

MODELING OF THE PASSAGE OF A SHOCK WAVE THROUGH THE BORDER OF THE SECTION OF DICOTYLEDONIC BIMETALLIC PARTICLES Cu-Au, Cu-Ni, Pt-Al

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SUMMARY. The method of computer modeling based on the molecular dynamics method is used to study structural changes in particles of Cu-Au, Cu-Ni, Pt-Al bimetals during the passage of a shock wave. The possibility of the formation of pore nuclei near the interface of metals is described. It is shown that the formation of pore germs near the interface of Cu-Au, Pt-Al is influenced by the size of bimetallic particles. No pores were formed in the Cu-Ni bimetal. The wave was initiated on the side of Au, Ni and Pt. The shock wave propagated along the not close-packed direction, the main part of the energy was scattered near the interface of the metals and led to the formation of pore germs. The dependence of the maximum pore size on the linear sizes of particles of dicotyledonic bimetals Cu-Au, Pt-Al is calculated. The evolution of pores with time is considered. The pores were formed from the side of Cu or Al, and not from the side of Au or Pt. This arrangement of pores is due to the lower binding energy between Al-Al or Cu-Cu atoms than between Pt-Pt, Pt-Al and Au-Au, Cu-Au.

KEYWORDS: bimetal, shock wave, pore, FCC crystal, misfit dislocation.

INTRODUCTION

Bimetals are a type of composite material consisting of two or more dissimilar metals linked together. They are used to save valuable metals, as well as to obtain materials with new properties. At the same time, a layer of cheaper metal, which perceives a power load, is called the main layer, and the more expensive layer, which provides special properties, is called the cladding layer. The use of bimetals can significantly increase the production of parts and equipment for the chemical, petroleum, agricultural, transport, energy and other engineering industries. With the transition to nano-sized materials, theoretical and experimental interest in bimetallic nanoparticles sharply increased. The unique physical and chemical properties of bimetallic particles are associated with their structural, electronic, and optical properties [1 – 3].

The structure of bimetallic nanoparticles is determined by the distribution of metals in it. Particles can be organized in the form of an ordered alloy, such as dicotyledonic bimetals (DBM), have an arbitrary composition, or have a core-shell architecture. The latter type is realized only at the nanoscale level and represents particles of one metal, coated with another.

Such materials attract considerable research interest in connection with their potential use in the field of heterogeneous catalysis, since they are often more active compared to their monometallic counterparts. Improving the properties of these systems is associated with the complex interaction of electrons of two metals and the effects of changing lattice parameters in bimetallic alloys or at the interfaces between two metals [4, 5]. Of particular interest in this regard is the compound Cu-Au, Cu-Ni, and Pt-Al.

Bimetallic nanoclusters are of practical importance for the formation of current and potential contacts in electronics elements due to the fact that the electron work function strongly depends on the actual structure of bimetals. In addition, thin coatings Cu-Au, Cu-Ni, Pt-Al are actively used when applied to the surface of parts that increase wear resistance, heat resistance and anti-corrosion [6 – 10].

Bimetallic compounds, in view of their use in various technological processes, can be subjected to various intense external influences, which can lead to energy and structural

transformations, which in turn affect the properties of such particles. The ability to control the properties and structure of nanoscale particles is an important task of modern materials science. One of the mechanisms for controlling the structure of bimetallic particles can be the effect of the flow of high-energy particles on a solid body, accompanied by the formation of shock post-stage waves formed as a result of a sharp expansion of a strongly heated cascade region.

A number of studies have shown that shock waves can affect the processes of self-diffusion in FCC crystals [11], cause the enlargement of vacancy pores [12, 13], and also participate in a number of other processes [14 – 16].

The initiation of shock waves can be carried out by means of high-power laser radiation, at intensity values within 10^{12} – 10^{13} W/cm², or by bombarding the metal surface with heavy ions [10, 16, 17].

The relevance of this study is also due to the need to create radiation-resistant structural materials that can work in extreme conditions without significant changes in their properties. Dimensional instability, manifested in the form of radiation creep phenomena or radiation swelling, is due to the development of a new defective structure as a result of creeping dislocations, as well as the growth of pores [18].

