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SIMULATION OF NANOPARTICLE FORMATION UNDER SYNCHRONOUS ELECTRIC PULSE EXPLOSION OF METAL WIRES

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Abstract. The paper is devoted to molecular dynamics simulation of the formation of bicomponent nanoparticles in simultaneous electric explosion of copper and nickel conductors. The influence of the distance between conductors on failure dynamics and nanoparticle formation is studied. It is shown that simultaneous electric explosion of metallic conductors makes possible the formation of bicomponent particles. Varying the distance between conductors allows one to control the structure of formed bicomponent particles. An increase in the viscosity of the environment in which conductors are exploded increases the size of formed particles.

1 INTRODUCTION

The method of simultaneous electric explosion of dissimilar metallic conductors is a promising technology for the synthesis of nanoparticles of given composition. This method enables the synthesis of composite nanoparticles consisting of crystallites of several metallic or non-metallic phases, due to which their physical and mechanical properties can change considerably and they can assume required performance characteristics [1–4]. Dispersion of conductors occurs as follows: when a high-density electric pulse (10^6–10^9 Å/cm^2) is sent through a metallic conductor, the conductor is rapidly heated, melted and then explodes. The explosion products disperse into gaseous atmosphere with the formation of nanoparticles. The

technology of electric explosion of metallic conductors has a range of important advantages over other nanopowder synthesis methods. Particularly, the energy transfer efficiency in electric explosion is very high because energy losses related to heating of the environment are very small. This method allows a flexible control of conductor dispersion parameters and hence synthesized nanopowder properties. The size of synthesized nanopowders falls within a small range; nanopowders are stable under normal conditions and have high activity in chemical reactions. Equipment for nanopowder synthesis has small dimensions. The explosive technology allows synthesizing a wide range of metal, oxide, nitride and other powders with complex internal structure. Notice that the internal structure of nanopowders influences their physical, chemical and mechanical properties [5–8]. It should be noted that the use of the method of particles in its various representations is promising for description of structural and phase transformations, generation of charged clusters, formation of gas phase and dispersion particles under the electric explosion of the conductors [9,10].

This paper studies the failure dynamics of dissimilar metallic conductors and formation features of bicomponent nanoparticles in simultaneous electric explosion. The influence of the distance between exploded conductors and environment viscosity on the structure of formed nanoparticles is studied. The solution of the formulated tasks is of both scientific and practical interest. For example, the investigation results can be useful in the development of a scientific basis for synthesizing nanoparticles of complex structural and phase composition with new physical and chemical properties.

2 CALCULATION RESULTS AND DISCUSSION

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

Copper and nickel crystallites of cylindrical shape were chosen as conductors for explosion. Each simulated conductor consisted of 50 000 atoms, the height of a cylindrical crystallite was about 30÷40 and the diameter was about 20÷25 lattice parameters. In view of the small size of the simulated crystallites, they were right rectangular prisms in external shape. 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 temperature 1000 K, and then the copper and nickel conductors were heated for 1 ps up to 7000 K and 9000 K, respectively. The distance between the conductors in different calculations varied within the range from 40 to 260 Å. The influence of the environment on the conductor dispersion was determined by the effective viscosity whose value varied from 1e-6 to 5e-4 eV*ps/Å^2.

The high-rate heating resulted in explosive failure of the conductors accompanied by the formation of nanosized particles (atomic clusters) and a gaseous phase. The cluster size was determined by assuming that atoms belong to one cluster if the distance between them is shorter than a threshold distance equal to 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.

Originally features of dispersion of copper conductors with a perfect structure and specimens containing grain boundaries under the electrical explosion were investigated. The analysis of simulation results suggests that after the simulated conductor has been heated, the process of dispersion occurs by stages. These stages are clearly defined on the time dependence of the simulated system temperature (Fig. 1).

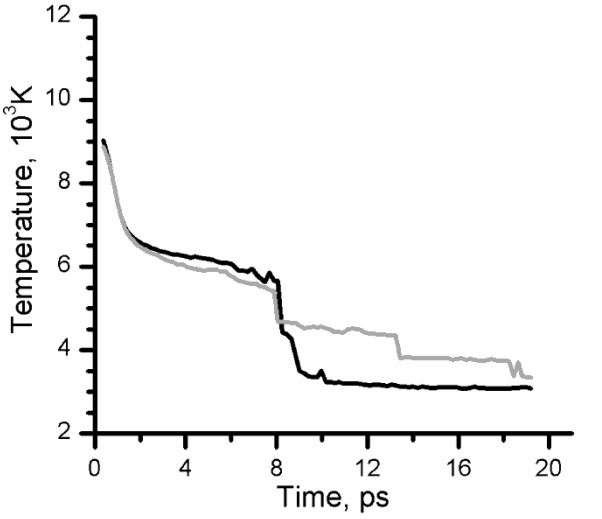


Figure 1: Variation in the temperature of the coper conducter by dispersion (black and gray curves correspond, respectively, to the original sample having ideal structure and to the sample having intergranular boundaries)

