High-speed collision of copper nanoparticles with aluminum surface: Inclined impact, interaction with roughness and multiple impact

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ABSTRACT

Using molecular dynamic simulation, we investigate the influence of the angle of incidence and surface roughness at the high-speed collision of copper nanoparticles with aluminum surface. Also, special attention is devoted to the consideration of several successive collisions. Nanoparticles with a diameter of 16.2 nm and a collision speed of 500 and 1000 m/s are considered. An increase in the angle of incidence of the nanoparticle leads to a lower defect structure in the surface layer of the substrate and reduces the adhesion of the deposited particle to the substrate. The presence of a roughness on the surface always leads to decrease in the total length of dislocations remaining in the substrate after collision; this decrease is due to the escape of some dislocations on the lateral surface of the protrusions on the substrate. The depth of the modified layer formed by several successive collisions of nanoparticles with the aluminum surface does not exceed the size of the nanoparticle. In the case of successive collisions of nanoparticles, the use of collision speed of 1000 m/s is optimal, since it ensures a minimum porosity of the formed copper layer. The hardness of the formed copper layer at successive collisions of nanoparticles is below the hardness of a copper single crystal by 30–45%. At the same time, the copper layer has good adhesion properties, which are comparable with the adhesion properties of copper atoms to a copper single crystal.

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1. Introduction

The collision of high-speed atomic clusters or nanoparticles with a solid surface [1,2] has numerous technological applications, such as hard [3], anticorrosive, conductive [4] or other functional coatings [5], surface nanostructuring [6], surface cleaning, dry etching, smoothing [7] and polishing [8,9]. At the present time, acceleration of nanoparticles by supersonic gas flow [5], as well as a combination of magnetron sputtering [6,10] or laser ablation [11] with subsequent acceleration by an electric field are used for the high-speed deposition of nanoparticles. The development of methods for obtaining high-speed nanoparticle flows and also combining the nanoparticle flows of various materials can offer the challenge for their use in additive technologies for the creation of multilayer coatings and products. Compared with traditional

additive methods of manufacturing, such as selective laser sintering, which is effective in the construction of monolithic products, the flow of high-speed nanoparticles can be advantageous in the manufacture of products with a complex internal structure.

Understanding the features of the high-speed particle interaction with the surface of various materials is critically important for the development of appropriate technologies. Experimental methods allow one to study only the final structure and properties of the treated surface. The collision process can be investigated using molecular dynamic (MD) simulation [12–19]. Despite the progress made in the research, there remain a number of questions that require further study. For example, collisions of relatively small clusters are considered in most MD calculations. Using a large-scale MD simulation, we showed in [20,21] that the collision of copper nanoparticles with diameter of 7–22 nm with the aluminum surface at velocities of 500–1000 m/s leads to their effective fastening on the surface due to substantial plastic deformation of the nanoparticles and the substrate.

In [20,21] we investigated the normal incidence of single nanoparticles of copper on a flat surface of aluminum. From the viewpoint of using the high-speed nanoparticle impact for coating

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formation and possible application in additive manufacturing, it is important to investigate the adhesion efficiency and the modification of the defect subsystem of substrate and nanoparticle in the case of oblique incidence, interaction with surface irregularities and multiple collisions of nanoparticles with substrate and with layers of nanoparticles deposited earlier. Such an investigation was carried out in this work using MD simulation.

2. MD setup

Simulation of the high-speed collision of nanoparticles with an aluminum surface is carried out using the molecular-dynamic package LAMMPS [22]. Angular dependent potential (ADP) potential [23] is used to describe the interaction of aluminum and copper atoms. This ADP potential is based on the embedded atom method (EAM) [24] and takes into account the angular dependence of the interaction energy. Visualization of the obtained atomic distributions is performed using the OVITO package [25]. An analysis of the defect structure of the substrate and particle is carried out by calculating the centrosymmetry parameter and CNA and DXA algorithms [26], which allow one to identify the type of crystal structure and dislocation lines in the calculated atomic configurations, respectively.

The initial state of the aluminum substrate and copper nanoparticles corresponds to an ideal single crystal. Crystallographic directions [1 0 0], [0 1 0] and [0 0 1] of the substrate are oriented along the axes Ox, Oy and Oz. We emphasize that unlike [20,21], in the present paper all calculations are carried out only for the case when the orientation of the copper nanoparticle lattice initially coincided with the orientation of the lattice of the aluminum substrate. The substrate size is $100 \times 150 \times 150$ of aluminum lattice periods ($41 \times 61 \times 61$ nm), which corresponds to 9 million atoms. In the direction Oy and Oz axes, periodic boundary conditions are superimposed on the system, and the free surface condition is set along the Ox axis. When considering one nanoparticle in a MD system, these boundary conditions physically correspond to the bombardment of flat aluminum nanolayer (41 nm of thickness) by a periodically ordered system of nanoparticles with a spacing of 61 nm between them. Bombardment surface of target is parallel to Oyz plane.

