Formation of 2D Nanoparticles with Block Structure in Simultaneous Electric Explosion of Conductors

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Abstract. A molecular dynamics simulation of nanoparticle formation in simultaneous electric explosion of conductors is performed. Interatomic interaction is described using potentials calculated in the framework of the embedded atom method. High-rate heating results in failure of the conductors with the formation of nanoparticles. The influence of the heating rate, temperature distribution over the specimen cross-section and the distance between simultaneously exploded conductors on the structure of formed nanoparticles is studied. The calculation results show that the electric explosion of conductors allows the formation of nanoparticles with block structure.

Keywords: electric explosion, molecular dynamics, nanoparticles

INTRODUCTION

Today, one of the promising technologies for synthesizing nanoparticles of a given composition is the method of simultaneous electric explosion of conductors. This method allows the formation of composite nanoparticles consisting of crystallites of several metallic or nonmetallic phases, which gives them additional new properties [1–4].

The aim of this paper is to study the failure dynamics of conductors and the peculiarities of the formation of nanoparticles with block structure in electric explosion. The solution to the given problem is of scientific and practical interest, e.g., for the development of the scientific and technological basis for the synthesis of nanosized particles with a complex structural and phase composition that defines novel physico-chemical properties of nanomaterials.

The tasks of the paper are solved on the basis of the molecular dynamics method. Interatomic interaction is described using potentials calculated in the framework of the embedded atom method [5, 6]. The used potentials allow describing with a good accuracy the surface properties, energy of structural defects, elastic characteristics and some other properties important for electric explosion simulation.

CALCULATIONS AND DISCUSSION

The specimen for the investigation consists of copper crystallites of cylindrical shape. The simulated specimen contains about 40 000 atoms; the height of the cylindrical specimen is about 30 lattice parameters, the diameter is 20. In view of the small size of the simulated crystallites, their external shape is a regular rectangular prism. Periodic boundary conditions are used along the cylinder axis, and the free surface is simulated in other directions.

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(a) (b)

FIGURE 1. Plane projection of the simulated specimen structure in t = 14.4 ps after loading (a) and after relaxation to room temperature (b)

The spatial temperature distribution governed by electric loading is specified by a linear law: temperature rises in the direction from the cylinder axis to the lateral faces. The temperature difference in the center and on the lateral faces during heating is 25%. The crystallite is heated up by linear scaling of atomic velocities with the preserved Maxwell distribution.

High-rate heating results in specimen failure accompanied by the formation of clusters. Atoms are assumed to belong to one cluster, provided that the distance between nearest neighbor atoms is smaller than a threshold distance. The threshold distance in the present paper is equal to the radius of the second coordination sphere in a perfect copper lattice. The cluster size is determined by the number of atoms in it.

Failure in electric explosion is simulated by heating the copper crystallite up to high temperatures (from 7000 K and higher). This heating regime is chosen so that to describe the main stages of the simulated crystallite failure for a "reasonable" computational time (within the molecular dynamics method). The calculation results show that two characteristic stages of the interatomic distance variation in the specimen with time can be distinguished. At the first stage of about 1 ps duration, the average interatomic distance increases rapidly to maximum without continuity violation in the specimen. At the second stage beginning after the maximum expansion of the crystallite without continuity violation, further specimen accommodation to high-rate heating occurs due to its failure with the formation of different-sized clusters and the gas phase. The conductor failure and cluster formation are accompanied by a rapid reduction of the interatomic distance in clusters as the kinetic temperature of atoms in the clusters starts decreasing rapidly. Notice that the time point from which the specimen's kinetic temperature starts decreasing correlates well with the time point when fragmentation begins.

The projection of the dispersed specimen structure at the time point 14.4 ps onto the plane perpendicular to the direction of periodic boundary conditions is illustrated in Fig. 1(a). It is seen from the figure that the initial specimen is broken into a multitude of fine clusters with gas phase formation. In the calculations, the influence of the environment on the specimen dispersion is not taken into account. Therefore, failure and grouping of the specimen explosion fragments at the stage of evolution will be determined by the following processes: (i) further failure of clusters, if their internal kinetic energy exceeds the energy of the formation of an additional free surface; (ii) evaporation of atoms from their surface; and (iii) collision with other clusters and gas phase atoms.

Analysis of the calculation results shows that dispersion is not finished for the simulated time but continues. The general trend of the system evolution is such that the gas phase fraction gradually increases, the size of large clusters reduces significantly due to evaporation of surface atoms and due to their failure upon collision with other clusters. Such behavior is governed by high temperatures of the formed clusters and by the absence of the environment resistance.

A decrease in the intensity of the thermal pulsed electric field leads to the formation of larger clusters. Figure 1(b) demonstrates the projection of the dispersed specimen structure after relaxation and cooling down to room temperature. The initial specimen was heated up by the above-described scheme with the maximum temperature T = 10 000 K in the center, then its failure for 24 ps was simulated, and then its temperature was reduced in steps down to melting and then room temperature using the artificial damping method. As is seen from Fig. 1(b), owing to this sequence of relaxation, larger clusters were formed in the simulated system (as compared to Fig. 1(a)), many of which have a complex shape with numerous thin bridges.

