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Peculiarities of structural transformations in metal nanoparticles at high speed collisions

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Abstract. A molecular dynamics simulation of nanosized particle collision under the electrical explosion of metal wires of different types was conducted. Interatomic interactions were described on the base of the embedded atom method. Used potentials allowed describing with high accuracy many mechanical and physical properties which are very important for the simulations of nanoparticle collisions with high velocities. The dynamics of the nanosized particle formation at the electric pulse explosion of metal wires of different types was studied. Features of particle collisions on the example of nanoscale particles of copper and nickel, whose velocities varied from 50 to 1500 m/s were investigated. The peculiarities of structural transformations in the colliding particles depending on the velocity of collision were determined. The intervals of collision velocities in which interaction between particles is elastic or leads to the formation of structural defects or melting were calculated. The analysis of the structure and distribution of chemical elements over the cross section of the particles which were synthesized under simultaneous explosions of different metal wires was carried out.

1. Introduction
Technologies based on pulsed processes with high rates of change of thermodynamic parameters of the system are widely used for producing nanoparticles with high value of their activity [1–4]. One such technology is electric explosion of metal wires. It is based on passing through the metal wire the current pulse with a high density of $10^6$–$10^9$ A/cm$^2$. As a result of such exposure, the wire is heated to the melting point, melted and explosively destroyed [5, 6]. Nanosized particles are synthesized during the scattering of the explosion products in gas atmosphere.

This technology allows obtaining a wide range of nanopowders of metals, alloys, oxides and nitrides of metals. The resulting nanoparticles have a relatively small size deviation. The average particle size typically ranges from $\approx$ 20 to $\approx$ 500 nm, and the area of their specific surface can vary from units to tens of m$^2$/g. They are stable in normal conditions and have a high activity in chemical processes. Experimental study of the process of nanoparticle synthesis at the electric explosive destroying is facing significant challenges that are associated with small spatial-temporal scale of this process. One of the most effective approaches to study dynamics of the electrical explosion of metal wires is the method of molecular dynamics [7–10]. Stages of the explosive destruction process, the influence of internal structure of metal wires on the explosion process, features of the simultaneous explosion of wires of different metals, the impact of the environment on the process of wire explosion and the synthesis of nanoparticles on the base of
this method were investigated in [11,12]. At the same time the process of nanoparticle formation by the collisions of the fragments of the exploded wires remains insufficiently investigated.

The aim of this work is study of peculiarities of structural transformations in nanoparticles synthesized from dissimilar metals by high-speed collisions of fragments of wires, which were electrically exploded.

2. Formalism
The study of the nanoparticle formation was carried out on the basis of molecular dynamics method with nve integration (microcanonical ensemble). Interatomic interaction was described in the embedded atom method [13]. Nanoparticles of copper and nickel were chosen as the studied objects. They had spherical shape and perfect crystal structure before their collisions. The colliding particles consisting of 30 000 or 100 000 atoms were heated to 300 K and 700 K. Nose–Hoover termostat was used in all temperature manipulations in the work. After collision particles were cooled to 300 K. Timestep was set to 10 fs for preparation and 0.5 fs for collision simulation. The process of central symmetric collisions of particles was simulated in this work. The velocity of the particles ranged from 50 to 1500 m/s. Analysis of the structural transformations in the particles during collisions was based on Common Neighbor Analysis [14]. The software OVITO was used for visualization of the simulation results [15].

3. Results and discussion
The calculations [11] showed that the process of electrical explosion of wires can be divided into three stages. The first stage is heating of metal wires without losing their continuity. The kinetic temperature of the simulated system reaches a maximum. Some atoms start to evaporate from the free surfaces of the metal wires. In the second stage the explosive destruction of wires resulting in the formation of fragments of various sizes takes place. Velocities of wire fragments can reach hundreds of m/s. Kinetic temperature of the simulated system abruptly decreases (almost 3 times). The processes of evaporation and deposition of atoms from the gas phase on the surface of the fragments occur in the third stage. The fragments of the explosion are colliding with a high velocities and begin to form nanoparticles. In the present work the structural transformations in these particles after their collisions were studied.

The following parameters of the simulated system were analyzed: a change in the distance between centers of mass for copper and nickel, temperature dynamics of the simulated system in the course of its evolution for different collision velocities. The calculation of the phase composition of the synthesized particles depending on the velocity, size and temperature of the colliding particles was carried out.

