Molecular dynamics investigation of behavior of grain boundaries under thermo-mechanical external impact.

Nikonov A.Yu [*], Dmitriev A.I., Psakhie S.G.

Institute of Strength Physics and Materials Science SB RAS. 634021, Tomsk, Russia

[*] nikonov@usgroups.com

Keywords: molecular dynamics, grain boundary, atomic scale.

Abstract. Molecular dynamics simulation of behavior of grain boundaries in bicrystal under shear loading were carried out. A variety of metals was investigated. The possibility of movement of the grain boundary in a direction perpendicular to the applied load was shown. The dependencies of the velocity of grain boundaries on the sample temperature are analysed. Results obtained in this paper help to understand the features of development of plastic deformation in polycrystals under shear loading.

Introduction

Polycrystalline materials on metal base with ultrafine grains have a number of unique strength and technological properties. Currently established that the unusually high mechanical properties of nanocrystalline materials are mainly caused by specific mechanisms of plastic deformation, which is closely related to the behavior of grain boundaries [1, 2]. This explains the large number of both experimental and theoretical works devoted to the behavior of the grain boundary under external dynamic influences, including shear. Note that the characteristic scale of the objects under study are comparable with the interatomic distances, so the experimental study of the behavior of grain boundaries requires high precision and expensive measuring equipment. Due to the complexity of experimental studies of mechanisms of motion of grain boundaries in recent years computer simulation methods are used for this purpose. Such studies allow to analyze in details various aspects of the investigated problem and to reveal the mechanisms of structural transformation of the crystal lattice in dynamics.

Studies carried out in [3] showed that under shear strain a defect structure, such as grain boundaries may move in the direction perpendicular to the applied load. Change the position of the boundary leads to an increase of one of the grains due to the atomic structure of the neighboring grains and, thus, leads to a redistribution of the configuration of structural defects and a change in deformation properties of the loaded material. Note that in mentioned study the boundary only at low temperatures was investigated, which are possible only in laboratory studies. At room, and especially at high temperature conditions, the behavior of grain boundaries may differ significantly.

In addition, in this paper studies were carried out for only one material that does not indicate the generality of the discovered phenomenon and requires further studies for other materials with FCC lattice.

Thus the aim of this study was to investigate the influence of temperature and the selected type of sample material on the behavior of grain boundaries of a special type under dynamic shear loading.

The object under simulation.

Calculations were performed using the method of molecular dynamics based on the program LAMMPS [4] which allows to use efficiently a parallel computing. Visual analysis of the structure was carried out using the program Rasmol [5]. The polycrystal consisting of two grains and containing a planar defect of type high-angle grain boundary in the plane XoZ, as shown in figure 1,

was selected as an object under simulation. To construct a special type of grain boundaries the algorithm proposed in [6] was used. Figure 1b shows the projection on the plane (001) of the bicrystals structure received as a result of the algorithm described above. This structure corresponds to the grain boundary of type $\Sigma=5(210)[001]$.
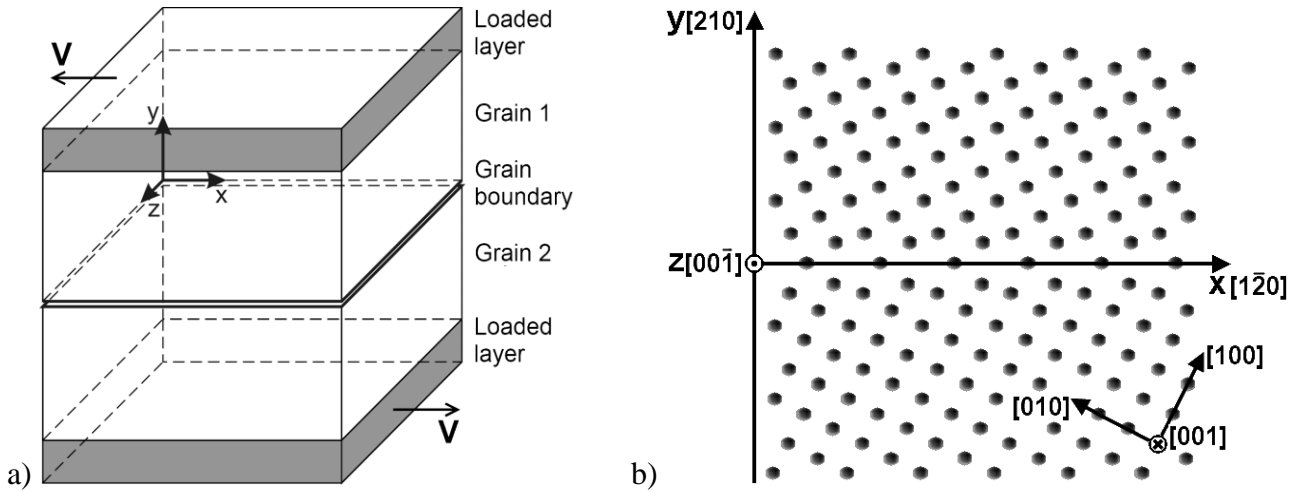

