Molecular dynamics study of the local frictional contact

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Abstract

In the paper simulation of the behavior of copper crystallite under local frictional contact was carried out using the method of molecular dynamics. Loading was realized by the movement of hard indenter along the surface of the sample. Following configurations were considered: initially defect-free crystallite, structure with a symmetrical tilt grain boundary $\Sigma 5$. Influence of the initial structure on the behavior of the crystallite under loading was analyzed. Nucleation of nanofragmentation of the surface layer was displayed. Atomic mechanisms of a process of nanofragmentation were investigated. A detailed analysis of the character of the atomic displacements in emerging blocks shown that they have a rotational nature. Further calculations showed that the amount of disorientation of formed nanoblocks along different directions is not more than 2 degrees. Despite what two limiting cases of arrangement grain boundaries in the material has been studied only, it can be assumed that the behavior of crystallites with defect disposed at an arbitrary angle relative to the free surface is a combination of processes that occur in these cases.

1 Introduction

In many modern applications the state of the surface layer, its hardness, wear resistance, mechanical behavior, processing quality and other characteristics are largely determine the performance properties of the various parts of machines. Therefore, the problem of studying the physical and mechanical properties of the surface and improve its performance by applying various treatment methods to pay close attention [1]. Despite the constant improvement of methods of experimental study, especially the evolution of structure in which these changes occur, are still poorly understood. These difficulties are caused by the simultaneous superposition of a large number of adverse factors occurring at different scales in contact area of the indenter with material surface. Effective solution to this problem, traceable in the modern literature is the use, in combination with experiment, different methods of numerical simulation. Molecular dynamics method still remains the main tool for the theoretical description of the behavior of the modeled system at the atomic scale. With the increasing performance of modern computing its contribution to the treasury of new knowledge acquiring is reinforced. New features allow us to study the

evolution of the atomic lattice under dynamic loading with the explicit consideration of the internal structure of the polycrystalline material. Thus, the purpose of the present study was to investigate with help of the method of molecular dynamics the characteristics of nucleation and development of structural defects in the crystalline material containing grain boundary under a localized loading conditions.

2 The model sample description

A fragment of polycrystalline copper, initially consisting of two grains separated by tilt grain boundary (GB) $\Sigma = 5(210)[001]$ was selected as an object of investigation. Two boundary position, along $X0Z$ and $Y0Z$ as shown in Fig. 1 were simulated. Note that early similar crystallite was used to investigate its behavior under shear loading as initially defect-free sample as well as containing the internal interface of various types [2, 3]. To describe the interatomic interaction the potential built in the framework of the embedded atom method was used [4, 5]. It was previously verified in a number of tests for the calculation of the elastic and energy characteristics.

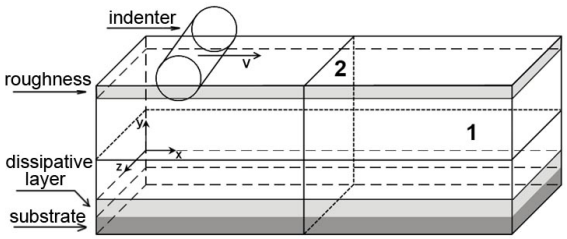

Figure 1: The scheme of the modeled sample.

Along the direction Z in a sample, periodic boundary conditions were set. Along the X-axis free surfaces were simulated. Thus, the considered sample can be represented as a single projection surface of an extended form (so-called pleated surface). The initial roughness of smaller scale was set additionally on the pleated surface. As a result surface stresses due to shear loading distributed unevenly and varied in different parts of the contact patch and further contributed to the redistribution of the local stresses and the formation of structural defects. The bottom layer of atoms (Figure 1) simulated unmovable substrate. Over the substrate a specific "damping" layer of atoms, which used the procedure reducing the kinetic energy was defined. By introducing of such a layer allow us to imitate the distribution of the kinetic energy deep into material along Y direction. The dimensions in the direction of the coordinate axes X, Y and Z were equal to $40.13 \times 24.95 \times 16.63$ nm, respectively. Total number of atoms exceeded 1500000. The equations of motion were integrated with a time step $\Delta t = 0,001$ ps.

Localized shear loading was applied by modeling the interaction of sample surface with microscopic counterbody, which acts as an absolutely rigid indenter. The indenter action has been realized through the force field described by the following formula $F(r) = K(r - R)^2$, where K – constant, r – distance from the center of the cylinder to the atom and the R – radius of the cylinder. At this at $r > R$ $F(r) = 0$. The sample was loaded with the indenter having a radius of 8 nm. The indenter

moved in X direction with a constant velocity $V = 10$ m/s, which is close to the maximal available rate of the surface finishing treatment.

