

THE MOLECULAR-DYNAMIC RESEARCH OF HETEROSTRUCTURE INTERFACE INFLUENCE TO THE MECHANICAL PROPERTIES

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ABSTRACT

In the work it is presented the results of molecular-dynamic research of the uniaxial tension of nano-length scale copper-silver heterostructure, and also the pure copper nanocrystal on the atomic level. It was realized the results comparison, it was revealed the influence of the interface on the results, it was found the critical deformation value. If the deformation become greater then critical one the heterostructure plastic modification takes place. During external effect it is revealed the formation such structural modifications as Luders-Chernov stripes.

INTRODUCTION

The experimental and theoretical works of the member of the Academy V.E. Panin [1-3] point to the special role of free surfaces and interfaces in the deformation and destruction processes of materials. It is stipulated the necessity of realization the molecular-dynamics researches on the materials interfaces. The numerical calculation of the heterostructure CuAg uniaxial tension to cryogenic temperatures have been made in the first stage of works devoted to the investigation of interface influence. The materials are chosen from the consideration of at most large differences of crystal cells values and in the same time the materials having the same crystal structure.

NOMENCLATURE

n_x	[-]	number of crystal cells along the X axe
n_y	[-]	number of crystal cells along the Y axe
n_z	[-]	number of crystal cells along the Z axe
a_{Cu}	[Å]	copper lattice constant
(x_i^0, y_i^0, z_i^0)	[Å]	coordinates of i-s atom after cooling
(x_i, y_i, z_i)	[Å]	coordinates of i-s atom
$V(\vec{r}_i)$	[erg]	harmonic external potential
k	[erg/grad]	Boleman constant

t	[sec]	calculation time
τ	[sec]	calculation time step, $\tau = 10^{-16}$ sec
v_0	[cm/sec]	speed of heterostructure moving edge
ε	[-]	percent elongation
ε_c	[-]	critical value of percent elongation
dU	[10^{-14} erg]	potential energy change
F	[10^{-11} N]	force acting to the crystal

PHYSICAL SYSTEM AND PREPARATION THE INITIAL DATA

The initial data: it is take the ideal copper crystal in the shape of rectangular parallelepiped with the number of crystal cells $n_x = 14, n_y = n_z = 4$ along the axes, and the similar silver crystal with sizes $n_x = 13, n_y = n_z = 4$. The silver crystal is set above copper crystal on the distance $a_{Cu}/2$ from the copper crystal plane along axe Z. The initial structure is shown on the Figure 1.

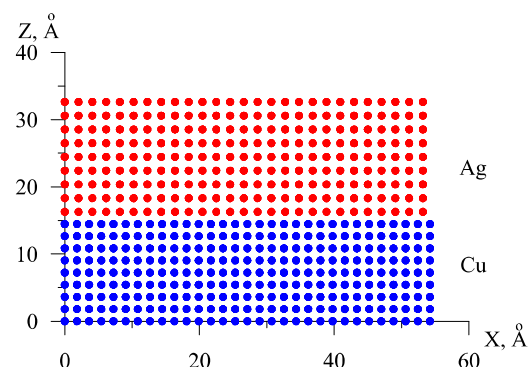


Figure 1 The initial heterostructure in the plane XZ

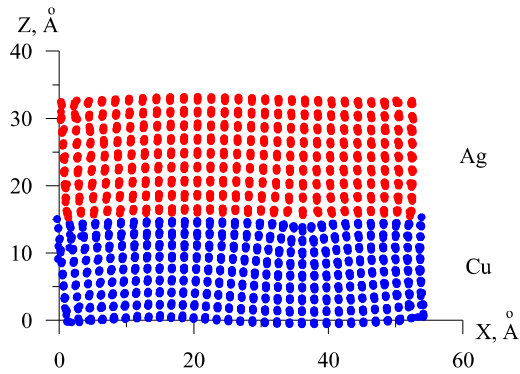


Figure 2 The cooled heterostructure in the plane XZ

The whole system is cooled with the help of the artificial viscosity method and the atoms positions are found in the global minima of the potential energy. The time step is 10^{-16} sec. On the Figure 2 the heterostructure is shown after cooling. The obtained atoms coordinates and impulses are used further as the initial data to the calculation of uniaxial deformation along axe X. component.

