Molecular Dynamics Study of Behavior of Symmetrical Tilt Grain Boundaries in BCC and FCC Metals under Shear Loading

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Abstract

Behavior of symmetrical tilt grain boundaries under shear loading was studied in the framework of classical molecular dynamics. Grain boundaries Σ5 and Σ9 in Cu and α-Fe were modelled. It was found that behavior of defect depends not only on the structure boundaries, but also on the type of crystal lattice. It is shown that under external stress grain boundary behaves differently in the BCC and FCC metal. Initially in the sample with GB Σ5 an elastic deformation of grains was observed in the condition of shear loading. That led to the formation near the defect structure different from BCC. With further loading, this structure is destroyed, which led to structural failure near the grain boundary. After that the defect is starting to move in a direction perpendicular to the applied loading. It was shown that grain boundary Σ9 behavior in α-Fe similar to the behavior of GB Σ5 in Cu: under an external influence defect begins to move without any changes in structure of GB. A comparison of the amount of displacement of GB with the amount of grain boundary slip due to shear deformation was performed. These results can help to understand the features of development of plastic deformation in polycrystals under shear loading.

1 Introduction

Studying the mechanisms of plastic deformation of polycrystalline materials is certainly one of the key problems of modern materials science. This issue is the subject of many both experimental and theoretical works. Established that the character of plastic deformation is determined by conditions of loading and the characteristic value of the grain structure of the material. For coarse material determining mechanism is dislocation one of deformation, leading to the emergence of localization bands. With decreasing grain size slip along the grain boundaries becomes the dominant mechanism of deformation. Earlier in [1] show that external shear deformation leads to restructuring of the crystal lattice near the grain boundaries, leads to an increase of one of the grains due to the atomic structure of the neighboring grains. These studies were conducted on a sample of copper containing tilt grain boundary Σ5(210)[001]. Later, similar studies have been performed for copper crystallite containing tilt grain boundaries, different from Σ5 [2]. Studies have shown that the behavior of the grain boundary $\Sigma 9(1\bar{2}2)[011]$ under shear deformation may differ from previously studied the behavior of the boundary Σ5.

To check the generality of the observed grain boundary sliding mechanism in the present study modeling of behavior of these grain boundaries under conditions of applied shear loading was conducted for a sample of nickel and α-iron.

2 Numerical model

Investigations were carried out in the framework of conventional molecular dynamics method using a software package LAMMPS [3]. 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 tilt grain boundary. Schematic representation of the sample shown in Fig. 1. The tilt grain boundaries $\Sigma5(210)[001]$ and $\Sigma9(1\bar{2}2)[011]$ were modelled using Coincidence Site Lattice (CSL) principle. The algorithm described in [4] used for modeling the grain boundaries. 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 determined by the type of defect. The second grain is the mirror image of the first in the plane XoZ, which becomes the plane of the defect. External shear loading was assigned by setting the constant velocity V atoms of the loaded layer. Direction of the velocity vector was specified as shown in Fig. 1. Speed of movement of atoms in the layers of the loading was $20m/s$. Thus, the resulting shear strain rate was $40m/s$. Sample with an initial temperature of $200K$ was simulated. Along the plane of the grain boundary (directions X and Z) modeled the periodic boundary conditions. Atomic interaction was described in the framework of the embedded atom method [5]. The total number of atoms was about 100000. 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. Velocity-Verlet integrator was used. The equations of motion were integrated with a time step $\Delta t = 0.001ps$.

