Computer simulation of metal wire explosion under high rate heating

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Abstract. Synchronous electric explosion of metal wires and synthesis of bicomponent nanoparticles were investigated on the base of molecular dynamics method. Copper and nickel nanosized crystallites of cylindrical shape were chosen as conductors for explosion. The embedded atom approximation was used for calculation of the interatomic interactions. The agglomeration process after explosion metal wires was the main mechanism for particle synthesis. The distribution of chemical elements was non-uniform over the cross section of the bicomponent particles. The copper concentration in the surface region was higher than in the bulk of the synthesized particle. By varying the loading parameters (heating temperature, the distance between the wires) one can control the size and internal structure of the synthesized bicomponent nanoparticles. The obtained results showed that the method of molecular dynamics can be effectively used to determine the optimal technological mode of nanoparticle synthesis on the base of electric explosion of metal wires.

1. Introduction

The electrical explosion of metal wires is one of the most promising technological approaches for the synthesis of nanoparticles of a given composition and internal structure. This approach allows synthesizing particles with complex internal structure consisting of several metallic and non-metallic phases which significantly influences their physical and mechanical properties [1–4]. The metal wire explosion occurs as follows: when a high-density electric pulse (10⁶–10⁹ A/cm²) is sent through a metallic wire, it is rapidly heated, melted, and then it explodes. The explosion products disperse into gaseous atmosphere with the formation of particles. This approach allows synthesizing a wide range of metals, oxides, nitrides and other powders with complex internal structure. It was shown that the internal structure of nanopowders influences their physical, chemical and mechanical properties [5–8]. Experimental study of the processes in electric explosion of wires has significant difficulties connected with ultrahigh temperature and high-velocity processes of explosion. It should be noted that the use of the particle method in its various representations is promising for describing structural and phase transformations, generation of charged clusters, formation of gas phase and dispersion particles under the electric explosion of wires [9, 10].

The purpose of this paper was the investigation of the synthesis of bicomponent particles as a result of simultaneous electric explosion of copper and nickel wires. The influence of the distance between
metal wires and viscosity of surrounding medium on characteristics of the synthesized particles and the distribution of chemical elements inside of them were studied.

2. Results of simulation and their discussion

Investigations in the paper were carried out using the molecular dynamics method [11–13]. The potentials calculated in the framework of the embedded atom method were used to describe interatomic interaction [14]. These potentials allow calculating with good accuracy the surface properties, energy of structural defects, elastic characteristics and other properties that are necessary for a correct simulation of electric explosion.

Copper and nickel specimens of cylindrical shape were chosen as conductors for explosion. Each simulated wire consisted of 110,000 atoms, the height of a cylindrical crystallite was about 50±60 and the diameter was about 25±30 lattice parameters. Each specimen consisted of two grains. In view of the small size of the simulated wires, they had a shape of rectangular prisms. Periodic boundary conditions were used along the cylinder axis, and the free surface was simulated in other directions. Loading was applied in the following steps: the system was kept at the temperature of 1000 K, and then copper and nickel wires were rapidly heated up to 7000 K and 9000 K, respectively. The thermostat was applied to the simulated system after 100 ps after explosion. The distance between the wires in different calculations varied within the range from 40 to 260 Å.

The high-rate heating resulted in explosive disintegration of the wires accompanied by the formation of nanosized particles (atomic clusters) and gaseous phase. The cluster size was determined by assuming that atoms belong to one cluster, if the distance between them is shorter than the radius of the second coordination sphere in a perfect lattice close to the melting point. The cluster size was defined by the number of atoms in it. The cluster of minimum size was assumed to contain no less than 13 atoms because the first coordination sphere in the fcc lattice consists of 12 atoms.

The analysis of simulation results shows that after the wire has been heated, the process of dispersion occurs by stages. At the first stage of dispersion process, the average interatomic distance rapidly increases; however, the thermal expansion of the specimens causes no loss of continuity. At the next stage, fast fracture processes occur in the specimens, which involve formation of clusters of different sizes and intensive surface evaporation of atoms. The fracture leads to abrupt decrease in the temperature of the simulated system. This is due to the fact that a significant part of the kinetic energy of the specimens is expended to break atomic bonds.

The change of the number of clusters and the number of atoms in the gas phase in the simulated system as a function of time is shown in Fig. 1. The figure shows that the number of the synthesized clusters in 70 ps starts to saturate. The fraction of the gas phase in the simulated system grows continuously until the beginning of cooling (100 ps), and then decreases due to deposition of atoms on the surface of forming clusters.