3 Results of simulation

Within the first stage the position of $\Sigma 5$ grain boundary, was oriented parallel to a plane X0Z and located in the center of the crystallite (position 1 in Figure 1). To analyze the changing of the crystal lattice structure the algorithm which allows identifying the local topology of inter atomic bonds [6], and reveals the formation of structural defects was applied. The simulation results show that, due to the motion of indenter a lot of stacking faults produced in the bulk of grain. The presence of GB leads to contain the spread of a defect in the neighboring grains. It was also found that as a result of external shear loading the grain boundary starts moving in the direction perpendicular to the plane of the defect. This effect has been studied and described in [2]. Analysis of the structure at different times showed that the motion does not observed for all parts of the defect simultaneously. Parts of the boundary which is located in front and under the indenter move only. This leads to a curvature of the plane of the defect and its output to the free surface. Fig. 2 shows the change in the structure of the simulated sample when the GB under the influence of external localized load rises up to the free surface. The figure marked only the atoms, which local topology of structural relations is differ from the initial fcc lattice. It can be seen that the defects are concentrated in the upper grain. Only after grain boundary beyond the free surface (Figure 2d), structural defects are formed in the lower grain.

Figure 3a demonstrates the position of the grain boundary at different time steps. It is clearly seen that the profile of the border is distorted due to indenter motion. Moving in the direction of the free surface takes place only in the part of the boundary which is situated in front of and under the indenter. Thus, the farther is the part of the border from the initial position of the indenter along the X axis, the longer time it is subject to shear deformation and the greater distance in the direction perpendicular to the applied stresses, it is shifted. According to the results at time $t = 2.5 \times 10^6 \Delta t$ a part of the grain boundary beyond the free surface. After passing the indenter the position of this section of the border over time remains unchanged.

To verify the correlation between the loading direction and the GB structure the similar sample containing a tilt grain boundary $\Sigma 5$, which structure was mirrored relative to the plane of the defect as compared with the above example was simulated. Figure 4 shows the structure of the sample at the same time steps as in Figure 2. It can be seen that the plane of the defect in this case is less distorted. This is because the distance between the grain boundary and indenter increases due to motion of defect far from the free surface in a direction perpendicular to the applied loading. According to the initial distribution of structural defects depicted on the Fig. 4a some defects form in the grain, located below the GB. Closeness to free side surface leads to further annihilation of its (Fig. 4b). So, plural structural defects form only in the grain, which are directly exposed to the action of the indenter (Fig. 4c and 4d).