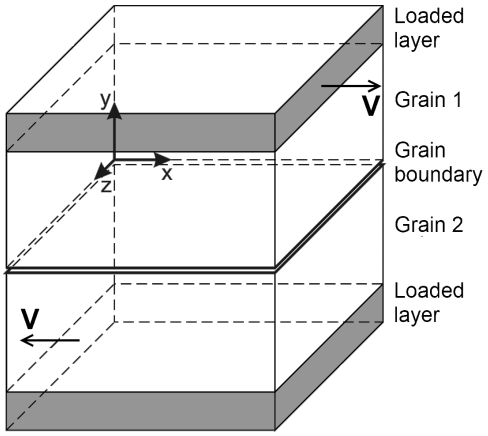
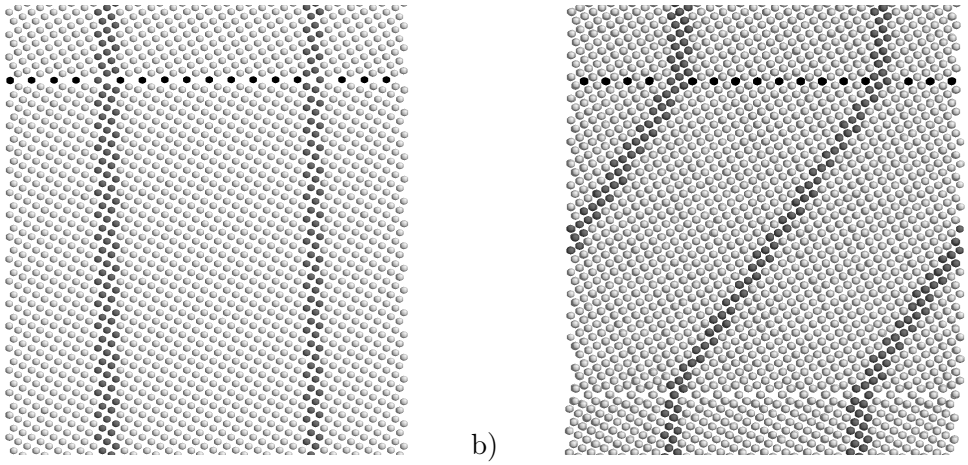


Figure 1: Schematic representation of the simulated sample

3 Simulation results for the sample Ni

Initially, we investigated the behavior of the sample of nickel containing grain boundary $\Sigma5$. Since the lattice Ni like Cu is FCC lattice, we should expect a similarity of response of Ni crystallite with grain boundaries on the external shear of loading of. Projection on the plane XoY of fragment of initial structure containing a planar defect is shown in Fig. 2a. Black color indicates the atoms lying in the plane of the defect, gray – atoms arranged in a plane perpendicular to the grain boundary. The results of modeling the behavior of grain boundaries $\Sigma5$ in the sample of nickel showed that in the conditions of shear strain relative sliding of interacting grains accompanied by displacement of boundary position in the direction perpendicular to the applied external loading. The resulting structure after

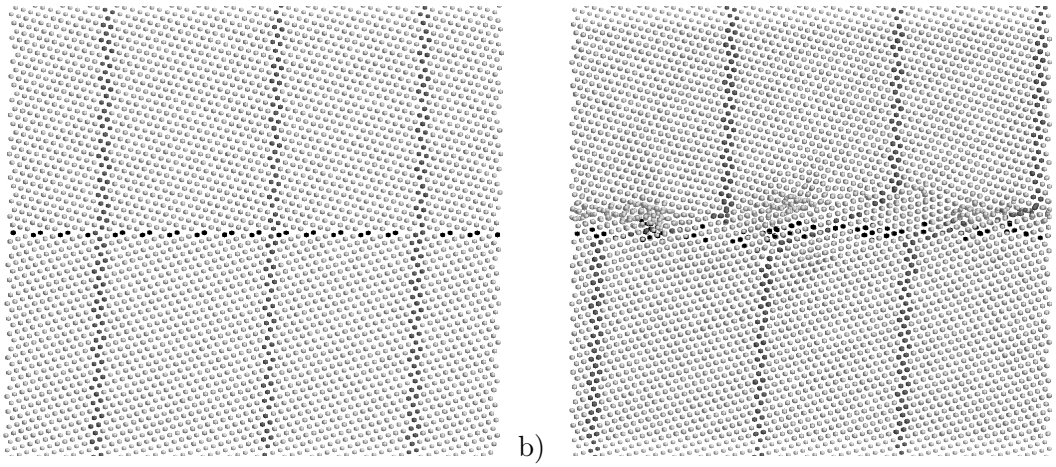
200000 steps of loading shown in Fig. 2b. Comparing the simulation results for the two Cu and Ni crystallites can be noted that the value of such movement, as previously [6] one and a half times greater than the amount of relative sliding of the grains. Thus, the behavior of the crystallite of Ni, containing tilt grain boundaries Σ5 identical to the behavior of similar bicrystal of Cu.



a) b)

Figure 2: The projection of structure atomic near the boundary on the plane XoY at the time a) $t = 0ps$; b) $t = 200ps$

The next stage of research was to model the behavior of the sample of Ni, containing a grain boundary Σ9. The resulting equilibrium atomic configuration near the plane of the defect is shown in Figure 3a. Feature of the structure of such a defect is its zigzag nature [7]. It was found that under conditions of shear deformation repositioning of the boundary plane along the axis Y does not occur. Observed only sliding of grains along the boundary accompanied by the curvature of the grain boundary plane. Fig. 3b shows the structure of the sample at time $t = 100ps$.