At the first stage of dispersion process the average interatomic distance rapidly increases; however, the thermal expansion of the crystallite causes no loss of continuity. At the next stage fast fracture processes occur in the crystallite, which involve formation of clusters of different sizes and intensive surface evaporation of atoms. The fracture causes a jump-wise decrease in the temperature of the simulated system, which is attributed to the bond rupture with the resultant significant expenditure of the kinetic energy of the system. Thus the disintegration of the largest cluster plots as a shoulder on the curve for times of 12 to 14 ps (see Fig. 1). The distribution of clusters with respect to size is demonstrated in Fig. 2 for two different instants of time, i.e. before and after the appearance of shoulder on the temperature curve.

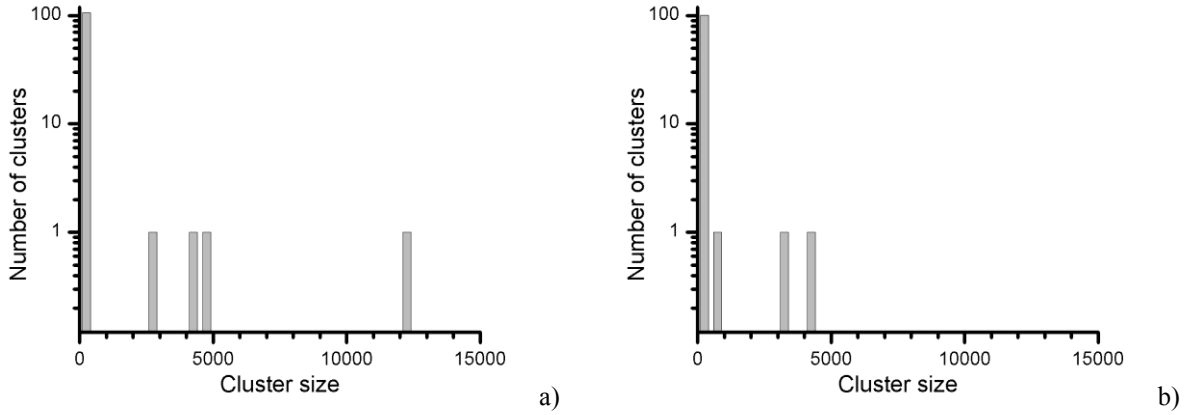


Figure 2: The number of clusters as a function of cluster size obtained for the simulated system for times of 13.6 ps (a) and 14.2 ps (b)

The variation in the number of clusters and in the fraction of gas phase with time is illustrated for the simulated system in Fig. 3. It can be seen that the curve representing the number of clusters formed flattens out with time. The curve representing the fraction of gas phase is an ascending one, which might be attributed to the high temperature of the simulated system, which exceeds the boiling temperature for time of 20 ps.