Fig. 1. a) Schematic geometry of simulated grain boundary, b) The fragment of the structure of the sample with the boundary of the type $\Sigma=5$

Loading was applied by set of constant velocities to all atoms of boundary layers, external to the modeled grain boundary. Atoms in loaded layers are moved so that their speed was directed parallel to the axis X. At that, velocities of loaded layers of different grains have been directed in opposite directions, as shown in fig. 1a. The thickness of each loaded layers corresponded to two cutoff radius of potential of atomic interaction, which is described in the framework of embedded atom method [7]. This choice was determined by the possibility to describe elastic and surface properties and energy parameters of the defects of the system with sufficiently high degree of accuracy. In the case of preservation of crystalline order a position of the boundary in the sample was defined as the y coordinate of the atoms in the plane of the defect (fig. 1b). In case of deviation of the crystal structure of the defect from the ideal configuration as a result of the thermo-mechanical effect, the position of the boundary was estimated as the average y-coordinate of the atoms forming the grain boundary. The equations of motion were integrated with time step $\Delta t=0{:}001$ ps. The total number of atoms was 133380. Along the plane of the grain boundary periodic boundary conditions were used. The distance between the loaded layers and grain boundary was more than 50 lattice parameters. A variety of metals is investigated.

The behavior of grain boundary $\Sigma = 5$ at low temperature.
In this paper, we simulated the behavior of grain boundary of a special type in copper for the different velocities of the atoms of the boundary layer. The velocity (V) in different tasks was varied in the range from 5 to 150 m/s. According to the results of simulation the behavior of the grain boundary of a special type $\Sigma=5(210)[001]$ under the shear loading essentially depends on the direction of the applied influence. So, under shear deformation along the X axis the grain boundary begins to move in a direction perpendicular to the applied loading (in our case along the axis Y), thus leading to a growth of one grain of a polycrystal.
In order to avoid induced effects associated with the symmetry of the ideal lattice, initially the equilibrium bicrystal "heated" to 100 K. For this purpose a special algorithm for scaling the velocities was used. At the initial time the procedure of random velocity distribution of atoms were

used. After reaching the equilibrium state was calculated actual kinetic temperature of the system from relations $3/2kT=mV^2/2$. Then, every appointed time span the velocity was scaled to achieve the desired temperature. The system at the stage of achieving the equilibrium configuration is considered as NVE (number of particles N, volume V and energy E were stored).