In accordance with the foregoing, this work is devoted to the study of the passage of shock waves through the interface between dicotyledonic bimetals Cu-Au, Cu-Ni, and Pt-Al.

MODELING TECHNIQUE

The processes studied in this work are distinguished by a high flow rate, which makes direct observations more difficult. In field experiments on the study of shock waves in metals, the initial and final states are often considered without studying the kinetics of the process. For a more detailed understanding of the essence of such processes, it is necessary to consider them in dynamics. Therefore, the use of computer simulation methods seems to be optimal. The method of molecular dynamics was chosen as a method of computer simulation, due to the fact that it allows one to conduct experiments with given atomic velocities and to describe the dynamics of the studied processes in real time. This method has proven itself well in the study of processes at the interface of the phases of metals and alloys [19 – 22]. The simulation was performed using a well-proven molecular dynamics package - LAMMPS [23]. This package was developed to apply to calculations on parallel computers. As an interatomic potential, we used the potential obtained by the embedded atom (EAM) method and included in the standard LAMMPS set proposed by the authors of [24]. The total energy of a crystal E can be expressed as:

$$E = \frac{1}{2} \sum_{i,j,i \neq j} \varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i), \quad (1)$$

where φ_{ij} represents the pair energy between atoms i and j separated from each other by the distance r_{ij} , and F_i is the energy of the embedded atom i in a local location with electron density ρ_i . The electron density can be calculated by the formula: $\rho_i = \sum_{j,j \neq i} f_j(r_{ij})$, where $f_j(r_{ij})$ is the electron density in the region of atom i located at a distance r_{ij} from atom j . The temperature of the computational cell was set by assigning random speeds to atoms in accordance with the Maxwell-Boltzmann distribution for the specified temperature. The step of numerical integration of the equations of motion was 1 fs.

In the present work, the study was carried out on a computational cell simulating Cu-Au, Cu-Ni, Pt-Al dicotyledonic bimetals having the shape of a rectangular parallelepiped, the number of atoms and cell size were varied to determine the influence of the size factor on the bimetal's behavior during the passage of a shock wave. To obtain dicotyledonic bimetals, two initial single-component crystals of different metals in the form of rectangular parallelepipeds were placed at a distance of about 2.5 Å from each other. After that, the structure was relaxed (Fig. 1). Free boundary conditions were set along all axes. In the process of relaxation, the calculation block was heated up to several tens of Kelvin. In view of the presence of free boundary conditions, some of the atoms near the surface moved to the adjacent metal. Table 1 shows the number of atoms in each model block of bimetals.

The number of atoms in the calculated cells of bimetals

Cu-Au		Cu-Ni		Pt-Al	
Cu	Au	Cu	Ni	Pt	Al
159000	254900	141000	222800	254900	159000

The following orientation of bimetallic particles in space was considered: the X axis is directed along the crystallographic direction, the Y axis along, and Z along $\langle 111 \rangle$.

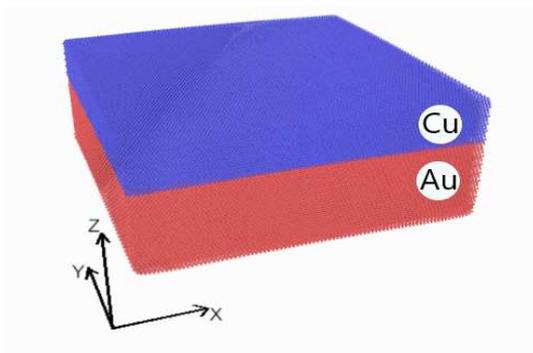


Fig. 1. An example of a volumetric view of a dicotyledonic bimetallic block (X axis is directed along the crystallographic direction, Y axis - along, Z - along $\langle 111 \rangle$)

At the interface of metals, a network of misfit dislocations was formed, due to the difference in the lattice parameters, the component of the DBM particle and the orientation in space of its components. In fig. 2 shows the grid of dislocation mismatches at the interface of dicotyledonic bimetallic particles Cu-Ni, Pt-Al, Cu-Au. In the process of structure relaxation, the DBM part of the dislocations shifted into the depths of Al and Cu, which is caused by a lower binding energy between Al-Al or Cu-Cu atoms than between Pt-Pt, Pt-Al and Au-Au, Cu-Au.