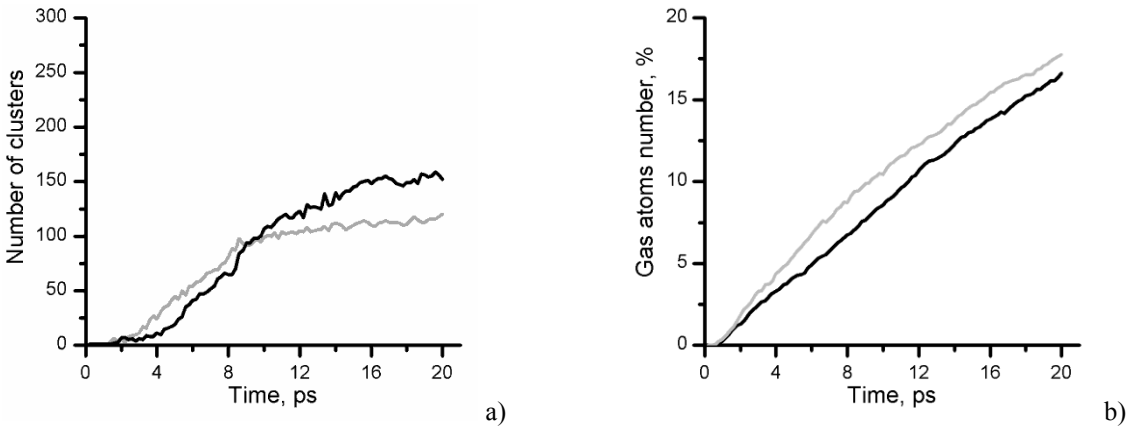
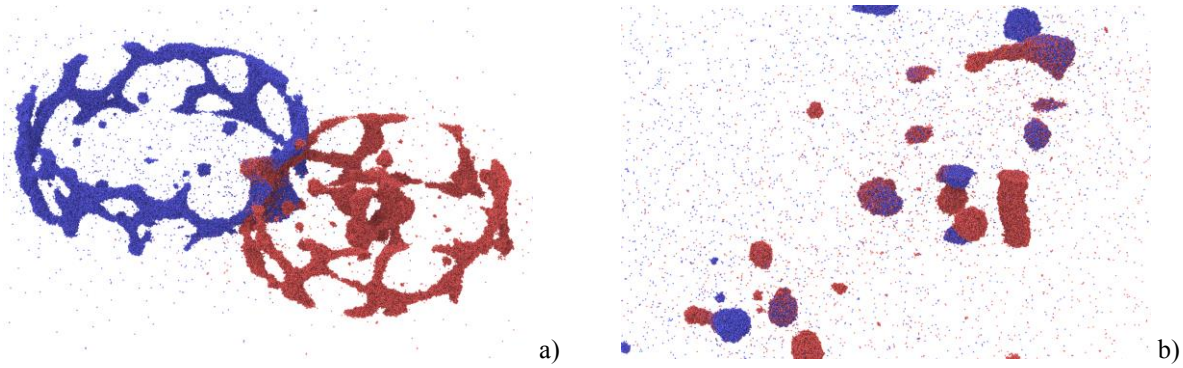


Figure 3: The number of clusters (a) and the fraction of gas phase as a function of time (b) (black and gray curves correspond, respectively, to the original sample having ideal structure and to the sample having intergranular boundaries)

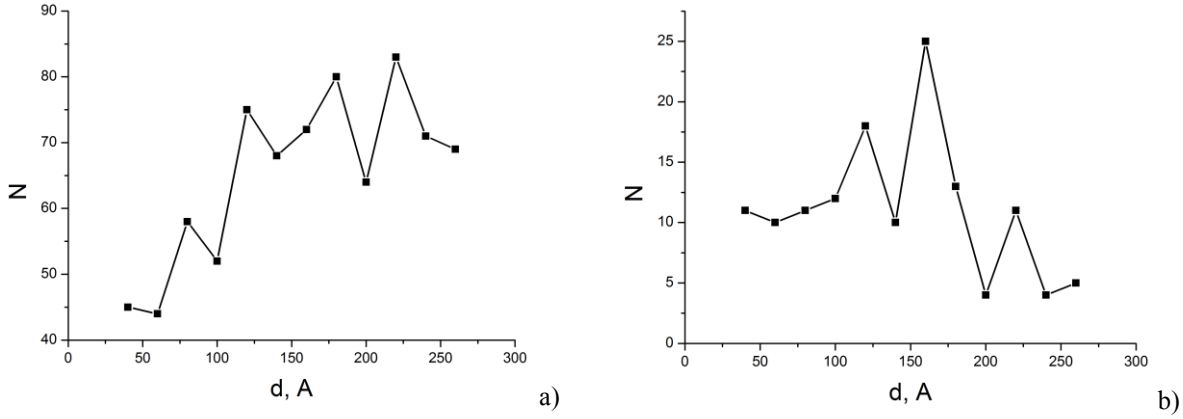
By giving high heating temperatures, we could describe failure of the simulated conductors and nanoparticle formation for a "reasonable" calculation time (within the molecular dynamics method). The structure of the simulated copper–nickel system at different time points after explosion is illustrated in Fig. 4. It is seen from the figure that bicomonent nanoparticles (red copper atoms, blue nickel atoms) are formed during dispersion.



a) b)

Figure 4: Structure of dispersed copper–nickel system at different time points after explosion: a) 30 ps; b) 100 ps

The calculation results showed that the distance between the exploded conductors has a strong influence on the number of formed clusters, their composition and structure, and on the fraction of the gaseous phase formed during dispersion. The total number of formed clusters and the number of bicomponent clusters depending on the distance between the conductors 100 ps after explosion are represented in Fig. 5. There is an optimal distance range for which the number of synthesized bicomponent particles is maximum. This range corresponds to 150–180 Å between the conductors prior to loading. It can be assumed that the optimal distance between conductors in bicomponent nanoparticle synthesis might to a great extent depend on the cross-section area of the conductors, their shape, and to a less extent on the heating mode and the environment in which the conductors are exploded.



a) b)

Figure 5: Dependence of the number of formed (a) and bicomponent (b) clusters on the distance between conductors

The distribution of the number of formed clusters with respect to their size, composition and distance between conductors is represented in more detail in histograms in Fig. 6. The distribution of clusters in the figure is given for the time point 100 ps after the beginning of loading. Analysis of the simulation results showed that the size of formed clusters slightly increases for a distance of about 160 Å between the conductors (Fig. 6a), among which are bicomponent particles (Fig. 6b).