As noted in [3] under certain conditions it is possible to rebuild the crystal lattice near the initial provisions of the defect, which is accompanied by a change in the position of a defect in the direction perpendicular to the applied load. This mechanism is associated with the movement of atoms of one grain under the conditions imposed shear deformation and rebuild by these atoms of the crystal lattice of opposite grain. Thus, the shear loading of grain boundaries of special type under certain conditions may lead to its displacement perpendicular to the applied load. A detailed study of this process of the motion is described in [3].
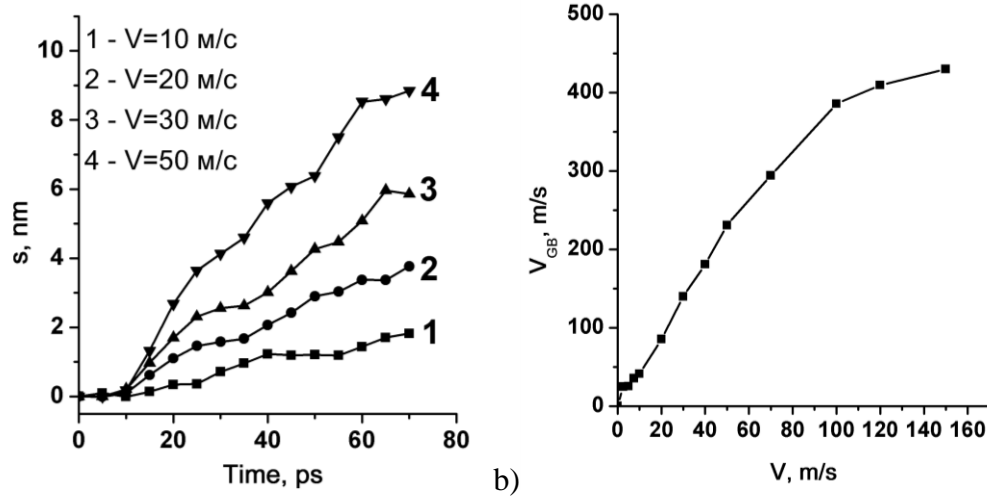

Fig. 2. a) The time dependence of grain boundary displacement for different values of the loading velocity V b) dependence of the velocity of the grain boundary motion in direction perpendicular to the loading on the value of loading.

It is obviously, that the direction of perpendicular motion of grain boundary is defined by lack of symmetry of the boundary in the plane YoZ. Therefore, it is expected that the change of loading direction should lead to a change in the direction of the boundary movement, as was confirmed later by simulation results. This means an increase in the effective speed of the grain boundary movement. Time dependencies of the Y-coordinates of the grain boundary for 4 different loading rates are shown in fig. 2a. One can see that when the loading velocity is 10 m/s the displacement of the boundary at t=72 ps is about 2 nm, while at the loading velocity 50 m/s the displacement reaches 10 nm at the same time. Comparative analysis of position of the grain boundary at different times for different strain rates showed that the grain boundary moves with the alternation of intervals of motion with constant speed and intervals of relative quiescence (fig. 2a). It is more visible at small values of shear velocity. Apparently, this alternation of motion is associated with the dynamics of loading and the features of rebuilding the crystal structure of the atomic lattice in the process of moving grain boundary. If to average obtained dependences, i.e. to take the difference of values of grain boundary displacements for the considered loading rates at the same time interval, it is possible to obtain the average values of the velocity of boundary motion as a function of the magnitude of the loading rate. On fig. 2b such dependence is presented. According to the simulation results, for the boundary of type Σ=5 effective speed of movement of the grain boundary is proportional to the load rate with factor k=4,59. However, the given dependence is valid only at low loading velocity (less than 100 m/s). At high-speed loading with increasing velocity of loaded layers increasing of velocity of boundary slows down and goes to a limiting value of ≈ 500 m/s. To all

appearance this limiting value is determined by the maximum velocity of gliding dislocations involved in the formation of the grain boundaries.

