Features of the behavior of the grain boundaries in the thermo-mechanical impact. Molecular dynamics study

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Abstract

Molecular dynamics simulation of behavior of grain boundaries in bicrystal of copper under shear loading were carried out. The influence of temperature of the sample on the behavior the grain boundaries was studied. The stability of discovered earlier effect of moving boundaries in a direction perpendicular to the applied loading was analysed. It was found that with increasing of temperature, the rate of such movement of the boundary decreases. As it was shown by studies of the structure, it is accompanied by a violation of order of the atomic structure near the boundary. The violation is caused by inconsistency of position of the grain boundaries in the various atomic layers. A similar effect was also found for other pure FCC metals (Ni, Ag). These results can help to understand the features of development of plastic deformation in polycrystals under shear loading.

1 Introduction

Considered to be reliably established that an unusually high mechanical properties of nanocrystalline materials are mainly due to the specific mechanism of plastic deformation, which is closely related to the behavior of the grain boundaries (GBs). In this regard, features of behavior of grain boundaries under of external influence has become a subject of extensive discussion in the literature with respect to the impact of this phenomenon on mechanical properties of ultra-fine-grained and nanocrystalline materials [1, 2]. Note that the characteristic scale of the objects under study are comparable with the interatomic distances, so the experimental study of the behavior of the grain boundaries requires precise and expensive test equipment. Recently, with the growth of computer technology that question is increasingly being studied using computer simulation. Such studies allow a detailed analysis of the various aspects of the investigated problem and research the mechanism of the structural transformation of the lattice in dynamics. In particular, results of molecular dynamics simulations show that under external shear deformation grain-boundary sliding in fcc crystals can be accompanied by the restructuring of the atomic configuration in the area of the defect, which leads to the displacement of the grain boundaries in the direction perpendicular to the applied load [3, 4]. It was noted that this effect is observed only under certain (special) conditions, namely, the low temperature of a crystallite, symmetrical boundaries of a special type, shear loading parallel to the plane of the defect. Obviously, in the real conditions behavior of grain boundaries under shear deformation may differ substantially. However, in spite of great practical importance, the question still remains unexplored. Thus, in [5] dependence of the mobility grain boundary on the crystal temperature observed, but reasons of the change speed of the defect movement with increasing temperature not investigated. Therefore the aim of this study was to investigate influence

of temperature of a crystallite containing a special type of grain boundary on the features of its plastic deformation under shear loading and understand the reasons for changes in grain boundary mobility with increasing temperature.

2 The model description

Investigations were carried out in the framework of conventional molecular dynamics method using a software package LAMMPS [6]. Modeled sample was a copper bicrystal consisting of two grains in the form of rectangular fragments and containing a planar structural defect such as high-angle grain boundary $\Sigma = 5(210)[001]$. The algorithm described in [7] used for modeling of the grain boundaries of a special type. The essence of the method is the following. Grain orientated in space in such a way that the external axis X, Y and Z correspond to the crystallographic directions [210], $[\bar{1}20]$ and [001], respectively. The second grain is the mirror image of the first in the plane XoZ, which becomes the plane of the defect.

Two types of boundary condition were imposed in the X-direction. In the fixed boundary condition, the grains are sandwiched between two slabs in which the atoms are fixed in their perfect-lattice positions relative to one another. The fixed atoms do not participate in MD simulations and only serve to impose interatomic forces on neighboring dynamic atoms. The thickness of each fixed slab is twice the cutoff radius of atomic interactions, which was described in the framework of the embedded atom method. Choice of potential was caused by the possibility to describe accurately the energy parameters of structural defects, the elastic and surface properties of the simulated sample. The fixed boundary condition restricts spontaneous translations of the grains. Lattice regions adjacent to the GB can still translate relative to each other but such translations are accompanied by elastic deformation of those regions. This boundary condition was used to apply a shear parallel to the GB by moving all fixed atoms of the upper grain with the same constant velocity V_x equal to $20m/s$, while the lower slab was moved with the same velocity in opposite direction. Thus, the resulting shear strain rate was $40m/s$. The equations of motion were integrated with a time step $\Delta t = 0.001ps$. The total number of atoms in the sample reached 150000. Along the plane of the grain boundary (directions X and Z) modeled the periodic boundary conditions. The distance between the loaded layers and grain boundaries was more than 50 lattice parameters.