Figure 1 shows how the distance between centers of mass for copper and nickel and the temperature of the simulated system depend on time. It is clearly seen in figure 1(a), that the distance between centers of mass after the collision with the velocity of 100 m/s oscillates around the value of 12.3 nm. The oscillations are eventually damped. Note that the radius of each particle before the collision was approximately 6.5 nm. Melting and subsequent uniform mixing of atoms in the particle has not happened at this value of collision velocity. The time dependency of temperature of the simulated system is characterized by abrupt changes. The first few steps on a curve in figure 1(b) are associated with the generation of structural defects. High velocities of collision lead to melting of the synthesized particles. The distance between the centers of mass for nickel and copper are virtually eliminated, which means a high degree of mixing of the metals, figure 1(c). The temperature of the simulated system initially increases substantially above the melting temperature, and then observed its abrupt decrease, which is connected with the explosion process, figure 1(d).

The calculations show that the distance between the centers of mass for copper and nickel in the synthesized particle decreases approximately linearly with the increase of the collision...
Figure 1. Time dependence of distance between the centers of mass for copper and nickel (D) and temperature (T) for collision velocity with 100 m/s (upper figures) and 2500 m/s (lower figures). Particles are consisted of 100 000 atoms, their initial temperature was 700 K.

velocity regardless of the size of the colliding particles and their temperatures, figure 2(a). The centers of mass for the metals at velocity collision of 2500 m/s coincide. The temperature of the synthesized particles monotonously increases with increasing collision velocity, figure 2(b). There are small kinks and slope changes of the curves at collision velocities in the interval from 1500 to 2000 m/s. It is connected with melting of copper blocks of particles which are synthesized at this interval of collision velocities.

The number of survived structural defects in the synthesized particle is determined by the temperature of the colliding particles and velocity of their collision. It is seen in figure 2(c, d) that the fraction of atoms with fcc symmetry of the nearest environment (the initial structure) is reduced and becomes zero with increasing of the collision velocity. The number of atoms with hcp symmetry has a characteristic maximum whose position depends not only on the initial temperature, but also on the particle size. Position of maximum number of atoms with hcp symmetry of the local environment in the synthesized particle shifts to the lower value of collision velocities with the increasing of the initial temperature and size of colliding particles, see figure 2(d). The formation of blocks with different phase composition is connected with the generation of shock waves at high-speed collision, leading to substantially nonuniform stress and density distributions in the volume of the synthesized particles [16,17]. The internal structure of the synthesized particle in different time moments of its evolution is shown in figure 3. The collision velocity of particles containing 100 000 atoms was 1300 m/s, the initial temperature was 300 K. The result-
Figure 2. Distance between the centers of mass for copper and nickel in the synthesized particle (a), its temperature (b), the fraction of atoms with fcc (c) and hcp (d) symmetry of their local environment versus collision velocity of particles. Red and blue correspond to 700 K and 300 K of the particles before their collision, respectively. Solid and dotted lines correspond to the collision of particles consisting of 30 000 and 100 000 atoms, respectively.

Figure 3. The structure of the synthesized particle at different points in time after the collision: (a) 4.5, (b) 6.5 and (c, d) 160 ps. The central part of the particles in the figures (a–c) is removed. Atoms with hcp, fcc, bcc and uncertain symmetry of the nearest environment are shown in red, green, blue and gray, respectively. Atoms of copper and nickel in (d) are shown in red and blue, respectively. Collision speed was 1300 m/s, initial temperature was 300 K.

ing particles had a block structure and their internal structure characterized by a large number of defects. As a rule particles with high density of defects possess high degree of activation.
Analysis of simulation results showed that the copper atoms in the synthesized particles tend to come to the surface, and the nickel atoms remain in the volume. The particle which was synthesized at the collision of copper and nickel particles containing 100,000 atoms is shown in figure 4. The velocity of particle collision was 2500 m/s and their temperature was 300 K. The segregation of copper and nickel in the synthesized particle is clearly seen.

4. Conclusion

The structure and chemical activity of the bicomponent nanoparticles synthesized by the collision of metal particles sufficiently depend on velocity of collision. It was shown that there is some optimal interval of velocity collisions for which the synthesized particles contain the maximum number of structural defects. This interval depends on the size of the colliding particles and their temperature. The presence of structural defects determines the activation ability of particles. The segregation effect in the synthesized bicomponent Cu–Ni particles was revealed. The copper atoms tend to be located near the free surface, and the nickel atoms occupy the region inside the particle.

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