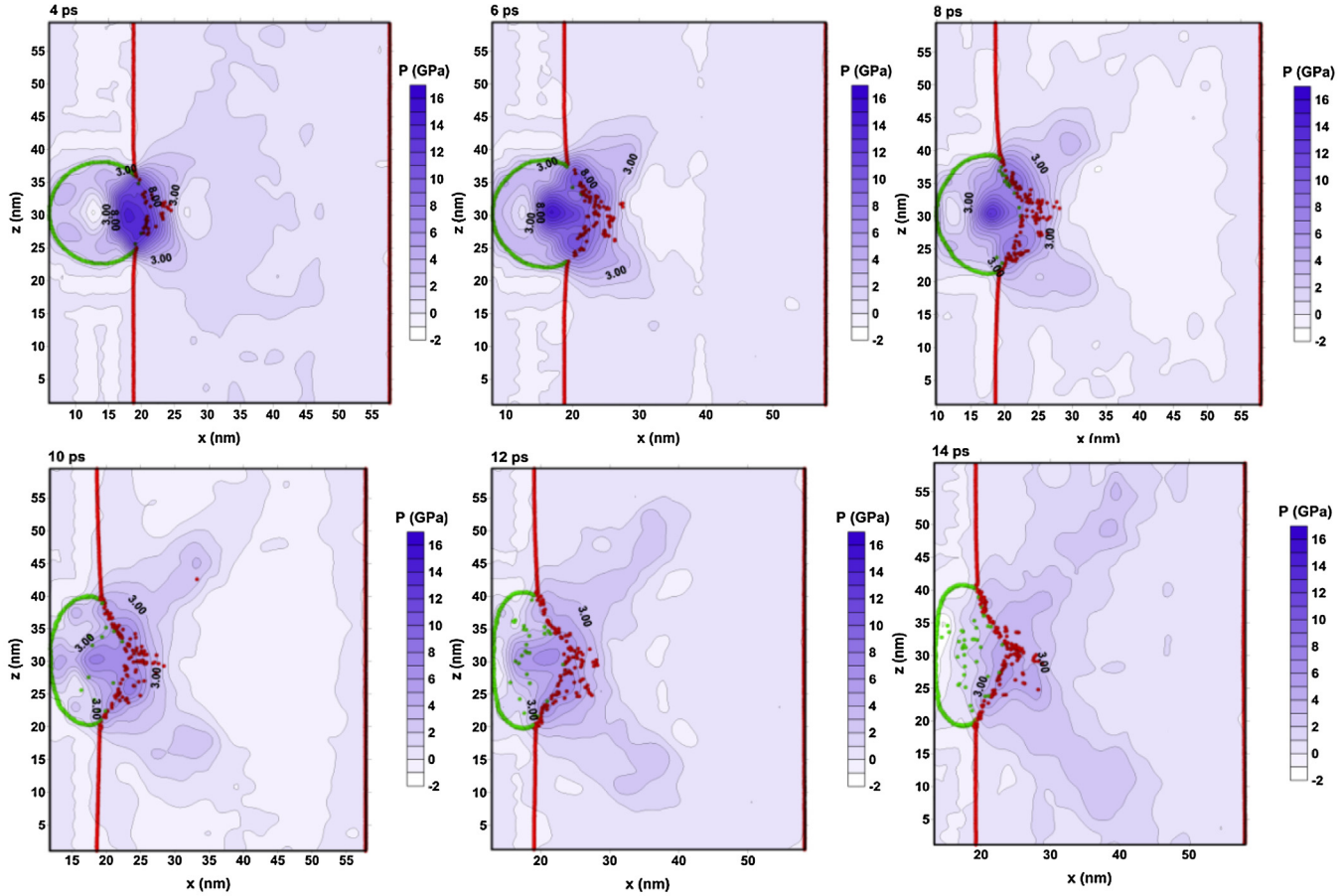

Fig. 1. Spatial distributions of pressure in the central cross-section of the system; the initial temperature of the system is $T_0 = 300$ K; the nanoparticle radius is $R = 20a_{Cu}$ (7.2 nm); the impact velocity is $V_0 = 1000$ m/s. Green line marks the position of Cu nanoparticle; red line marks the position of aluminum surface; separate green and red points mark atoms with the most defective lattice in the surrounding area. Lattice directions [100], [010] and [001] of copper nanoparticle coincide with *x*, *y* and *z* axes, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

for producing of a modified deposition layer with desired properties.

One of the effective investigation methods of the high-speed nanoparticles interaction with solid surface is the molecular dynamics (MD) simulation. There is a number of works devoted to MD simulation of the high-speed nanoparticle collision with solid surface [5,6,18–26] and also with matter nanolayers [27,28].

Hsieh and Averback [18] investigated the collision of copper clusters consisting of 13 and 19 atoms with a copper substrate; a difference between the interaction of a cluster with a surface and the interaction of single atom with the same surface was shown. Interaction of the copper clusters of 13, 18, 38 and 55 atoms with copper surface (111) was investigated by Alamanova, Grigoryan and Springborg [20]. Simulations showed that the change of structure for large clusters is less than that for small clusters. When initial energy of the clusters is equal to 0.5 eV/atom, the structures of the deposited clusters have minimal likeness to the initial structure, and monolayers of incident atoms are formed. Increase in the initial energy of the clusters leads to formation of the more difficult structures on the metal surface. Normal impact of bigger Cu clusters containing up to several hundreds of atoms with Cu (100) substrate was investigated by Fang, Kang and Liao [21] at various substrate temperatures. Dislocation slip inside substrate was reported, intensity of the slip increases together with the cluster size increase. Plastic deformation of substrate led to the formation of crater on the impact site.

Zhang et al. [25] simulated a deposition of copper clusters Cu_{55} on an iron surface Fe (001). Effects of the initial energy of cluster and the substrate temperature on the number of embedded atoms, the defect quantity in the substrate, the structural parameter and the spreading index were investigated. Araghi and Zabihi [24] investigated a cobalt nanocluster collision with copper substrate Cu (001). It was indicated that the incident cluster energy rather than the cluster size and substrate temperature mainly affected the penetration and diffusion processes, but the structural parameter of the cluster was affected by the cluster size, incident energy and substrate temperature. Kang and Hwang [19] simulated the aluminum cluster deposition on the aluminum substrate (100). They determined the dependence of the maximum substrate temperature and time of its achievement from the cluster size. Hong, Hwang and Fang [26] simulated the low-energy iron and cobalt cluster deposition on the copper substrate (001). It was shown that the substrate roughness is reduced together with the increase in the initial cluster energy and substrate temperature, at the same time, the mixing of atoms on the surface is increased. Bombardment of Ni clusters onto Cu (001) surface was simulated by Lin et al. [23]; the cluster size was up to 214 atoms. It was shown that the cluster size increase leads to an increase in both the penetration depth and the substrate surface damage at a given energy per atom, it means, at a given impact velocity. Also, the substrate temperature growth raises the penetration depth and the rate of diffusion. Yoon et al. [27] simulated impacting of graphene by supersonic projectiles, the energy of penetration was obtained in comparison with experiments [15], the cracking of graphene was initiated from formation of 5/7 Stone-Wales defects; also, the influence of initial graphene structure defects was studied. In paper [28] authors determined the