The boundary condition is modeled next way. The atoms of planes normal to axe X are set into the harmonic potential having the form:

$$V(\vec{r}_i) = \frac{k}{2}(x_i - x_i^0 - v_0 t)^2 + \frac{k}{2}(y_i - y_i^0)^2 + \frac{k}{2}(z_i - z_i^0)^2 \quad (1)$$

Here (x_i^0, y_i^0, z_i^0) are the coordinates of i-s atom after cooling.

The speed of the left edge equals zero, and the right edge speed is 10^3 cm/sec. It is allowed to simulate fixed and moved clamps with the generalized potential.

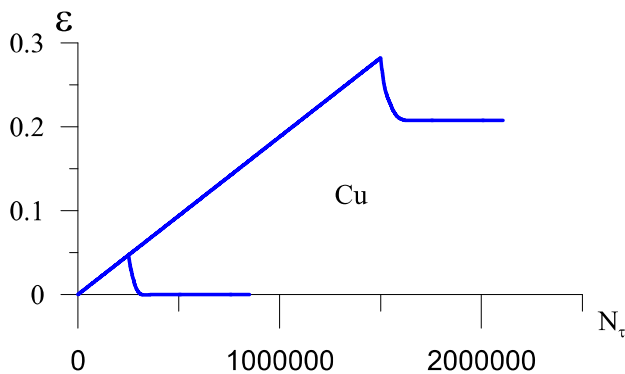


Figure 3 The dependence of percent elongation of copper crystal on the time steps number

THE SIMULATION OF HETEROSTRUCTURE TENSION

To analysis of the heterostructure uniaxial tension it were calculated such system macrocharacteristics as the forces acting from moved clamp to the copper and silver subsystems, the total percent elongation and the change of subsystems potential energy. In addition the coordinates and impulses arrays were saved after each 10000 time steps.

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from moved clamp to the copper and silver subsystems, the total percent elongation and the change of subsystems potential energy. The force has linear dependence from the heterostructure percent elongation, and the potential energy has the parabola shape up to value of the heterostructure percent elongation $\epsilon_c = 0.074$. Therefore this interval (from 0 to 0.074) is the heterostructure elastic deformation interval. The analysis of deformation type for $\epsilon \geq \epsilon_c$ is more convenient to carry out by the indication of reversibility of the geometrical form of structure after unloading.

The simulation of this process is carried out in the next way. In the fixed time moment the external potential was cut off and the system relaxes to the potential energy minimum (statically equilibrium state) by means of artificial viscosity. The dependences of percent elongation and the potential energy change from time are represented on the Figure 3, Figure 4, Figure 5, Figure 5. As initial data were took the atoms coordinates and impulses in the time moments when the deformation was 0.05 (5%) (i.e. $\epsilon < \epsilon_c$ - the elastic area) and 0.285 ($\epsilon > \epsilon_c$). One can see in the first case the final percent deformation equals zero, i.e. the system returns to the initial state, and in the second case the significant residual deformations take place. It means that at the deformation $\epsilon > \epsilon_c$ the plastic modifications take place.

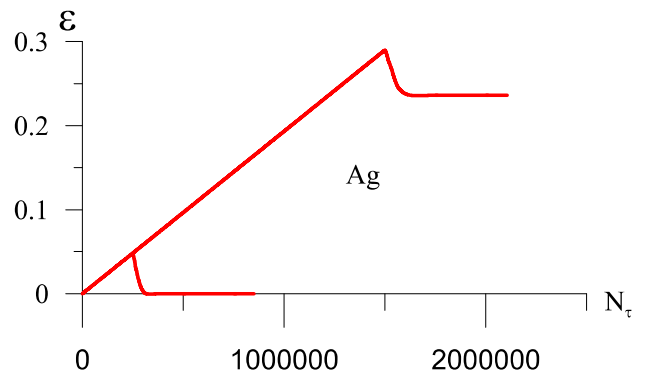


Figure 4 The dependence of percent elongation of silver crystal on the time steps number

The analysis of the heterostructure energy gives the same. In the region of elastic deformation the crystal potential energy equals initial one, and in the region of plastic modification the crystal potential energy greatly exceed the initial value. The analysis of the heterostructure external shape after cooling also approves the plastic deformations at the $\epsilon > \epsilon_c$.

The analysis of geometric structure in the different time moments (or at the various deformation values) is of interest. Before elastic deformations limit, at the $\epsilon_c = 0.066$ in the copper crystal the local deformation stripes appear which spread at the angle of 45° . The transfer to the plasticity region (Figure 7) is characterized that the Luders-Chernov stripe sharply increases the intensity and crosses all heterostructure.