a) b)

Figure 3: Projection of atomic structure of the sample containing a grain boundary Σ9 at time a) $t = 0ps$; b) $t = 100ps$

To analyze the features of atomic configuration near the boundary the algorithm to search of local structural changes was used [8]. It allows one to identify the appearance of defects such as dislocations and stacking faults in the FCC lattice, and also to identify the local configuration of the crystal lattice (FCC, BCC and HCP) near the selected atom

by the location of its neighbors. Fig. 4a shows the projection of the fragment structure of the sample containing grain boundaries after 100000 integration steps. Atoms with different local configurations of the crystal lattice marked by various shades of gray and sizes. Bright dots indicate the atoms forming the defect-free FCC lattice. Atoms with local HCP lattice marked by large gray circles. The appearance of such a structure corresponds to the formation of stacking fault. Black dots indicate the atoms whose local configuration differs from the crystal lattice defect-free FCC, BCC and HCP. Such atoms are located near the free surfaces, grain boundaries, vacancies, dislocations, and many other structural defects.

With further loading of crystallite formation separate fragments of material near the plane of the defect and the curvature of grain boundaries is observed. This is clearly seen in Figure 4b.

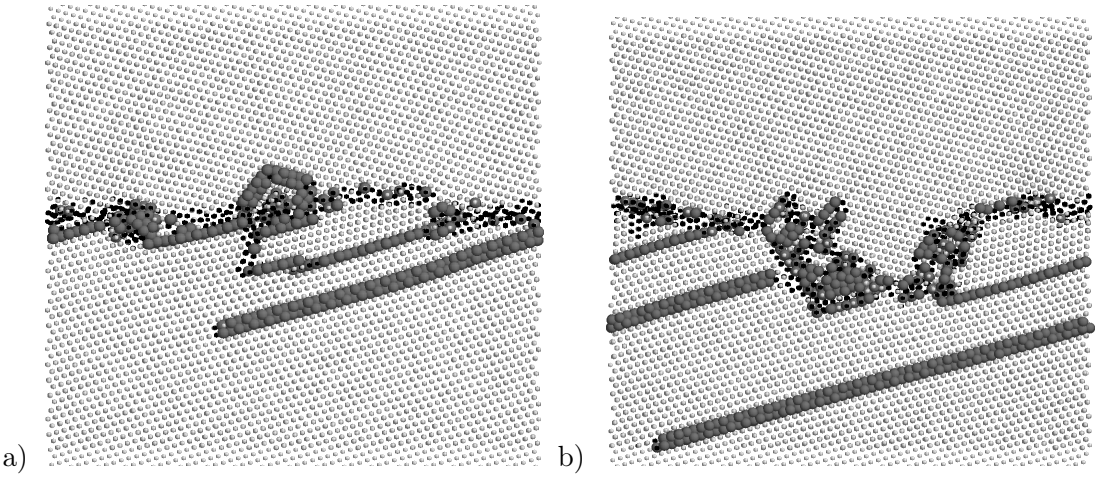


Figure 4: Projection of the structure of the sample on the plane XoY at time a) $t = 100ps$; b) $t = 160ps$.

Comparing the behavior of the investigated grain boundaries in sample of copper and nickel may be noted that, as expected, the identity of the crystal lattices of the two metals leads to that the simulation results are in good qualitative agreement. It can be assumed that a similar behavior is observed in other metals with face-centered cubic lattice.

4 The behavior of the tilt grain boundaries in the iron sample.

To test the universality of the observed phenomenon of displacement of a grain boundary under shear deformation investigation of the behavior of metal with a BCC structure containing tilt grain boundaries was carried out. A sample of α-iron with grain boundaries $\Sigma5$ and $\Sigma9$ was modeled. Initially boundary $\Sigma5(120)[001]$ was generated. Similar to that described above algorithm was used to initialize the structure. At the first stage, necessary orientation of the crystal structure of the grains was set. Later the minimum energy of the simulated ensemble of atoms was located by the relative displacement of grains. Shift vector for grain boundary $\Sigma5$ was $\overrightarrow{t} = (1,28;0;0)$. Projection on the plane XoY of fragment of obtained equilibrium configuration of the crystal lattice of α-iron containing grain boundaries is shown in Figure 5. Velocity of the atoms of loaded layers was set equal to $20m/s$.