Clearly, the evolution of the simulated system to equilibrium and the formation of nanoparticles would continue with the decreasing rates and on longer time intervals. As computational resources are limited, the process of the system evolution to equilibrium cannot be described within the molecular dynamics approach without some approximations. An effective approximation is to use viscoelastic boundary conditions that model the properties of the environment in which the metallic conductors are exploded, and to increase the integration step while the temperature of the simulated system decreases.

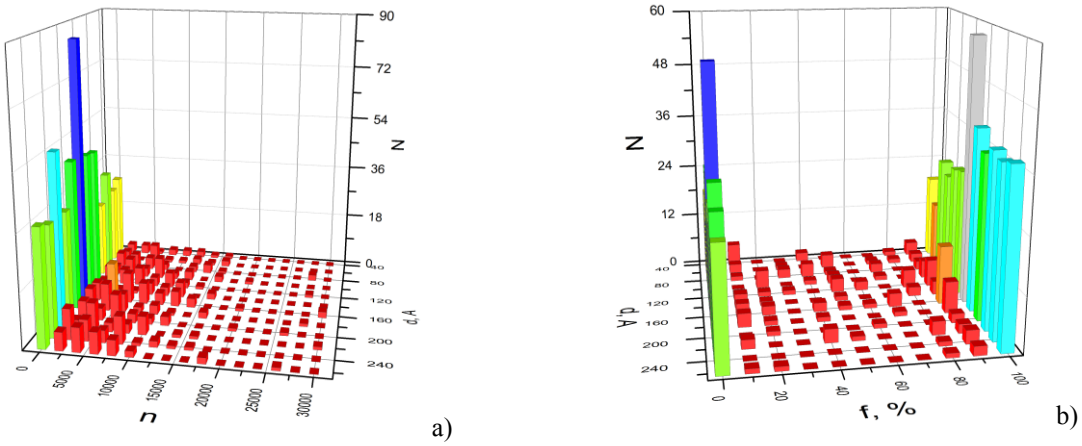


Figure 6: Distribution of formed clusters (N) with respect to their size (n) and distance between dispersed conductors (a). Distribution of clusters with respect to copper content in them (f) for different distances between conductors (b)

According to the performed calculations, the number of formed particles, including bicomponent ones, reduces with the growing viscosity of the environment in which the conductors are exploded (Fig. 7). The size of formed particles increases with the viscosity growth (Fig. 8). This feature of the evolution process is first of all related to the growing rate of heat rejection from the simulated system with the viscosity increase. As a result of introducing viscous boundary conditions, the processes of failure of the conductors and their fragments, evaporation and melting of formed particles subside considerably.

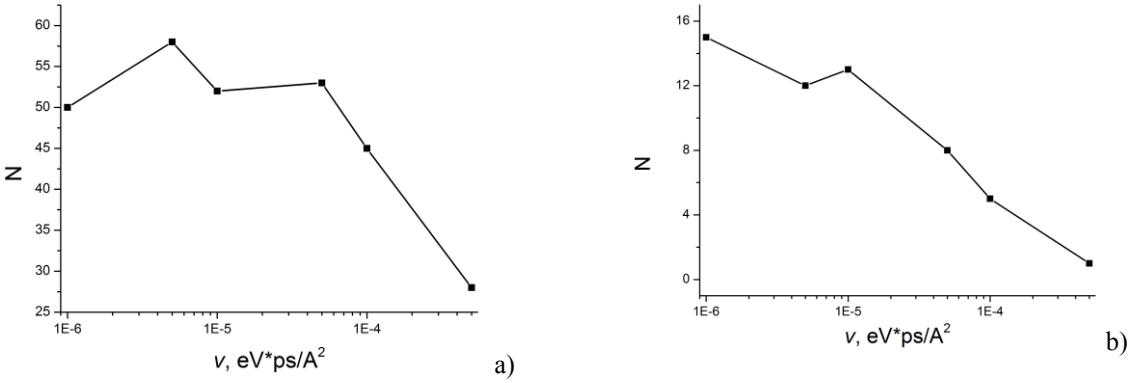


Figure 7: Dependence of the total number of particles (a) and bicomponent particles (b) on effective viscosity of the environment