The influence of temperature on the behavior of grain boundary.
The studies described in [3] were carried out at low temperatures, which are possible only under laboratory conditions. This was done to reduce the influence of thermal effects on the behavior of atoms. Investigation of the influence of sample temperature on the features of its behavior under shear loading was carried out by the example of copper bicrystal containing a grain boundary of type $\Sigma=5(210)[001]$. Loading rate was V=20 m/s. The sample temperature was varied in the range of temperatures from 0K to 1000K. A definite temperature was specified at the initial time and during the subsequent loading could be varied. Under condition of the imposed shear strain observed a slight increase of the kinetic temperature of the sample over a time of simulating (within 10K).
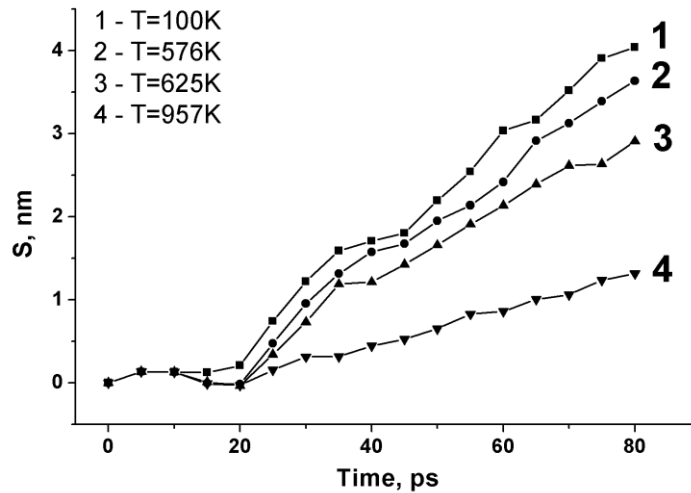

Fig. 3. Time dependence of the movement of the grain boundary at the variation of initial temperature of the simulated bicrystal.

The results showed that at temperatures up to 550K the behavior of grain boundaries is not change. Speed of movement of the boundary in the direction perpendicular to the applied loading under otherwise equal conditions remains practically unchanged. There are minor changes in the atomic structure in the plane of defect, as shown in fig. 4a. The figure shows the projection of all atomic layers on the plane XoY, calculated position of the boundary is indicated by the solid line. This form of boundary explained by the fact that due to temperature fluctuations the position of atoms in each layer may vary, and there is a "blurring" of the lattice sites on the projection of all layers. This is particularly noticeable in the area of the defect structure. With a further temperature rises, other things being equal conditions of the loading a rate of vertical movement of the boundary, and, consequently, its resultant displacement sharply decreases (see the transition from curve 2 to curves 3 and 4 in fig. 3). Analysis of the structure showed that if by variation of temperature in the range from 100K to 576K values of the boundary displacements remain almost unchanged (from 4.04 nm to 3.63 nm), then at a temperature of 625K resultant displacement of the defect was 2.9 nm. And at a temperature of 957K – only 1.3 nm. In this case the calculated velocity of the grain boundaries also decreases. In the investigated temperature range, this change was almost three times: from 61 m/s to 21 m/s. This is accompanied by increase of the width of the boundary, which is caused by a violation of the ordered crystalline structure of the sample (fig. 4b).
In fig. 4b by the dashed lines indicate the atomic planes, the appropriate boundaries of a defect in the direction of the axis OY.
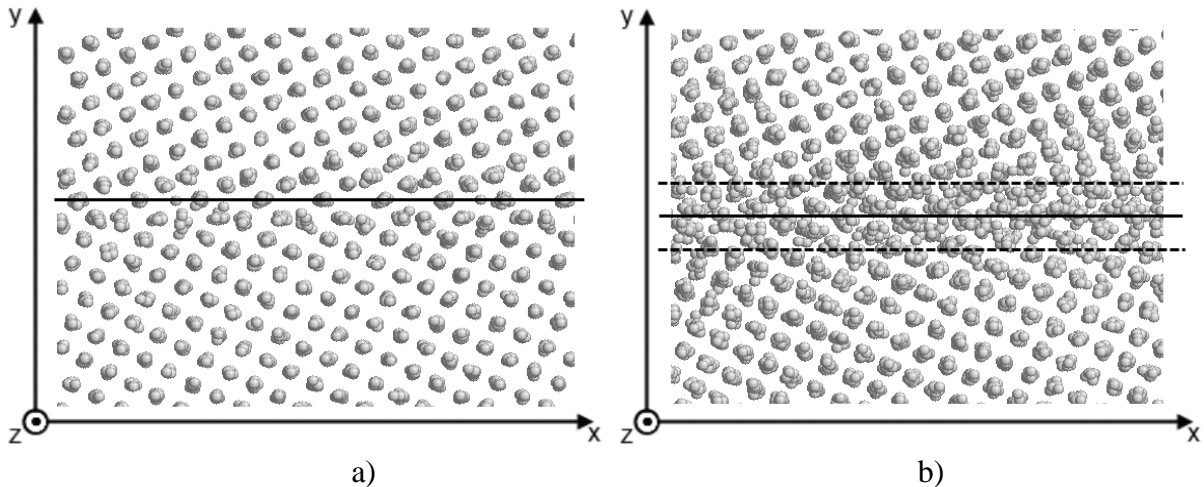
a)   b)

