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 velocities of impact is equal to 500 or 1000 m/s. Dislocation analysis shows that a large quantity of dislocations are 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 of the initial kinetic energy or increase of the layer thickness lead to restriction of the penetration depth of the dislocation net; formation of separate dislocation loops are observed in this case. Increase of 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.