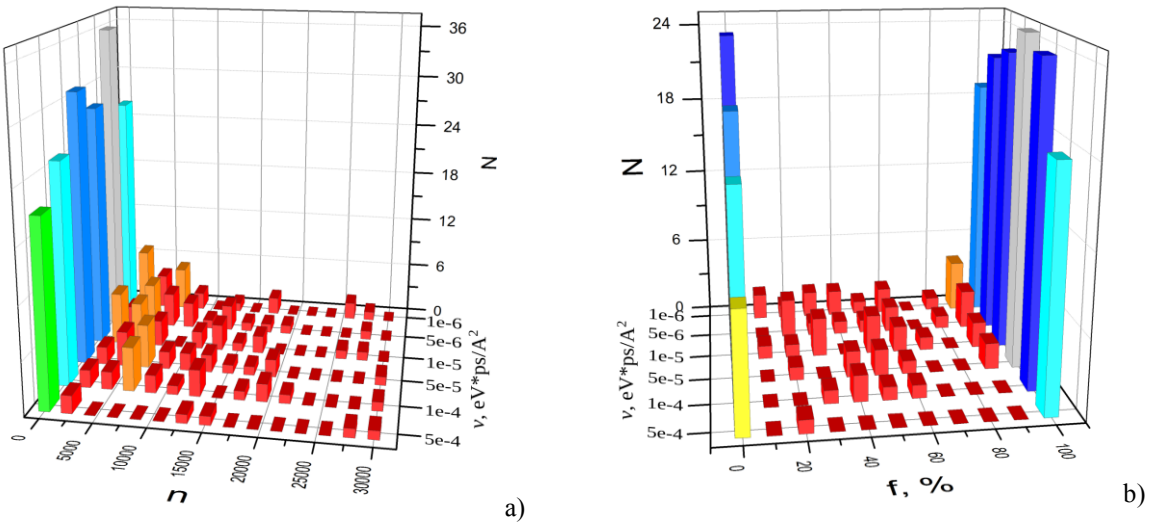


Figure 8: Distribution of particles (*N*) with respect to size (*n*) versus effective viscosity variation (a). Distribution of bicomponent particles with different copper content (*f*) versus effective viscosity variation (b)

The characteristic distribution of particles after the application of viscous boundary conditions and cooling of the dispersed system down to 1000 K is illustrated in Fig. 9.

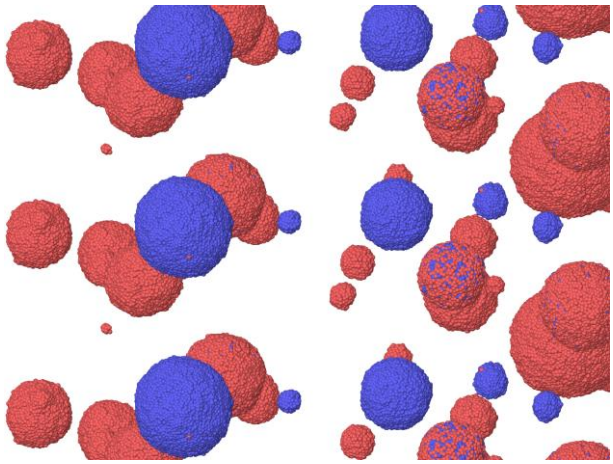


Figure 9: Formed clusters. Distance between conductors – 80 Å, effective viscosity – 1e-4 eV*ps/Å^2, copper atoms are red, nickel atoms are blue

Notice that the dynamics of kinetic temperature variation of the simulated conductors during dispersion has a feature. Its value decreases abruptly about 6 ps after the high-rate heating stops. This behavior of the simulated system is due to the failure of the conductors and formation of clusters. During failure of the conductors the area of free surfaces in the simulated system increases and a large part of kinetic energy converts to potential energy. In this case, a decrease in the intensity of thermal pulse loading leads to the formation of larger-sized clusters. Our calculations showed that the high-rate electric pulse loading of the crystalline conductors can significantly increase their volume without continuity violation (in

the calculations the atomic volume increased abruptly by about 9 %). Such behavior of the crystalline conductors might be related to a lower rate of accommodation processes in the internal structure as compared to the loading rate.

3 CONCLUSIONS

The paper demonstrates that the molecular dynamics method is promising for the development of a scientific basis of nanoparticle synthesis in electric explosion of conductors. This approach can be used not only to study the nanoparticle formation dynamics, but also to find optimal loading modes, distances between exploded conductors, and to select an environment with particular viscosity to synthesize particles of necessary size and composition.

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