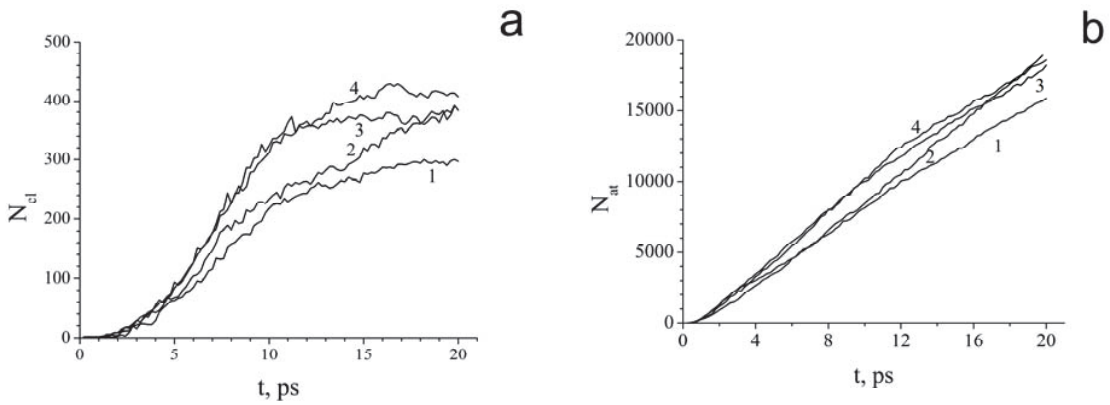

FIGURE 2. Time-dependence of the number of clusters (N_{cl}) (a) and the number of gas phase atoms (N_{at}) (b) in the dispersed system. Heating temperature 10000 K. The curves correspond to the following distances between conductors: 5 (*1*), 150 (*2*), 400 Å (*3*). Curve *4* corresponds to the doubled number of clusters in dispersion of an isolated conductor

The formation of the complex-shape clusters at a more realistic cooling procedure should lead to the formation of nano-sized particles with internal block structure [7–9].

A promising approach to the formation of nanoparticles with different phase composition and block structure is the simultaneous electric explosion of conductors. The calculation results show that the distance between exploded conductors has a significant effect on the number of formed clusters and on their structure (Fig. 2(a)). It is seen from the figure that for the distance between simultaneously exploded conductors 5 Å the number of formed clusters in 20 ps after the beginning of failure is by approximately 30% lower than in the case of explosion of two isolated, remote conductors (curves *1* and *4*).

The fraction of the gas phase formed during failure also strongly depends on the distance between simultaneously exploded conductors (Fig. 2(b)). The dynamics of the kinetic temperature variation in the simulated conductors during dispersion has a specific feature manifested as an abrupt drop in the curves of Fig. 3 in about 6 ps after loading. Such behavior of the studied systems is related to failure of the heated conductor and cluster formation, which causes an increase in the free surface area in the simulated system and transfer of a large amount of kinetic energy to potential one.

The performed calculations suggest that under high-energy loading the chosen methods of spatial temperature distribution over the simulated crystallite cross-section do not qualitatively change the electric explosion development. The high-rate thermal pulsed loading of the crystalline specimen can lead to a significant increase in its volume without continuity violation (in the performed calculations the atomic volume increased by 9%).

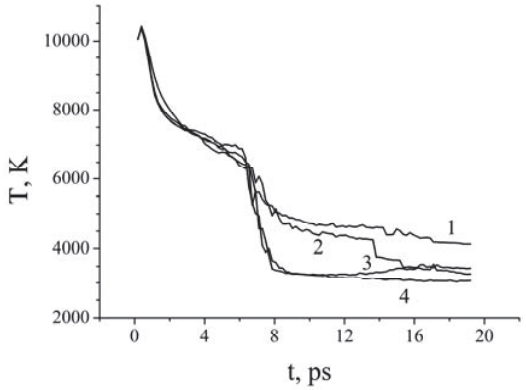

FIGURE 3. Dynamics of the kinetic temperature variation in the dispersed systems. Heating temperature 10000 K. The curves correspond to the following distances between conductors: 5 (*1*), 150 (*2*), 400 Å (*3*). Curve *4* corresponds to the kinetic temperature in dispersion of an isolated conductor

Such behavior of the crystalline specimen is possibly due to a lower rate of internal structure accommodation as compared to the loading rate. In the absence of the environment resistance the crystalline specimen failure in electric explosion is accompanied by the formation of clusters and the gas phase. The initially formed clusters are broken into finer clusters, and atoms are evaporated from their surface until their kinetic temperature decreases below the boiling temperature.

By varying the distance between conductors in simultaneous explosion, the process of nanoparticle formation can be effectively governed to change the size and internal structure of nanoparticles. For a more realistic simulation of processes in electric explosion of conductors, the effects of viscous resistance of the environment must be taken into account. The performed calculations show that the molecular dynamics method can be effectively used to choose the best technological mode of producing nanoparticles with block structure by electric explosion.

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