Modeled crystallite was investigated in the temperature range from $0K$ to $1300K$. For comparison performed previously estimate of defect-free crystallite melting point of copper with the same interaction potential demonstrated the importance of $\approx 1350K$. Selected temperature was specified using scaling algorithm of atoms velocities based on equality energies

$$\frac{3}{2}kT = \sum \frac{mV_i^2}{2},$$

where i is atom number. At the initial time a random distribution of velocities of the atoms was being specified, and their correction was carried out at the points of minimum potential energy. To include the effect of thermal expansion, prior to MD simulations the block was expanded uniformly by the lattice thermal expansion factor at the desired temperature T. Modeled sample was considered as NVE ensemble that maintains the number of particles N, the occupied volume V and the energy of the system E.

3 Results of simulation

The simulation results show that can be identified three stages according to nature of response of the simulated crystallite to external shear load. At the first stage at initial temperatures up to $\sim 500K$, the behavior of the studied grain boundary is identical to what was noted in [4, 5]. Namely, in the conditions of shear strain in addition to the relative sliding of interacting grains the displacement of boundary position in the direction perpendicular to the applied external loading was observed. Change the position of the boundary leads to an increase of one of the grains due to the atomic structure of the neighboring grains. The speed of the displacement of the boundary in this temperature range remains approximately unchanged and exceed the speed of the relative displacement of loaded layers 1.5 times. The resulting displacement of the boundary in the direction of Y was $10.43nm$ and $10.38nm$ at the beginning and end of the interval of temperatures, respectively. It should be noted that with increasing temperature, there is a slight change in the structure in the plane of the defect, as shown in Fig.1a, but this is not affected on the dynamics of the whole process.

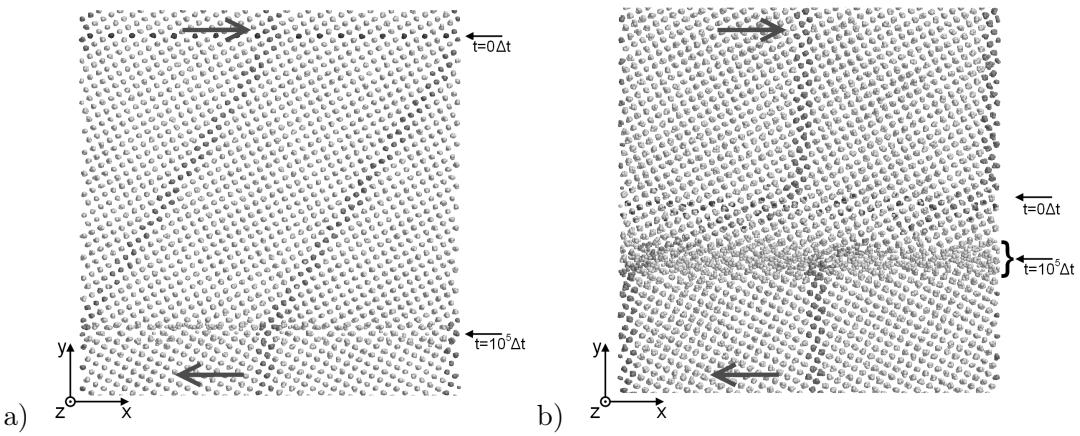


Figure 1: Structure of the sample fragment near the grain boundary at time $t = 10^5\Delta t$ at different initial temperatures of a) $500K$; b) $1000K$. To visualize the effect of moving the grain boundaries in the initial structure of the sample were highlighted two atomic layer thickness of two atomic planes and oriented parallel to the plane YoZ.

In the temperature range from $\sim 500K$ to $\sim 700K$ second stage can be identified, when the speed of displacement of the boundary in the direction perpendicular to the applied shear loading, and, consequently, the resulting amount of displacement of grain boundary in the Y direction sharply decrease. Thus, at a temperature of $600K$ resultant displacement of planar defect in the same period decreased to $6.57nm$. When the temperature raises to $700K$ the resulting displacement of the boundary is only $4.21nm$. In this case, calculated speed of boundary motion decreased almost in 3 times to $58m/s$ to $23m/s$. This is accompanied by increasing of the width of the grain boundary, which is caused by a violation of the ordered crystalline structure of the sample close to the plane of the defect. In Fig.1b marked region adjacent to the plane of the defect, where a violation of the regularity of the crystal lattice was observed. At that, the Y coordinate of the defect was assumed to mean the specified area.