The subsequent deformation growth up to 0.133 leads to the appearance of new intense stripes of local deformation and to the displacement of the matter in the form of blocks. With the

deformation reaches the value 0.286 the copper crystal begins to failure in the interface area along the zone boundary of local deformation. At the deformation increase to 0.381 the crack in the copper crystal grows with the simultaneous flowing the silver into the crack. At the deformation $\varepsilon_c = 0.572$ the crack cuts through whole copper crystal at the simultaneous healing of crack by silver atoms (Figure 8).

COMPARATIVE ANALYSIS: UNIAXIAL TENSION OF COPPER CRYSTAL

To reveal the interface role in the heterostructure the comparative analysis was carried out: the calculation of uniaxial deformation of copper crystal, which is the accurate copy of copper part of the heterostructure. The boundary condition totally coincides with the heterostructure case. The dependence of the potential energy change and the force acting to the moving crystal edge from the deformation value are shown on the Figure 8, Figure 8.

One can see that to the pure copper the upper limit of elastic deformation interval is increased to 0.15, after that the sharp decrease of force and potential energy takes place. The crystal shape analysis allows interpreting this fact.

The crystal has the well-ordered FCC-structure form with the deformation along X axe without the local deformation stripes. The exceeding of elastic deformation limit leads to the crystal destruction (Figure 8), which is accompanied by abrupt reduction of the crystal potential energy and the force on the moving crystal edge.

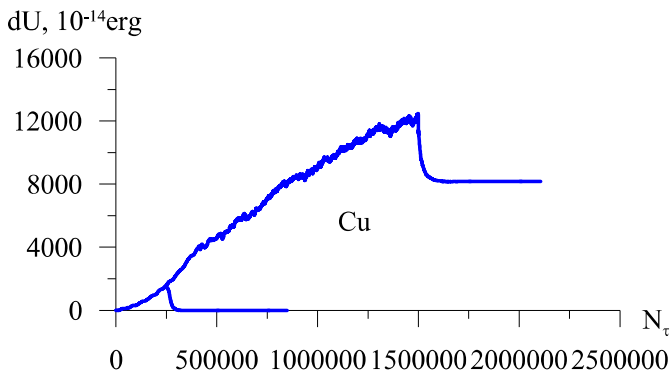


Figure 5 The dependence of potential energy change of copper crystal on the time steps number

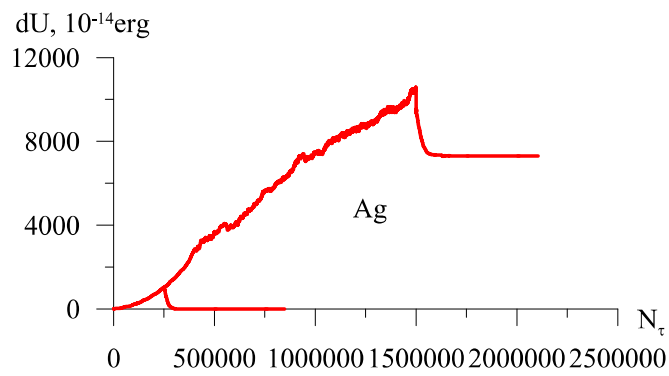


Figure 6 The dependence of potential energy change of silver crystal on the time steps number

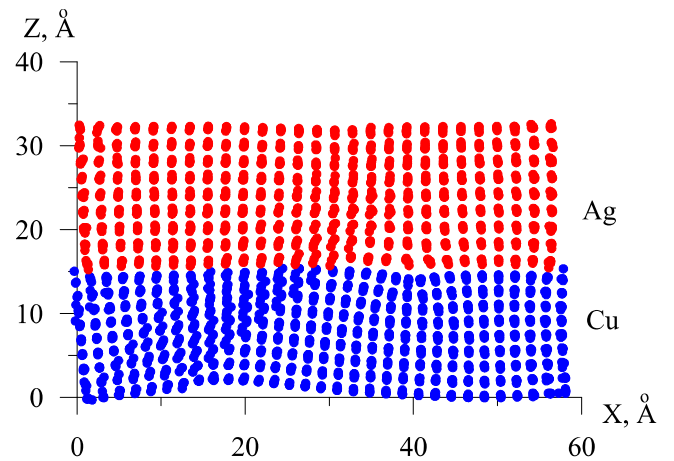


Figure 7 The heterostructure is in the plane XZ. The initial data correspond to the total percent elongation is equal to 0.285