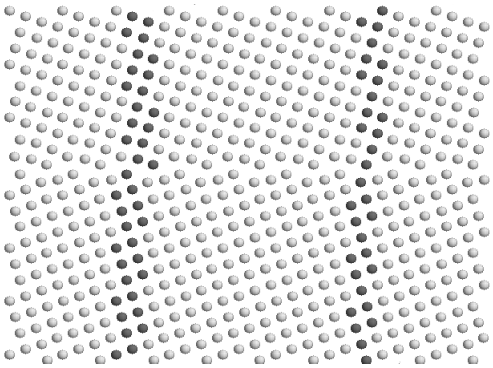


Figure 5: Projection of the structure of the sample of iron that contains grain boundary at time $t = 0ps$

The results show that the response of the simulated crystallite containing the boundary $\Sigma 5$, differs from previously investigated crystallites of Ni and Cu. According to the results, the external action of the shear loading initially only leads to elastic deformation of the crystal lattice outside the plane of the defect. Near the original position of the plane, defect formation of the crystal structure that is different from the initial one is observed. It is possible to select the layer thickness of 4-5 interatomic distances, where the arrangement of atoms close to the close-packed configuration. In Fig. 6a this layer highlighted by dashed lines. Figure 6b shows a fragment of three layers of the crystal structure parallel to the plane YoZ marked by numerals in Fig. 6a. This structure is a structure close to the FCC configuration of atoms.

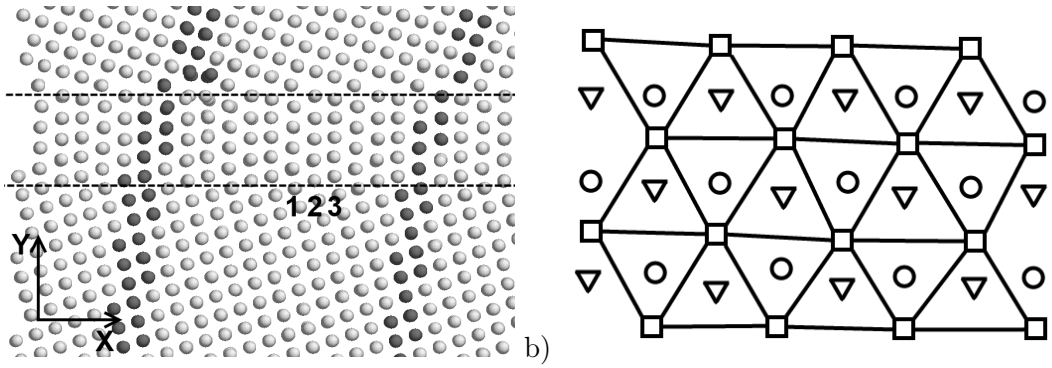


Figure 6: a) Projection of atoms of fragment of structure near the grain boundary on the plane XoY at the time $t = 60ps$; b) layer structure, taken in the plane YoZ, figures represent layers: the square – layer 1, circle – layer 2, triangle – layer 3

The observed crystal structure is non-equilibrium and on further loading of the sample its restructuring is observed. This is accompanied by a violation of the ordered structure near the grain boundaries is similar to that observed in the sample of copper with grain boundary $\Sigma 5$ at high temperatures of the sample or imperfect initial structure of boundary. After that, the grain boundary begins to moving in the direction perpendicular to the applied external loading. Analysis of the structure at different time points showed that, despite the disordered structure near the defect, the boundary moves uniformly with constant speed (Fig. 7), which is 1.2 times higher than the rate of external loading. The resulting configuration fragment of structure of the sample that contains grain boundaries after 200000 integration steps shown in Fig. 8.

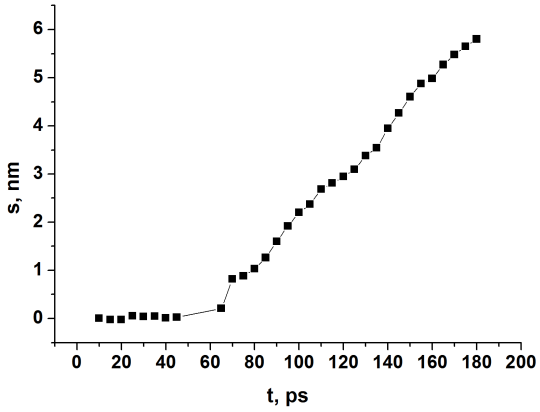


Figure 7: The dependence of the boundary displacement from the initial position of the time