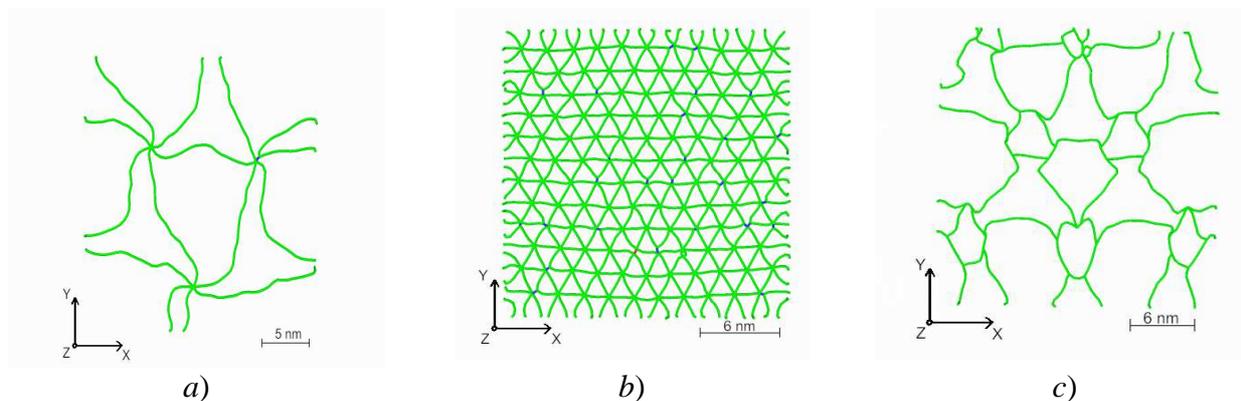


Fig. 2. Grid of misfit dislocations at the interface of dicotyledonic bimetallic particles: a) Cu-Ni; b) Pt-Al; c) Cu-Au

The special features of the shock wave are the large amplitude of atomic displacements, as well as the small width of the front, commensurate with the lattice parameter of the crystal. In addition, shock waves propagate in matter with velocities exceeding the speed of sound. Therefore, to create a wave, a group of atoms in the border area of the computational cell (one extreme atomic layer) was assigned a velocity c , exceeding the speed of sound waves from the material along the crystallographic direction of the corresponding Z axis. The speed of the atoms was assigned so that the wave propagation velocity estimated by the front waves of ten interatomic distances, was in the range from c to $1.5c$. As a result, a shock wave was formed, passing through the boundary of bimetals Cu-Au, Cu-Ni, Pt-Al.

THE DISCUSSION OF THE RESULTS

As shown on 2D and 3D models of Ni-Al, Ni-Fe bimetals [16, 25], the passage of shock waves is accompanied by their diffraction on misfit dislocation cores near the metal interface. The grid of misfit dislocations for a three-dimensional case has a complex structure, so the distribution of interference maximum (minimum) also has a more complex form.

The wave was initiated on the side of Au, Ni and Pt. The shock wave propagated along the not close-packed direction - $\langle 111 \rangle$. In the case of a Cu-Ni bimetal, its speed varied from 60.46 \AA / ps to 87.79 \AA / ps , in the case of Cu-Au from 45.84 \AA / ps to 53.25 \AA / ps and in the case of Pt-Al from 48.75 \AA / ps to 57.23 \AA / ps in accordance with the tabular values of the speed of sound in Pt, Ni, Al and Cu crystals [26].