As distinct from the works [17–19], we do not use absorbing boundary conditions and temperature control to mimic the effect of a large substrate. We already consider a large substrate, for which the propagation time of the thermal wave through this substrate is much longer than the cooling time of the deposited nanoparticles. Also, the size of the substrate is chosen in such a way that the resulting dislocation structure does not reach the rear surface of the substrate to exclude the effect of a free back surface as an absorber of dislocations.

At a distance of approximately 1 nm from the substrate or layer of previously deposited nanoparticles, resting copper nanoparticles with a diameter of 16.2 nm are placed. After this, the whole system is maintained at a constant temperature and a pressure of 1 bar during time interval from 5 to 10 ps for relaxation. Then, the copper atoms obtain an initial velocity of 500 or 1000 m/s. In the study of inclined incidence, the velocity is directed at different angles to the normal to the surface of the substrate; velocity vector is directed in the Oxy plane; normal incidence corresponds to the motion of the particle along the Ox axis. In the study of inclined incidence and interaction with irregularities, the module of initial velocity of the nanoparticle is 500 m/s. In the case of the application to a multilayer coating, two problem statements are considered: (1) three successive impacts by five nanoparticles at a speed of 500 m/s; (2) the first impact with a speed of 500 m/s and two subsequent ones with a speed of 1000 m/s. After the beginning of the collision,

the NVE ensemble is used, which ensure the conservation of the total energy of the system.

Adhesive properties of the resulting multilayer coating are investigated using the technique proposed in [20]. The atomic distributions obtained during the collision of a nanoparticle with a substrate are used as the initial state of the system. To each atom of the nanoparticle located above the surface of the substrate, a force normal to the surface of the substrate is applied. This force linearly increases over time with a proportionality coefficient 7.2 pN/ps. The time of detachment of the area, to which the force is applied, makes it possible to judge the quality of adhesion. In these calculations, the NVE ensemble is used, that is, the total energy of the system is conserved, taking into account the work of the applied external force.

The nanohardness of the coating formed during multiple collisions of nanoparticles is also estimated. For this purpose, the nanoindentation process is simulated. We consider a ball consisting of aluminum atoms with a radius of 6 nm as an indenter. During the calculation, the speed of motion of the indenter to deep into the substance is maintained at 20 m/s. The condition of non-deformability is given for the indenter. The distribution of nanohardness over the depth of the coating is investigated, details are described in Section 3.4.

3. Results and discussion

3.1. Inclined incidence

Fig. 1 illustrates the dynamics of the collision of a copper nanoparticle with an aluminum substrate at an incidence angle of 45°. Fig. 2 shows the state of the system at various incidence angles of nanoparticles at a time point of 100 ps, to which a stationary state is reached, that is, the motion and deformation of the particle and substrate ceased. The surface of the substrate and the impacted nanoparticle is shown, as well as the formed dislocation structure inside the substrate.

In the case when the angle of incidence differs from zero, the particle turns for some angle before a complete stop; it is due to the presence of a velocity component parallel to the substrate surface. In this case, the aluminum layer adheres to the surface of the copper particle and rotates together with it, leaving a stria on the substrate (Fig. 2); this behavior is associated with good adhesion properties of copper and aluminum atoms. As the angle of incidence increases, the rotation angle of nanoparticle increases and the nanoparticle moves away from the place corresponding to the normal impact.

Dislocation analysis shows that when a nanoparticle of copper collides with an aluminum substrate, a large number of dislocations form in the impact region, which is determined by the kinetic energy of the nanoparticle. With an increase in the angle of incidence and, correspondingly, a decrease in the fraction of the kinetic energy that goes into the deformation of the system, the length of formed dislocations decreases. Over time, under the influence of stresses formed during collision, the dislocations penetrate deep into the substrate; at small angles of incidence, dislocations penetrate to a greater depth. In all calculations, there is a tendency to form dislocation loops. Initially, dislocation half-loops arise on the interface between copper and aluminum, which then expand to form a dislocation structure. This situation is similar to the situation at the beginning of the plastic growth of an already existing pore in an aluminum single crystal under tension [27]. The energy of dislocation formation is less near the interface [27], which is also a crystalline defect. In addition, the pressure and shear stresses are maximal near the interface. Both these factors determine the position of the dislocation sources. The active growth of the dislocation