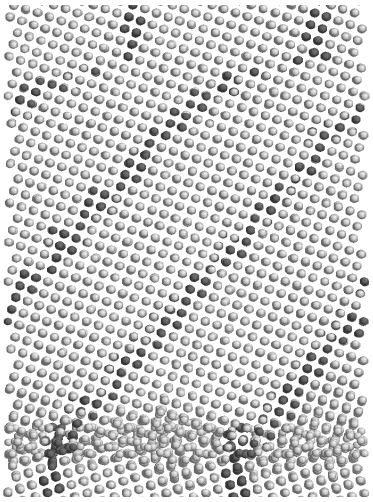


Figure 8: The structure of boundary at time $t = 200ps$

The next stage of research was to model the boundary Σ9. For this type of grain boundary vector of relative shift is $\overrightarrow{t} = (10,17576; 0,5325; 1,04988)$. Figure 9 shows the resulting structure of the boundary after a relative shift and the subsequent relaxation of the sample. Behavior of such a defect in iron similar to the behavior boundary Σ5 in FCC metals. As a result of deformation synchronous restructuring of the entire surface of the defect occurs, thereby resulting to the displacement of the boundary. At that the structure of the defect is not violated. The simulation results showed that under loading the boundary begins moving with constant speed (Fig. 10). Calculations showed that at overall rate of loaded layers of $40m/s$ boundary moves with a speed of $70m/s$.

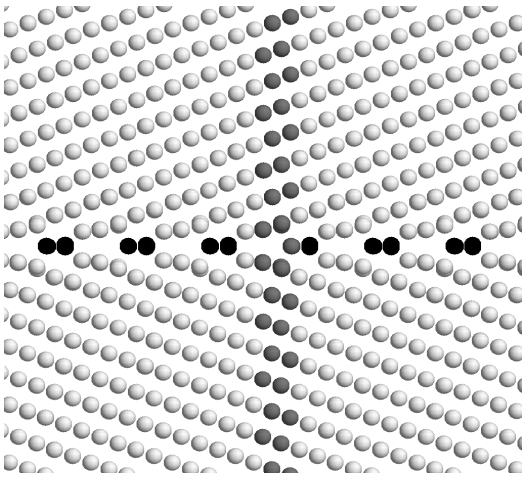


Figure 9: Projection of atoms of fragment of structure of grain boundaries Σ9 on the plane XoY

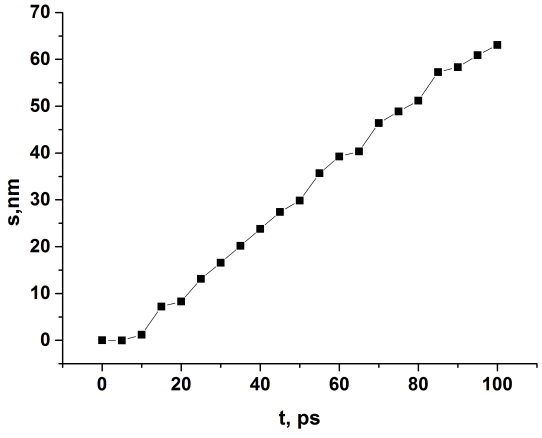


Figure 10: The dependence of the boundary displacement from the initial position of the time

5 Conclusions

Using computer simulations features of development of grain boundary sliding mechanism was discovered on the scale of individual atoms on the example of large angle tilt boundaries $\Sigma 5$ and $\Sigma 9$ in crystals of Ni and α-Fe. It is shown for the certain orientation of a grain boundary under shear loading grain boundary sliding may be accompanied by rearrangement of the atomic configuration in the plane the defect, which leads to efficient movement of position of the boundary in a direction perpendicular to the applied load. At that speed of displacement of the boundary can be several times higher than the rate of loading. During the research it was found that the dynamic properties of the boundary depends on the features of its structure and type of the crystal lattice. In particular, the "mobility" boundary $\Sigma 5$ under shear deformation disappears in the crystallite α-Fe, and vice versa – "fixed" boundary $\Sigma 9$ when changing the type of the lattice begins moving in the direction perpendicular to the applied loading. Note that in this paper we study only elementary grain boundary sliding mechanism that is realized on stage deformation. The influence of possible sources of resistance to movement in the direction of slip, such as triple junctions are not obviously taken into account. Nevertheless, these results can be used to understand features of plastic deformation polycrystals under dynamic loads.

Acknowledgements

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