At sufficient energy of the wave, pore germs were formed in Al and Cu in the case of consideration of bimetallic compounds Pt-Al, Cu-Au. For example, the evolution of pore germs in Fig. 3 shown for Cu-Au. With time, coagulation of pores occurs in one large pore in the center of the computational cell (Fig. 3, c). In the future, this pore is collapsing. When considering the bimetallic compound Cu-Ni, the formation of pore germs did not occur. This is due to the lower density of inconsistency dislocations (Fig. 2, a), which is due to the minor difference in the lattice parameter of the components of the bimetallic particle, as well as the orientation of the crystals chosen by us.

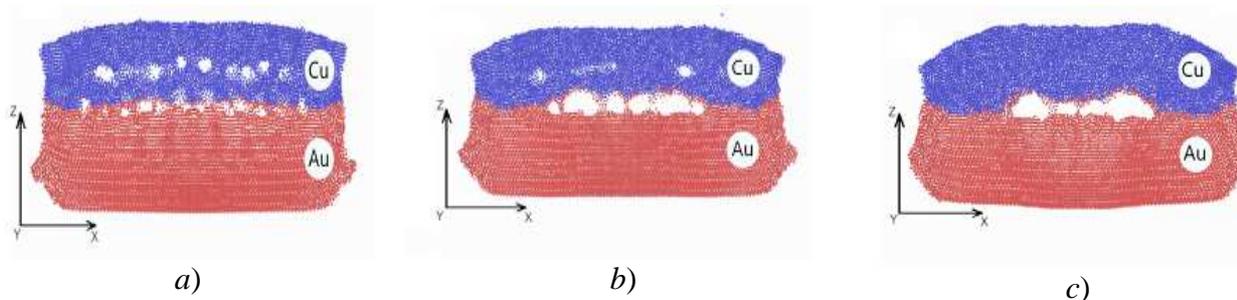


Fig. 3. Evolution of the structure of nanopores near the boundary of the Cu-Au bimetal: a) after 3.7 ps from the beginning of the experiment; b) after 6.2 ps from the beginning of the experiment; c) after 9.6 ps from the beginning of the experiment. 5 nm thick layer was visualized

For the entire range of velocities, the formation of pore germs took place near the boundary of the metals. Experiments have shown that the initial velocity of the shock wave influenced the size of the pore germs, which were formed on the side of Cu and Al (Fig. 4). The graph shows the value of the maximum linear pore size along the Z axis of the DBM Cu-Au and Pt-Al components. The sizes of the pore germs were rather large, since there was a more dense arrangement of misfit dislocations at the interface of metals. Also, the dispersion of the energy of the shock wave after the passage of the boundary was promoted by a non-close-packed direction in the crystal.

At the same time, the distribution of pores and the rate of their collapse in the bimetal depended on the linear dimensions of the particle model were considered. Note that for particles smaller than 8 nm, pores did not form in any of the bimetals. This is due to the influence of the bimetal free surface and a smaller number of dislocations at the interface. For bimetals ranging in size from 8 to 15 nm, two or three pores are located in the regions of the first and second interference minimum of the shock wave at misfit dislocations. For large cell sizes, the number of pore germs was increased. The size of the DBM particles influenced the pore collapse time. In fig. 5 shows dependence for the Cu-Au and Pt-Al bimetal on the linear dimensions of the cell along the X and Y axes.

The influence of the free surface decreases with increasing linear dimensions of the cell. The possibility of the formation of pore germs is largely determined by the size of dicotyledonic bimetallic particles.

