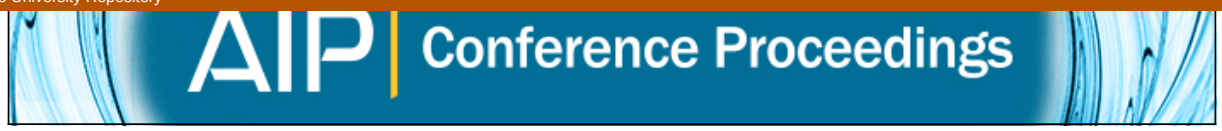

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Citation: AIP Conference Proceedings **1783**, 020237 (2016); doi: 10.1063/1.4966531
View online: http://dx.doi.org/10.1063/1.4966531
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1783?ver=pdfcov
Published by the AIP Publishing

Features of Particle Synthesis at Metal Wire Dispersion

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Abstract. Features of particle synthesis under simultaneous dispersion of copper and nickel wires were investigated using a molecular dynamics method. The dynamics of wire dispersion, the size and phase composition of synthesized particles depend on the internal structure of dispersed metal wires and the distance between them. The main mechanism of particle synthesis was agglomeration of sputtered clusters, which predominated over the atom deposition from the gas phase on the particle surface. Synthesized particles were characterized by a nonuniform distribution of chemical elements along their cross section. The subsurface region had a higher concentration of copper in comparison with the particle volume. The molecular dynamics simulation of the metal wire dispersion allows finding optimal loading parameters for the synthesis of particles with desirable size and internal structure.

INTRODUCTION

The dispersion of metal wires under electric pulse explosion has been widely used since 1946 for the synthesis of particles of the given composition, block structure and size. This perspective technology enables a synthesis of composite particles consisting of crystallites of several metallic or non-metallic phases, due to which they can possess required performance characteristics [1–5]. Dispersion (explosion) of wires occurs as follows: when a high-density electric pulse (10^6–10^9 A/cm^2) passes through a metallic wire, it is rapidly heated, melted, and then explodes. The explosion products disperse into the gaseous atmosphere with the formation of particles. The explosive technology allows synthesizing a wide range of metal, oxide, nitride, and other powders with complex internal structure.

It was shown that the internal structure of nanopowders influences their physical, chemical and mechanical properties [6–8]. It should be noted that the use of the method of particles in its various representations is promising for the description of structural and phase transformations, generation of charged clusters, formation of gas phase and dispersion particles under the electric explosion of wires [10–13].

The aim of this paper is to investigate the atomic level of the formation dynamics of particles under simultaneous electric explosion of copper and nickel wires. The influence of the loading scheme (in particular, distances between metal wires) on the size and composition of the synthesized particles is studied.

MATERIALS AND METHODS

The process of the metal wire dispersion and particle formation was investigated on the base of the molecular dynamics method [11–16]. Many-body potentials calculated in the framework of the embedded atom method were used to describe interatomic interaction [17]. 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.

Advanced Materials with Hierarchical Structure for New Technologies and Reliable Structures 2016
AIP Conf. Proc. 1783, 020237-1–020237-4; doi: 10.1063/1.4966531
Published by AIP Publishing. 978-0-7354-1445-7/$30.00

Copper and nickel specimens of a 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 were shaped to 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 1000 K and then copper and nickel wires were rapidly heated up to 7000 and 9000 K, respectively. The thermostat was applied to the simulated system in 100 ps after explosion. The distance between the wires in different calculations varied within the range from 4 to 26 nm.

The high-rate heating resulted in explosive failure of the wires 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 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 smallest cluster was assumed to contain no less than 13 atoms because the first coordination sphere in the fcc lattice consists of 12 atoms.

RESULTS AND DISCUSSION

The analysis of the simulation results shows that after the simulated wire has been heated, the process of dispersion occurs by stages. At the first stage of the 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 the formation of clusters of different sizes and intensive surface evaporation of atoms. The fracture leads to an abrupt decrease in the temperature of the simulated system. This is due to the fact that a significant part of 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. 1a. The figure shows that the number of the synthesized clusters in 70 ps starts to go to saturation. A fraction of the gas phase in the simulated system grows continuously until the beginning of cooling (100 ps), and then decreases due to the deposition of atoms on the surface of forming clusters.

Note that the set high temperature of heating allowed for a "reasonable" computational time (using the molecular dynamics method) to describe the dispersion of the simulated wires and the particle synthesis. The analysis of the structure of the simulated copper-nickel system at different points in time after the explosion shows that bicomponent particles were formed during dispersion.

The results show that the distance between dispersing wires has a significant influence on the number of generated clusters, their composition and structure as well as on the fraction of the gas phase, which is formed during explosion. The total number of formed clusters and the number of bicomponent clusters as a function of the distance between wires after the relaxation process are shown in Fig. 1b. The figure clearly shows that for the simulated system there is an optimum distance interval, at which the maximum number of bicomponent particles is synthesized. This interval corresponds to 80–160 lattice parameters between wires before loading.

