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MOLECULAR DYNAMICS MODELLING OF BOUNDARY MIGRATION IN BICRYSTALS UNDER NANOBURNISHING

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Abstract. The paper reports the molecular dynamics simulation results on the behavior of a copper crystallite in local frictional contact. The crystallite has a perfect defect-free structure and contains a high-angle grain boundary of type Σ5. The influence of the initial structure on the specimen behavior under loading was analyzed. It is shown that nanoblocks are formed in the subsurface layer. The atomic mechanism of nanofragmentation was studied. A detailed analysis of atomic displacements in the blocks showed that the displacements are rotational. Calculations revealed that the misorientation angle of formed nanoblocks along different directions does not exceed 2 degrees.

1 INTRODUCTION

The state of the surface layer, its hardness, wear resistance, strength properties, quality, and other characteristics are crucial for a whole range of modern applications. They to a large extent determine the operating properties of various machine components. That is why much attention is given to the investigation of physical and mechanical properties of the surface and improvement of its properties by various treatment methods [1, 2]. Despite continuous improvement of experimental methods, the structural evolution features that accompany these improvements are still poorly explored. The difficulties are due to the simultaneous effect of a large number of different-scale secondary factors occurring in contact between the indenter and indented material. Today this problem is efficiently solved using various numerical simulation methods combined with experiment. The molecular dynamics method remains the main tool for the solution of atomic-scale problems which theoretically describes the simulated system behaviour. With the increasing performance of modern computing systems, the molecular dynamics method greatly contributes to the generation of new knowledge. It

has become possible to study the evolution of the atomic subsystem under dynamic loading with an explicit representation of the internal structure of a polycrystalline material.

The objective of this work is to study the generation and development of structural defects in a crystalline material with a grain boundary under localized surface plastic deformation. To achieve this, the numerical modelling of the nanostructuring burnishing process was undertaken with help of molecular dynamics method.

2 NUMERICAL MODEL

The object of investigation was a fragment of a copper polycrystalline that initially consisted of two grains divided by a planar defect such as a high-angle boundary of special type $\Sigma = 5$ (210)[001]. Two positions of the boundary along X0Z and Y0Z were simulated (Fig. 1). The copper polycrystalline was chosen because we have accumulated experience in simulating this metal both in the initial defect-free state and with internal interfaces of different types [3, 4]. Interatomic interaction was described using an interatomic potential calculated in the framework of the embedded atom method, which had earlier been verified in test problems on the calculation of elastic and energy characteristics [5, 6].

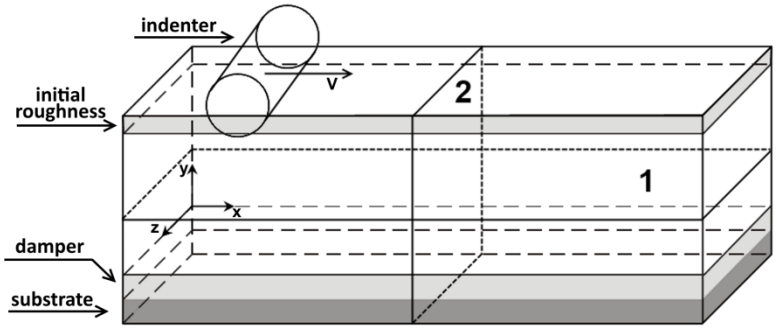

Figure 1: Schematic of the simulated specimen

Periodic boundary conditions were given along the Z axis, and the free surfaces were simulated along the X axis. The simulated specimen was thus a single elongated asperity on the surface (a fold on the surface). The microasperity had smaller-scale roughness on its surface, owing to which stresses arising in the crystallite under localized shear loading were not distributed uniformly but varied in different contact spot areas, which favored local stress redistribution and structural defect generation. The lower atomic layer imitated the substrate (Fig. 1). A special "damping" atomic layer was placed above the substrate for which a procedure of kinetic energy reduction was used. Using the layer that absorbs kinetic energy allowed us to simulate energy propagation deep into the material bulk along the Y axis. The simulated specimen measured 40.13×24.95×16.63 nm along the coordinate axes. The total number of atoms exceeded 1 500 000. Motion equations were integrated with the time step $\Delta t = 0.001$ ps.

Localized shear loading was performed by simulating contact between the microasperity surface and a counterbody that was an absolutely rigid indenter. The action of the indenter was simulated by a force field and described by the formula $F(r) = –K(r-R)2$, where K is the constant, r is the distance from the cylinder center to an atom, R is the cylinder radius, and

F(r) = 0 at r > R. The simulated material was loaded by an indenter of radius 8 nm. The motion of the indenter was simulated along the X axis at the constant speed V = 10 m/s, which is close to speed limits in surface finishing.