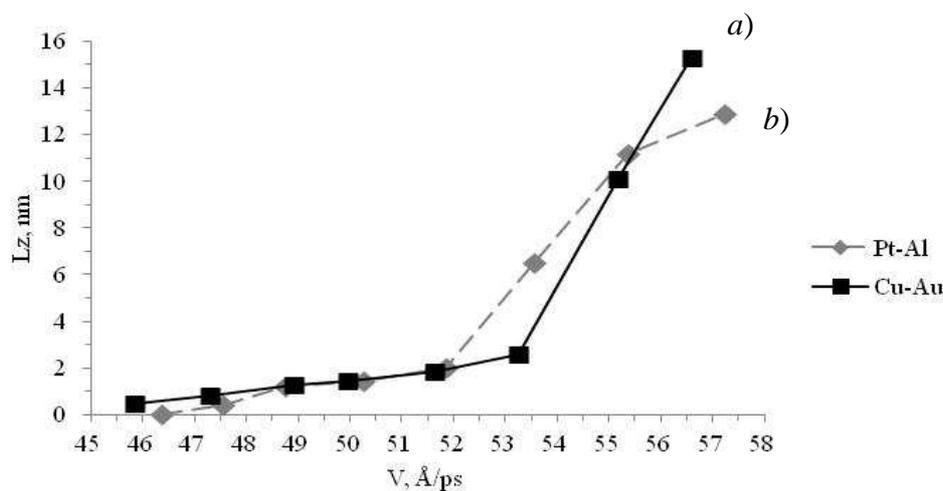


Fig. 4. The dependence of the maximum linear pore size along the Z axis on the shock wave velocity for a bimetal: a) Cu-Au bimetal, the bimetal linear dimensions along the X and Y axes were 24.8 nm, along the Z axis 9.7 nm; b) Pt-Al bimetal, the bimetal linear dimensions along the X and Y axes were 24.8 nm, along the Z axis 10.1 nm

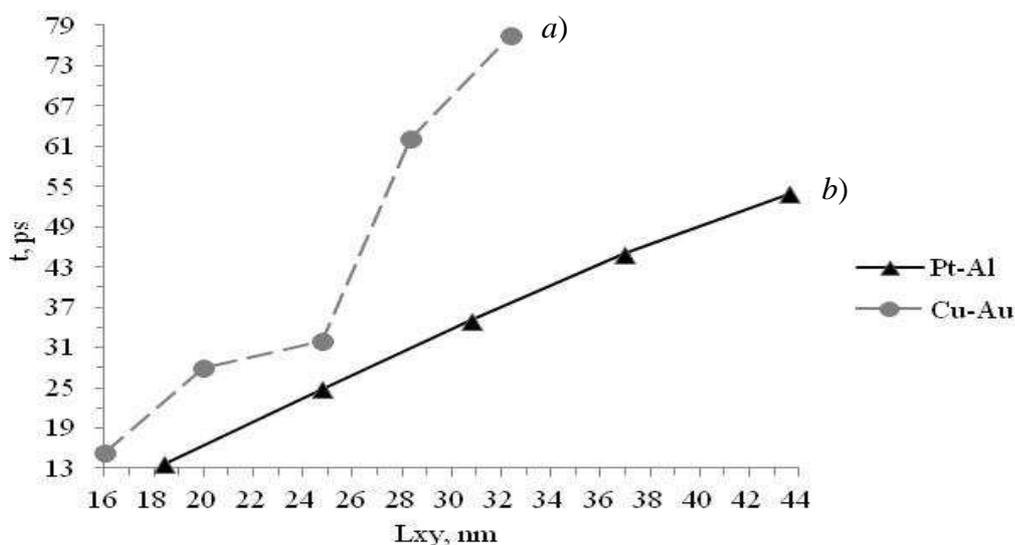


Fig. 5. Dependence of the time of pore collapse on the linear dimensions of a bimetallic cluster along the axes X и Y: a) Cu-Au; b) Pt-Al

CONCLUSIONS

Computer simulation carried out by the molecular dynamics method showed a significant effect of the shock wave on the structure of the DBM Cu-Au, Cu-Ni, Pt-Al interface and the crystal surface. It has been established that one of the determining factors for the formation of pore germs near the interface of Cu-Au and Pt-Al is their size. In the case of DBM Cu-Ni, the pore germs are not formed. The wave was initiated on the side of Au, Ni and Pt. The shock wave propagated along the not close-packed direction, the main part of the energy was scattered near the interface of the metals and led to the formation of pore germs. The pores were formed from the side of Cu or Al, and not from the side of Au or Pt. This arrangement of pores is due to the lower binding energy between Al-Al or Cu-Cu atoms than between Pt-Pt, Pt-Al and Au-Au, Cu-Au.

The results obtained can be useful in the ultrasonic processing of materials, nano-engineering, as well as in radiation materials science.

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