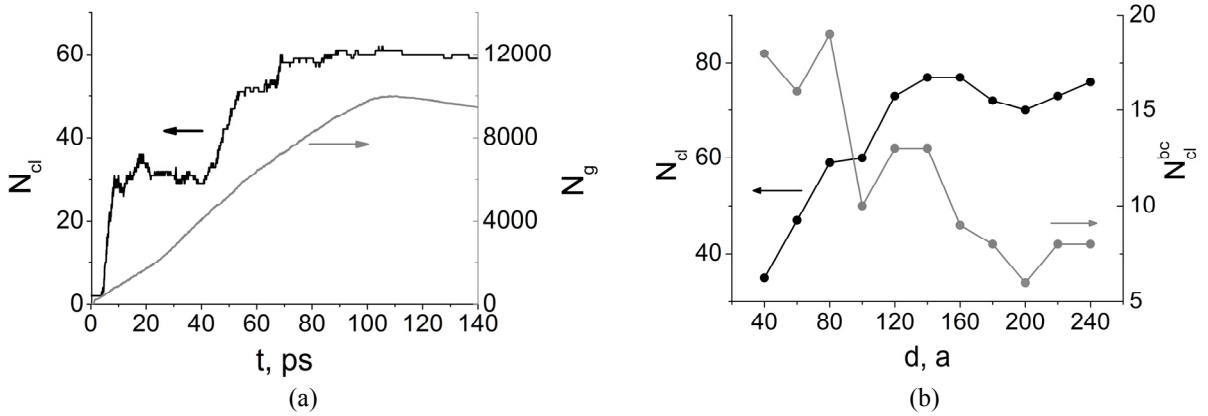
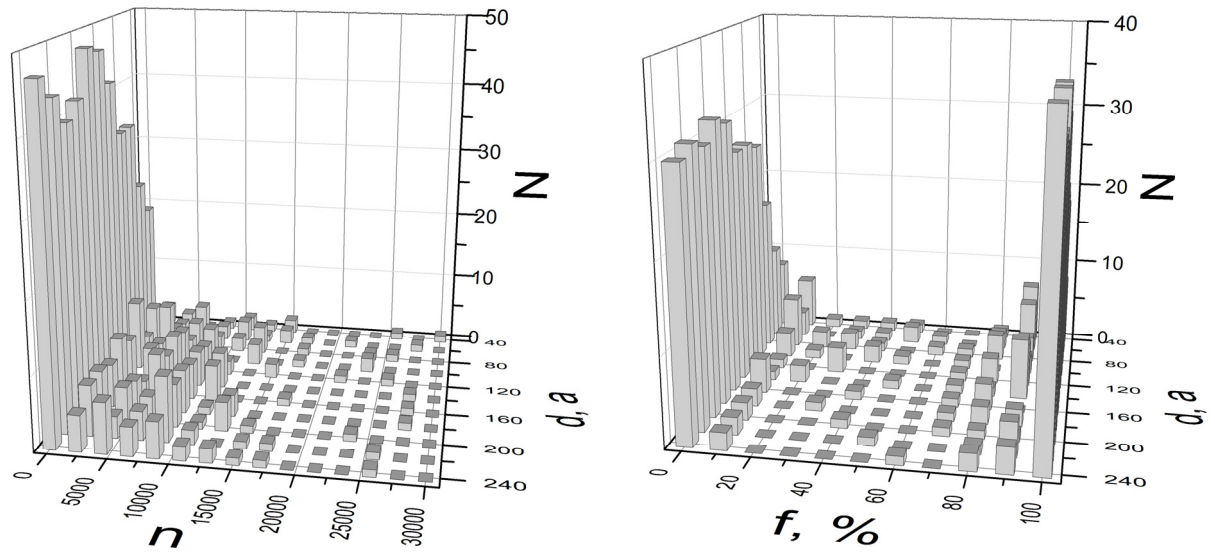


FIGURE 1. Dependencies of the cluster number N and the number of atoms N_g in the gas phase (a) on the time. The distance between wires before explosion was 80 lattice parameters. The total number of formed clusters N_{cl} and bicomponent clusters N_{cl}^{bc} versus the distance d between wires (a stands for the lattice parameter) (b)



(a) (b)

FIGURE 2. The number of formed clusters *N* versus: their size *n* and distance *d* between wires (a), the copper concentration in them *f* and distance between the (b)

It can be assumed that the optimum distance between 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.

A more detailed picture of the cluster distribution by their size and the component composition depending on the distance between wires at the end of the calculations is shown in Fig. 2. The figure shows that a large number of clusters with a high concentration of the second component are formed for small distances between dispersing wires. It is obvious that the evolution of the simulated system closer to the equilibrium state and the particle formation will continue with slowing rates for longer time intervals. In view of the limited computer resources, the evolution of the system towards equilibrium cannot be described within the molecular dynamic approach without using some approximations. A quite efficient approach is to use viscoelastic boundary conditions that simulate properties of the environment in which metal wires are dispersed and an increase in the integration step with lowering temperature of the simulated system.

The calculations showed that the basic mechanism of the particle formation is agglomeration of smaller clusters, but not the deposition of atoms from the gas phase on the particle surface. It should be mentioned that the chemical composition of the formed particles varies in a wide range. Moreover, the chemical composition along the cross section of bicomponent particles varies strongly. The concentration of copper atoms near the surface of bicomponent particles is much higher than in the bulk.

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

CONCLUSION

It was found that the particle formation under metal wire dispersion realizes on the base of two processes. The key role is played by an agglomeration process of small clusters formed by explosion of metal wires. An atom deposition from the gas on the free surface of particles gives a smaller contribution to their formation. The

distribution of chemical elements is heterogeneous along the cross section of formed particles. In particular, the concentration of copper atoms in the volume is smaller than that in the subsurface layer. It should be noted that the distance between exploding wires is one of the main parameters that sufficiently determines the internal structure, size, and chemical element distribution of synthesized particles. The molecular dynamics approach allows finding optimal loading conditions of the metal wire explosion for particle synthesis.

ACKNOWLEDGMENTS

The work was carried out at the support of RFBR Project No. 15-01-06585.

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