Fig. 4. The structure of the sample near the boundary after the load at a) 500К; b) 1000К.

Analysis of the structure of atomic lattices in various atomic planes showed that in each plane the violations of atomic order near grain boundary does not occur. It is possible to distinguish quite clearly the structure of each of the grains as well as grain boundary (fig. 5). However, the shape of the boundary is not straight but has a complex shape. It is obvious, that the complex form leads to an increase in the length of grain boundaries in a separate atomic plane, and the mismatch of the structure of atomic planes mean a general increase of the area of the defect. This in turn means an increase in energy of the defect, so should be a reason of the increased resistance to movement of boundary under external influence.
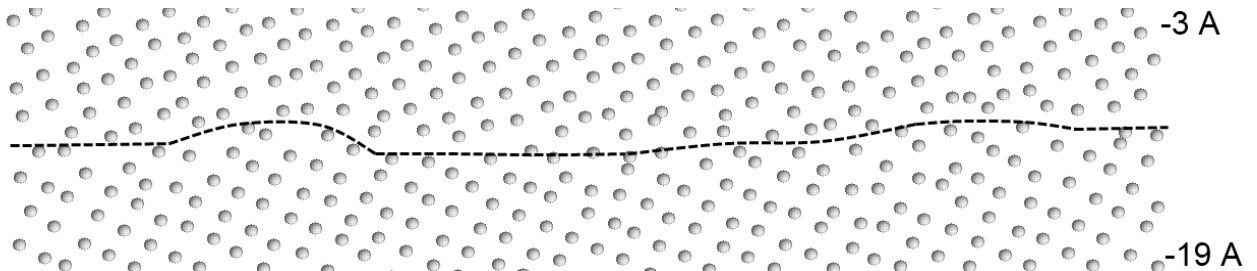

Fig. 5. The structure of grain boundary in atomic plane parallel to the plane XoZ.

For a detailed study of the effect of temperature bicrystals of different materials are simulated. Samples of Cu, Ni, Al, Ag are examined. All samples contained a grain boundary of type $\Sigma = 5$ (210) [001], the number of atoms in all bicrystals was 133,380. Only an overall size of the samples is differed. Samples were subjected to load at varying temperatures ranging from 0K up to 0.7-0.9 of the melting temperature of the material. The possibility of moving boundaries, the path traveled as a result by such movements and the width of the interface during displacement of the defect were investigated (fig. 6). The simulation results showed that the grain boundaries in the investigated samples behave similarly. In all materials with increasing temperature there is a decrease magnitude of the displacement boundary and an increase in the width of the boundary are observed.