![Figure 1](image_url)

Figure 1. The dependencies of the cluster number (a) and number of atoms in the gas phase (b) on time. The distance between the wires before detonation was 80 lattice parameters.
Figure 2. Structure projection on plane normal to cylinder axis of exploded system at different time points after explosion: a) 30 ps; b) 100 ps. The distance between the wires before the explosion was 80 lattice parameters.

Note that setting a high temperature heating allowed for “reasonable” computational time (in the framework of molecular dynamics method) to describe the dispersion of the simulated wires and the particle synthesis. The structure projection of simulated copper-nickel system at different points in time after the explosion is shown in Fig. 2. The figure shows that the bicomponent particles were formed in the process of dispersing (copper atoms are shown in red, nickel – in blue).

The results show that the distance between the dispersing wires has a significant influence on the number of generated clusters, their composition and structure, as well as the fraction of gas phase, which is formed in the process of explosion. The total number of formed clusters and number of bicomponent clusters as a function of the distance between the wires after relaxation process are shown in Fig. 3. The figure clearly shows that for the simulated system there is optimal distance interval, at which maximum number of bicomponent particles is synthesized. This interval corresponds to 40-160 lattice parameters between the wires before loading. It can be assumed that the optimum distance between the wires for the synthesis of bicomponent particles will depend largely on the wire thickness, their form and, to a lesser extent on the mode of heating and environmental properties, at which dispersion takes place.

Figure 3. The total number of (a) formed clusters and (b) bicomponent clusters versus the distance between the wires (a is lattice parameter).
The cluster distribution by their size and component composition depending on the distance between the wires at the end of the calculations was analyzed. It was found that a large number of clusters with a high concentration of the second component was formed for small distances between the dispersing wires. It is obvious that the evolution of the simulated system closer to equilibrium state and particle formation will continue with the slowing rates for a longer time intervals. In view of the limited computing resources, the evolution of the system towards equilibrium cannot be described within the framework of molecular dynamics method without using some approximations. A quite efficient approach is the use of viscoelastic boundary conditions that simulate the properties of the environment in which metal wires are dispersed, and the increase of the integration step at lowering temperature of the simulated system.

Typical particle distribution after the application of viscoelastic boundary conditions and cooling the dispersed system down to 2000 K is presented in Fig.4. The analysis of simulation results showed that the basic mechanism of particle formation is the agglomeration of smaller clusters, but not the deposition of atoms from the gas phase on the particle surface. It is seen in Fig. 4 that the chemical composition of the formed particles varies in a wide interval. Moreover, the chemical composition along the cross section of the bicomponent particles varies strongly. The concentration of copper atoms near the surface of bicomponent particles is much higher than in the bulk of the particles (Fig. 5).

It should be noted that temperature dynamics of the simulated system has a feature. The temperature abruptly decreases after high-rate heating. This behavior of the simulated system is connected with fracture processes of the wires and particle formation. The process of the wire fracture is accompanied by an increase in the free surface area of the simulated system and leads to the transition of a significant part of the kinetic energy into potential energy. The decrease in the intensity of the thermal pulse loading leads to the formation of particles of larger size. The calculations showed that the wire heating at high-rate electric pulse can lead to a significant increase in their volume without discontinuity (the jump of the atomic volume was about 9%). Such behavior of the crystalline wires might be related to a lower rate of accommodation processes in the internal structure as compared to the heating rate.

Figure 4. Structure of dispersed copper–nickel system in 150 ps. The distance between wires before the explosion was 80 lattice parameters.

Figure 5. The cross-section of the bicomponent cluster (the copper atoms are marked in red, the nickel atoms in blue). The cluster contains around 10 000 atoms, the concentration of copper in it being 30%.
3. Conclusion
The results of simulation show that there are two mechanisms of particle formation at metal wires explosion: agglomeration and deposition from the gas on the particle surface. The first one is agglomeration of small clusters and it prevails over the process of atom deposition from the gas on the free surface of the particles. The chemical composition of the formed particles is heterogeneous along their cross section. So, the concentration of copper atoms near the particle surface is higher than in the volume. It was found that the distance between dispersing wires greatly affects the process of particle formation. On the basis of the performed calculations one can conclude that the molecular dynamics metod can be used effectively to determine the optimal loading conditions of wire explosion to synthesize particles with desired composition and size.

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