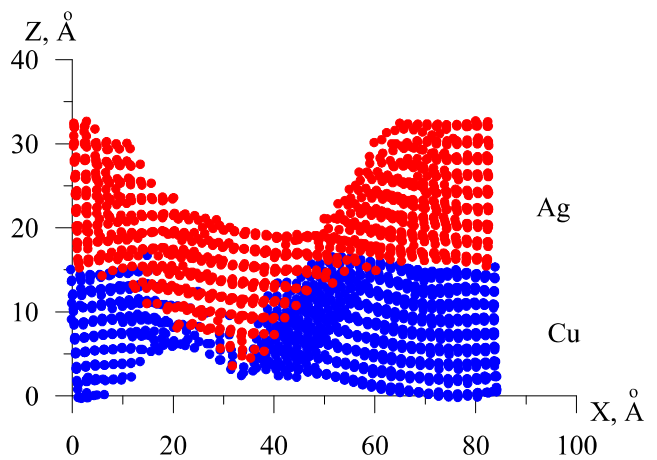


Figure 8 The heterostructure is in the plane XZ. The total percent elongation is equal to 0.572

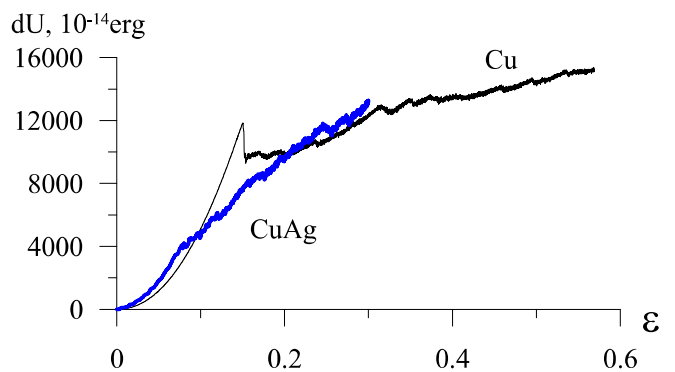


Figure 9 The dependence of potential energy change of separate copper crystal on the deformation – black line. The dependence of potential energy change of copper part in the composition of heterostructure on the deformation – blue line

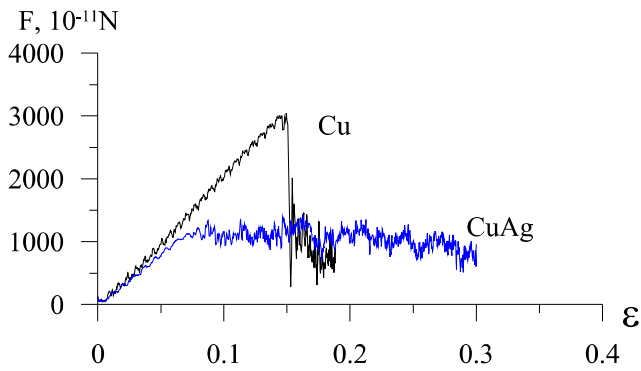


Figure 8 The dependence of the force acting to the separate copper crystal on the deformation – black line. The dependence of the force acting to the copper part in the composition of heterostructure on the deformation – blue line

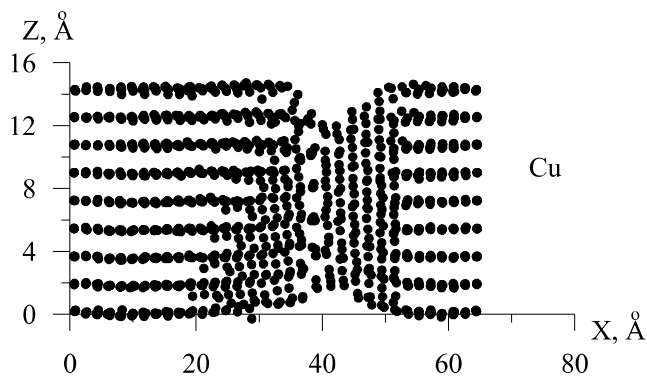


Figure 8 The copper crystal is in the plane XZ. The total percent elongation is equal to 0.208

CONCLUSION

So the interface cardinally changes not only mechanical characteristics of individual parts of heterostructure, but also the processes character taking place in it at the external mechanical influence.

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