Since the materials have different properties, for a quantitative comparison of the numerical parameters of the phenomenon is convenient to use the relative temperatures, which is reduced to its melting point for each material. In fig. 7 shows graph of the reduced temperature dependence of displacement of the boundaries for the investigated bicrystals. It is seen that the reduction of the displacement occurs in the temperature range from 0.45 T_{melt} to 0.6 T_{melt} (fig. 6). A sample of silver

is behaves in a special way at low temperatures. To study this feature further investigation is required.
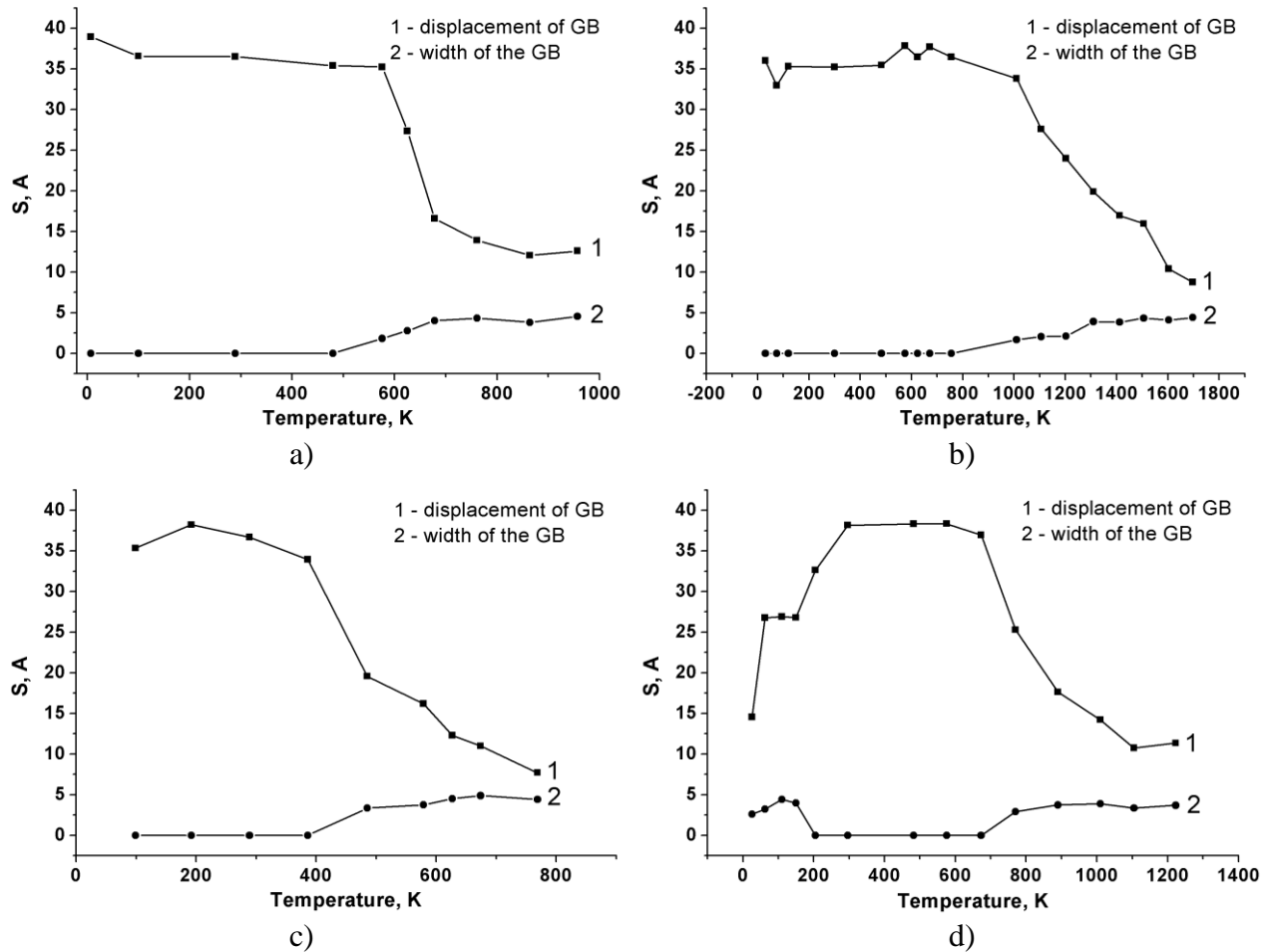