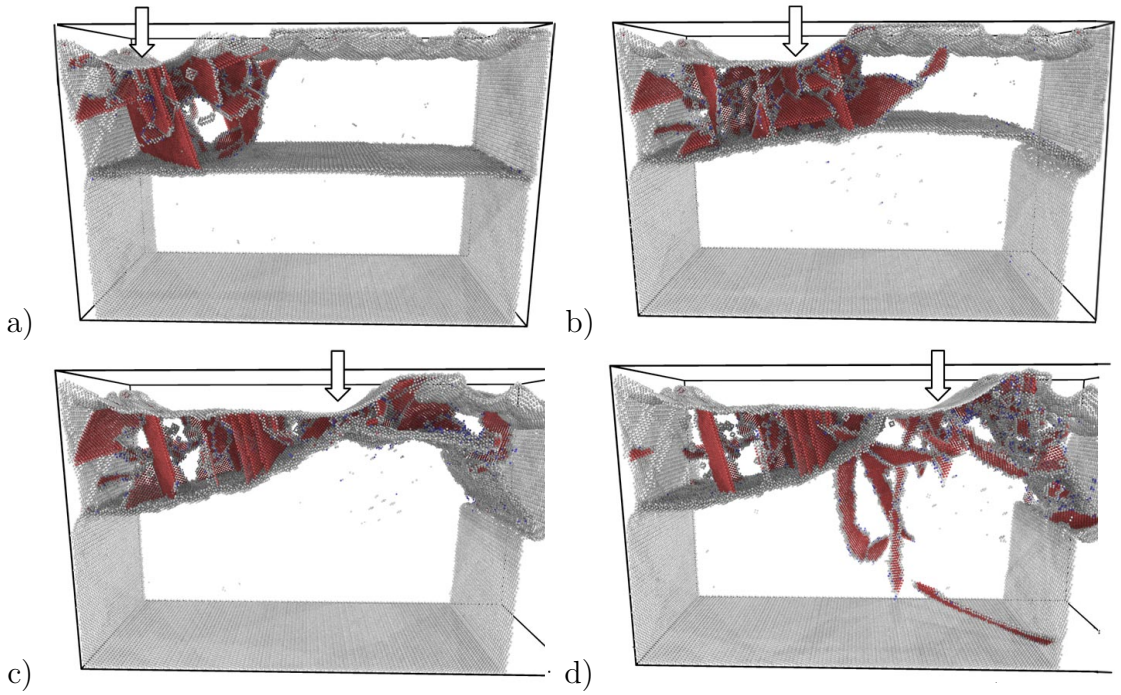

Figure 2: The structure of the modeled fragment at different time steps: a) 0.15 ns, b) 1.0 ns, c) 2.0 ns, d) 2.5 ns. Red spheres indicate position of atoms with hcp local topology of atoms relation; gray spheres depict atoms located at the border and close to GB. Hereafter arrows indicate the position of indenter.

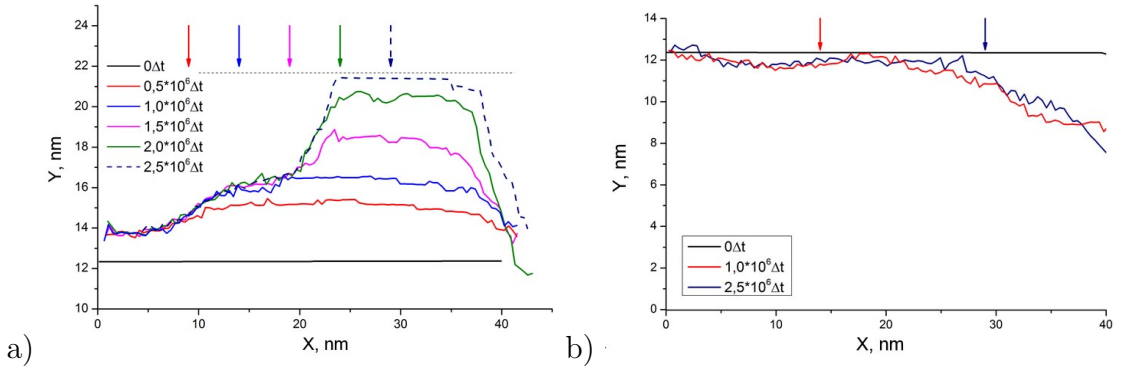

Figure 3: The projection of the grain boundary location on plane X0Y at different time step.

Figure 3b shows the position of the GB for the described case for two time steps: at the beginning and close to final of the loading. It is seen that in contrast to the previous configuration the resulting position of the grain boundary at the end of loading stage changes only slightly in a direction from the free surface to the substrate. The offset position of the boundary grows up as the distance of this part of the defect increases from the initial position of the indenter. This is due to the peculiarities of redistribution of stresses and strains during the formation of defects in the system containing the grain boundary. Subsequent movement to the grain boundary from free surface to the lower grain is constrained by the presence of a