At temperatures above $\sim 700K$ dynamics of the boundary behavior changes. Rate of change of displacement decreases with increasing temperature, and the resulting displacement of the position defect in the Y direction for the considered time interval reaches a

minimum near the value of $1.3nm$. At that the width of the area where violation of the regularity of the atomic lattice near the plane of the defect was observed, in the third stage remains almost unchanged at $0.5nm$. In Fig.2 the total value of shift and the resulting width of the border were shown as a function of the initial temperature of the simulated sample. It can be seen that the sharp decrease of the resulting shift of the defect and the broadening of grain boundary occurs in the temperature range of the sample $\approx 500-600K$. Note that these temperatures correspond to the initial values of the temperature of the sample and during the loading they rise. According to the results of modeling, these temperature changes can be neglected, since it is about $20K$ for all the cases examined. Further heating of the sample to a temperature close to the melting point leads to a sharp increasing of the width of the layer of disordering and the decreasing of the shift of the defect to 0.

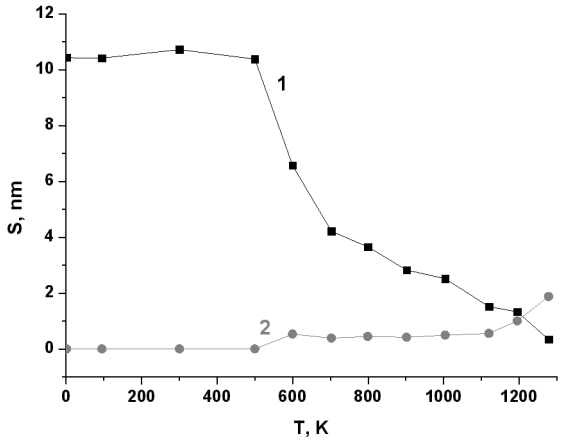


Figure 2: The influence of the sample temperature on the resulting shift of the grain boundaries along the Y axis during the analyzed time period (1) and the thickness of the layer with the violation of a regular packing of atoms close to the plane of the defect (2).

Layer-by-layer analysis of the resulting atomic structure of the simulated sample in the plane lying parallel to the plane XoY, showed that even at high temperatures in each layer only minor violations of the order of atomic lines near the grain boundaries are found. It is possible to clearly distinguish the structure of each of the grains and grain boundaries. However, the shape of the border is not a line. Thus, the apparent violation of the regularity of the atomic lattice packing in the simulated defect (Fig.1b) is due to a mismatch of in the position of the boundary line different atomic layers perpendicular to the direction Z. Note that a similar result was observed in [3], where features of behavior of grain boundaries with imperfect structure under shear deformation was studied. Mismatch of position of grain boundaries in different atomic layers can be clearly seen in Fig.3, which shows the structure of one of the selected atomic layers parallel to the plane XoY, and dashed line 1 marks the position of the boundary in this layer. Position of the grain boundaries in the other two atomic layers marked by dashed lines 2 and 3. One can see that in some areas discrepancy of position of grain boundaries can exceed the size of the lattice parameter.

Investigation of the structure of atoms near the grain boundary showed that at high temperatures the proportion of grain boundary sliding mechanism attended by perpendicular movement grain boundaries decrease. Result of this is the dominance of rigid relative slip along the grain boundary. Thus, revealed staging of simulated crystallite response to