Fig. 6. The displacement of the boundary and width of the interface at the variation of initial temperature in the sample of a) Cu; b) Ni; c) Al; d)Ag.
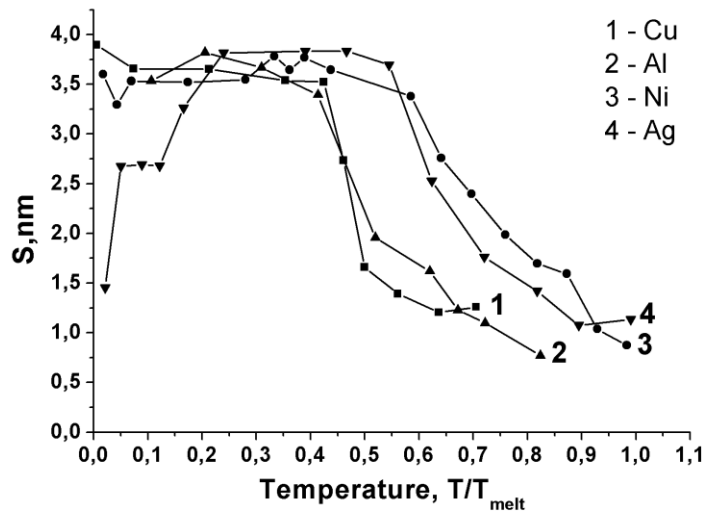

Fig. 7. The displacement of the boundary at the variation of initial temperature in the sample

Conclusions

The mechanism described above of movement of grain boundaries confirms one of the existing hypotheses that the movement of grain boundaries associated with the cooperative movement of group of atoms [8]. According to the results of simulation dynamic properties of the boundary depend on the temperature of the sample. Low temperature significantly increases the mobility of boundary at other things being equal. At temperatures above the 0.45 of melting point the mobility of the boundaries may be significantly reduced. The studied features of the behavior of grain boundaries were observed in a number of metals with fcc structure, which might suggest that there are generality of the observed phenomenon. Results obtained in this paper help to understand the features of development of plastic deformation in polycrystals under shear loading. The observed behavior of the boundaries may influence on the changes of the microstructure of the material, and as a consequence, on its properties and behavior under load.

References:

[1]   G.A. Malygin Plasticity and strength of micro-and nanocrystalline materials (Review) // Physics of the solid state. 2007. V. 49, No. 6. P. 961–982.

[2]   Gutkin M. Yu., Mikaelyan K. N., Ovidko I. A. Grain growth and collective migration of grain boundaries during plastic deformation of nanocrystalline materials // Physics of the Solid State, 2008, V.50, No.7, P.1261-1265.

[3]   A.I. Dmitriev, A.Yu. Nikonov and S.G. Psakhie Atomistic mechanism of grain boundary sliding with the example of a large-angle boundary S = 5. Molecular dynamics calculation // Fiz. Mezozekh. – 2010. – V. 13. – No. 4. - P. 15-24.

[4]   S.J. Plimpton Fast Parallel Algorithms for Short-Range Molecular Dynamics // J. Comp. Phys. 1995. V. 117. No. 1, P. 1–19.

[5]   H. J. Bernstein RasMol and OpenRasMol [Electronic resource] – Mode of access: http://rasmol.org (05.05.2012).

[6]   A. Suzuki, Y. Mishin Atomistic modeling of point defects and diffusion in copper grain boundaries // Interface Sci, 2003. V. 11, № 1. P. 131–148.

[7]   S.M. Foiles Embedded-atom and related methods for modeling metallic systems // MRS Bull, 1996. V. 21, № 2, P. 24−28.

[8]   Gorkaya T., Molodov D.A., Gottstein G. Stress-driven migration of symmetrical h100i tilt grain boundaries in Al bicrystals // Acta Materialia, 2009, V.57, P.5396-5405.