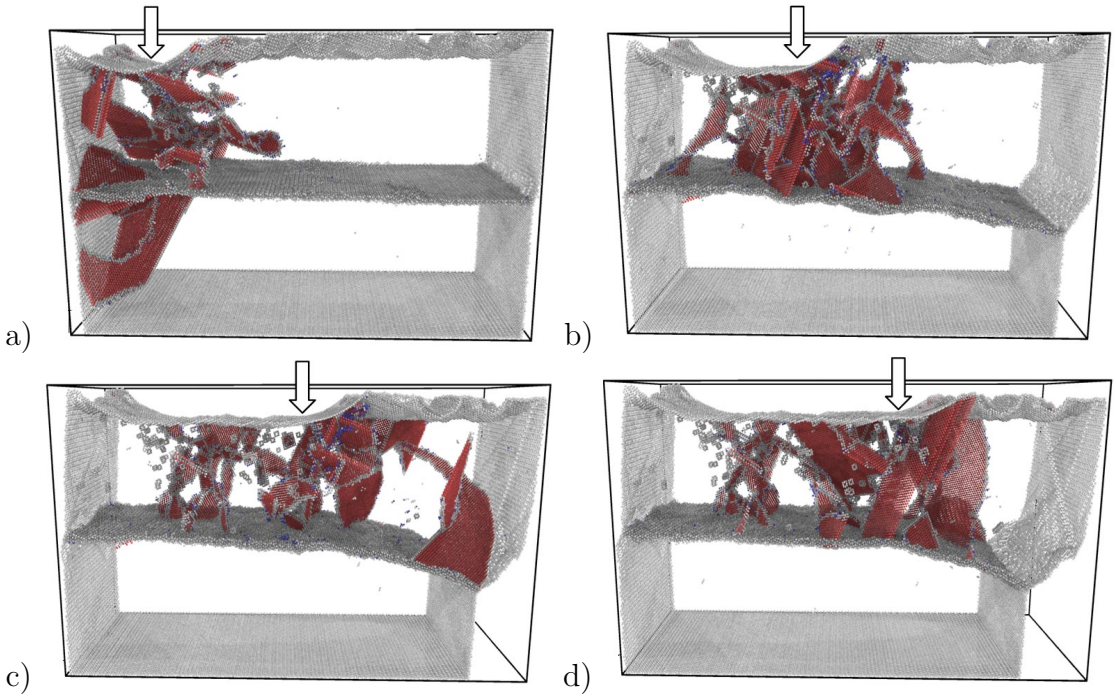

Figure 4: The structure of the modeled sample in which GB was mirrored relative to the plane of the defect as compared with the example shown in Fig. 2 at different time steps: a) 0.15 ns, b) 1.0 ns, c) 2.0 ns, d) 2.5 ns. Red spheres indicate position of atoms with hcp local topology of atoms relation; gray spheres depict atoms located at the border and close to grain boundary.

fixed substrate.

The results showed that for both sample configurations the local shear loading leads to formation of numerous structural defects in the volume of the loaded grain. This advantageously stacking faults. Formation numerous defects in the surface layer can also mean a possibility of surface nanofragmentation. In order to identify possible mechanisms leading to the formation of the fragmented structure of the material in the volume of loaded grain atomic displacements at different time intervals for the central layer of the sample were analyzed. The thickness of the selected layer was equal to three atomic planes and its orientation was parallel to the X0Y plane. Figure 5 shows the displacement of the atoms in the central layer of the bicrystal at the time moment near 0.5 ns and during the time interval of 50 ps. The structure of building blocks in the upper grain, located in the area close to the indenter is clearly visible.

A detailed analysis of the character of the atomic displacements in forming blocks showed that they can carry rotational type. Figure 5 shows enlarged view for one of the blocks forming in the structure. It is clearly seen that the block as a whole is rotated about an axis parallel to the direction Z. Further calculations showed that the value of such rotations along different directions for forming nanoblocks is no more than 2 degrees.

Similar conclusions can be done by analyzing the displacements of atoms for selected central layer in the subsequent time intervals, depicted in Figure 6.

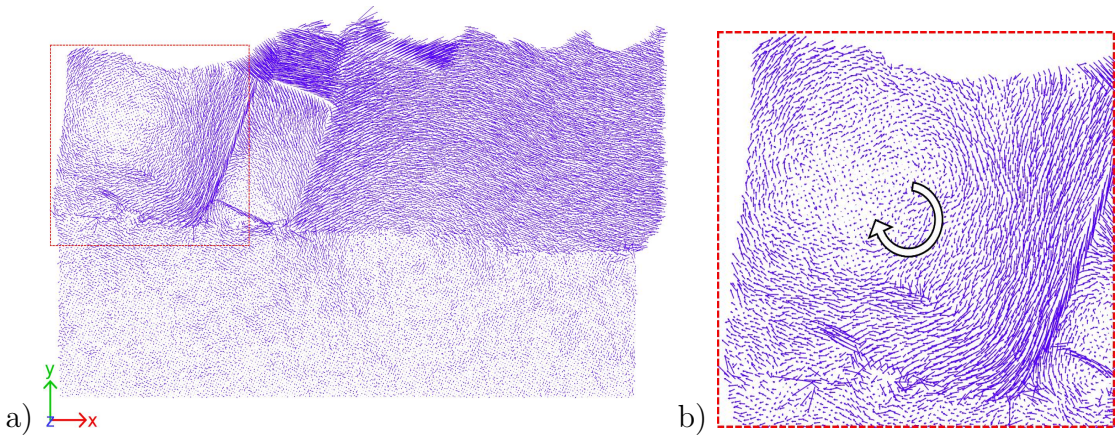

Figure 5: The map of displacements at the time interval $(0.50 - 0.55)$ ns for the atoms of the central cutting of the modeled bicrystal with the thickness of 3 atomic layers. The size of segments is increased up to 5 times for the better visualization. The arrow in zoomed fragment indicates the direction of rotation.