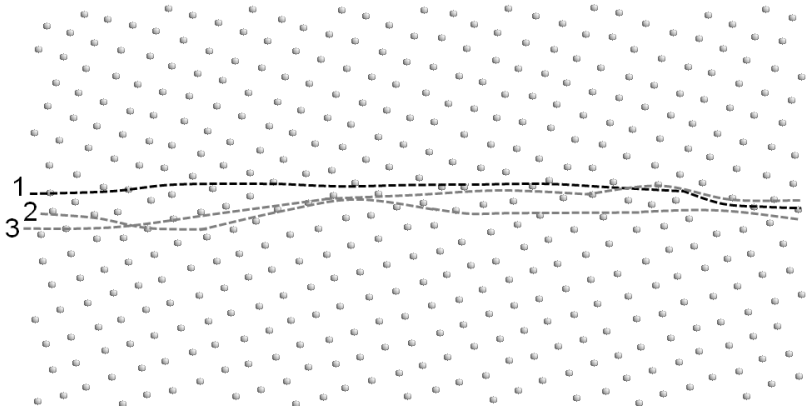
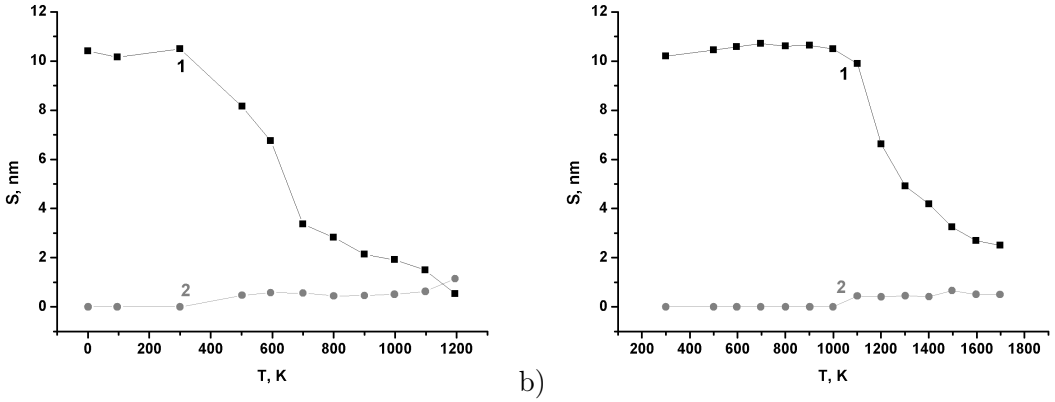


Figure 3: The structure of the grain boundary in selected atomic layer parallel to the plane XoY. The dashed lines indicate the position of the grain boundaries in the selected layer and in two other atomic layers.

external shear loading in a wide range of temperatures can be related to the manifestation of various mechanisms of grain boundary sliding for the considered type of planar defects, as a transitional stage accounted for the change of the mechanisms. As a criterion of change may be a degree of mismatch of the atomic structure of grain boundaries caused by the change temperature background or other external influence, as well as changes in the lattice parameter due to thermal expansion of the lattice.

To study the temperature effect more detailed the same investigatione for other materials were carried out. Bicrystal samples of Cu, Ni and Ag were examined. All samples contained a grain boundary type $\Sigma = 5(210)[001]$, and the number of atoms was the same, about 150000. 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.4). 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.



a) b)

Figure 4: The displacement of the boundary and width of the interface at the variation of initial temperature in the sample of a) Ag; b) Ni.

Since the materials have different properties, for a quantitative comparison of the nu-

merical parameters of the phenomenon is convenient to use the relative temperatures, which is reduced to its melting point for each material. In fig.5 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 $0.45T_{melt}$ to $0.6T_{melt}$.

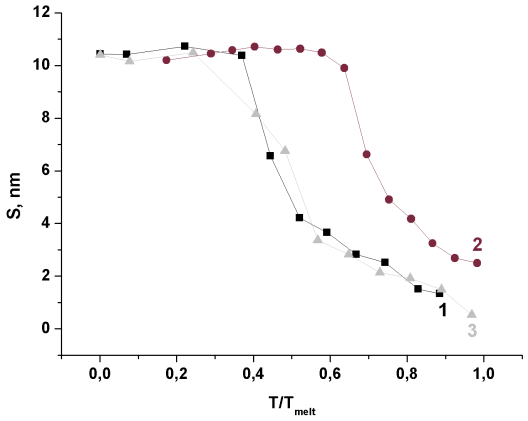


Figure 5: The displacement of the boundary at the variation of initial temperature in the sample of Cu (1), Ni (2), Ag (3).

4 Conclusions

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.

Acknowledgements

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