Simulation of nanoparticle formation under synchronous electric pulse explosion of metal wires

K.P. Zolnikov*[1,2], D.S. Kryzhevich[1,2], A.V. Korchuganov[1], S.G. Psakhie[1,3,4]

[1] Institute of Strength Physics and Materials Science (ISPMS)
2/4, pr. Akademicheskii, Tomsk, 634021, Russia
e-mail: sp@ms.tsc.ru, web page: http://www.ispms.ru/en/

[2] Tomsk State University (TSU)
36, Lenina Avenue, Tomsk, 634050, Russia
e-mail: rector@tsu.ru, web page: http://tsu.ru/english/

[3] Tomsk Polytechnic University (TPU)
30, Lenin Avenue, Tomsk, 634050, Russia
e-mail: tpu@tpu.ru, web page: http://tpu.ru/en/

[4] Skolkovo Institute of Science and Technology,
100, Novaya St., Skolkovo, 143025, Russia
web page: http://www.skoltech.ru/en/

ABSTRACT

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. The purpose of this work is connected with investigation of fracture dynamics of different metal wires in the course of the synchronous electric pulse 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 nano-sized particles with a complex structural and phase composition that defines novel physical-chemical properties of nanomaterials. The investigation was carried out using the molecular dynamics approach. Atomic interactions were described using the potentials calculated within the framework of the embedded atom method. These potentials allowed describing the surface properties, defect structure energy, elastic characteristics and a number of other propetries to a high accuracy, which were critical for the simulation of the explosion process. Simulation of fracture in the course of synchronous electric pulse explosion was performed by heating of metal crystallites to high temperature within a short time step. The metal wires under study had cylindrical shape and contained about 100 000 atoms, with the height of the cylinders being around 30 and the diameter – 20 lattice parameters. Periodic boundary conditions were used along the cylinder axis, and the free surface was simulated in other directions.

Failure in electric explosion was simulated by heating the metal wires up to high temperatures (from 7 000 K and higher). This heating regime was 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 showed 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 increased 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 occurred due to its failure with the formation of different-sized clusters and the gas phase.

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 more realistic simulation of processes in electric explosion of wires, the effects of viscous resistance of the environment must be taken into account.

The work was supported by RFBR, grant No.15-01-06585.