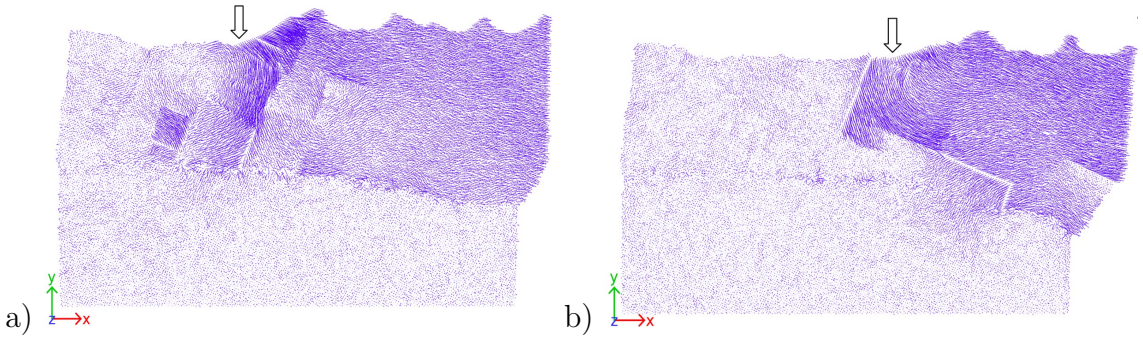

Figure 6: The map of displacements at different time intervals for the atoms of the central cutting layer of the modeled bicrystal with the thickness of 3 atomic layers: a) $(1.0 - 1.05)$ ns, b) $(2.0 - 2.05)$ ns. The size of segments is increased up to 5 times for the better visualization.

In the next stage of the research the sample in which the GB was located parallel to the plane Y0Z (position 2 in Figure 1) was generated. Simulation results have shown that the similar action of the indenter on the grain boundary movement along the X axis is not observed. The presence of GB, prevents to the spread of structural defects as in the previous case, but only until the time where the indenter locates at a quite far distance from the position of GB. When the indenter approaches the GB stacking faults occur in the next grain as well. The structures of the modeled fragment for the respective time steps are shown in Figure 7.

4 Conclusion

In conclusion, we note that the results of computer simulation on the scale of individual atoms revealed the mechanism of plastic deformation of a material with an internal structure in terms of the local shear loading. According to the results,

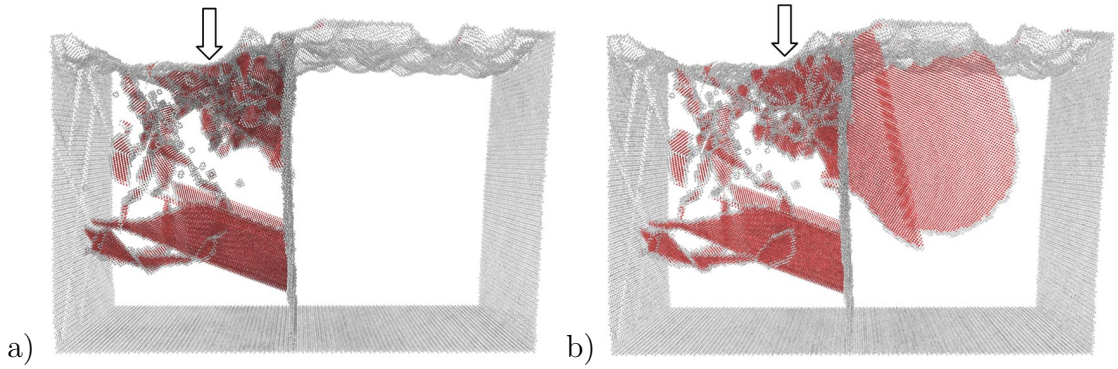

Figure 7: The structure of the modeled fragment with vertical orientation of the GB at different time steps: a) 0.8 ns, b) 0.9 ns. Red spheres indicate position of atoms with hcp local topology of atoms relation; gray spheres depict atoms located at the border and close to grain boundary.

this process can occur through the formation of multiple intersecting planar defects – stacking faults. This leads to the formation of separate fragments of nanoscale size separated by an interface between them. It was found that the displacements of atoms in forming of fragments can have rotational character. Thus, the resulting structure of the modified surface layer is the system of disoriented nanoblocks.

With the help of computer simulations it was shown that the presence of GB in the crystal can limits the propagation of defects into the volume of the sample under shear load and can lead to recrystallization of individual grains only. Despite what it has been studied only the two limiting cases of grain boundaries arrangement in the material, it can be assumed that the behavior of defective crystallites disposed at an arbitrary angle to the free surface is a combination of processes that occur in these cases.

The obtained results can be use as well to understand the process of nanostructuring of the surface during for example finishing treatment.

Acknowledgements

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