3 RESULTS OF SIMULATION

First we considered a specimen with a grain boundary of type Σ5 lying in the X0Z plane in the middle of the crystallite (position 1 in Fig. 1). The crystal lattice structure was analyzed using a common neighbor analysis [4, 7] which reveals the formation of structural defects. The simulation results showed that the motion of a microasperity on the counterbody surface causes the formation of numerous stacking faults in the grain bulk. The grain boundary inhibits the defect propagation to the neighboring grain. External shear loading makes the grain boundary to move along the direction perpendicular to the plane of the defect. This effect was studied and described by Dmitriev et al. [8]. Analysis of the structure at different points of time showed that the boundary motion is not simultaneous. Parts of the grain boundary which located in front and under the indenter are 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 the grain boundary beyond the free surface (Figure 2d), structural defects are formed in the lower grain.

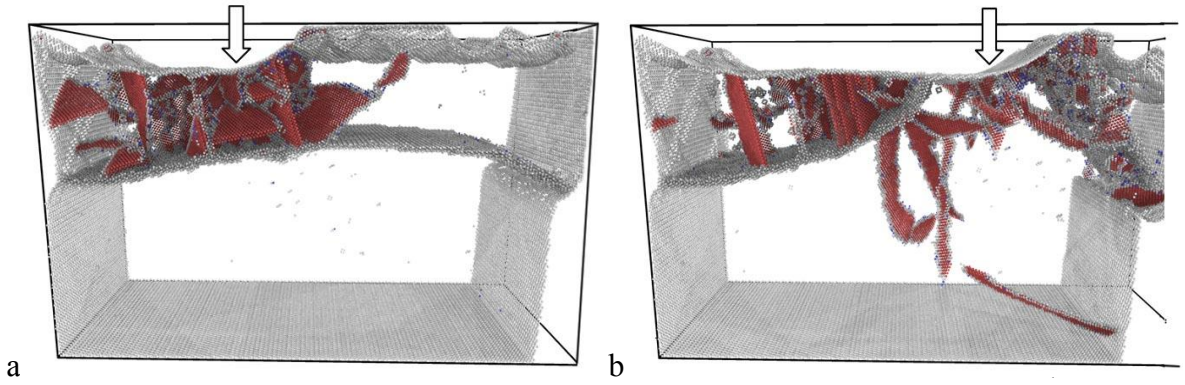

Figure 2: The structure of the modeled fragment at two consecutive time steps: a) 1.0 ns, b) 2.5 ns. Hereafter atoms with hcp local topology of atoms relation are marked by red; gray color depicts atoms located at the border and close to the GB. Blue spheres denote atoms with undetermined local topology.

Figure 3a illustrates the grain boundary position at different points of time. It is clearly seen that the boundary profile is distorted with the passage of the indenter. The only part of the boundary that moves to the free surface is in front of and beneath the indenter. The farther from the initial position of the indenter is a part of the boundary along the X axis, the longer is the period of its shear deformation and the larger is the distance to which it is shifted in the direction perpendicular to the applied load. According to the obtained results, a part of the grain boundary reaches the free surface at the time point t = 2.5×106Δt. After the passage of the indenter the position of this part of the boundary does not change with time.

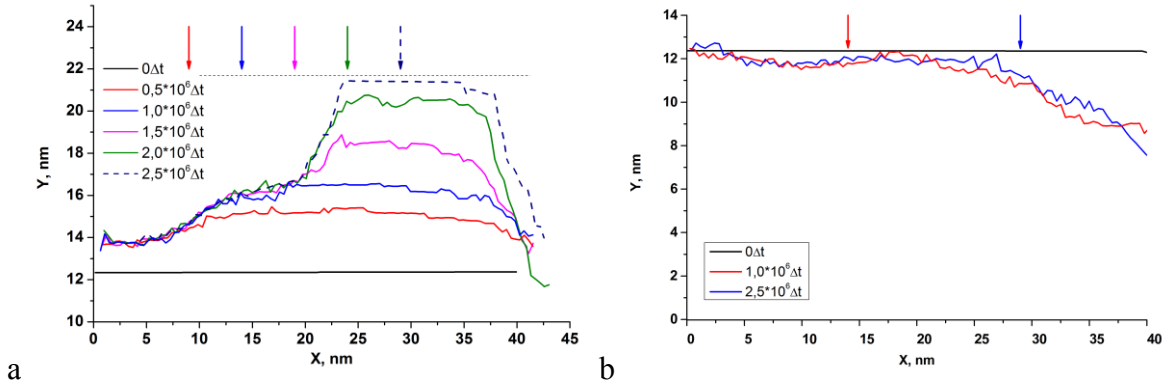

Figure 3: Grain boundary position at different points of time. Arrows indicate the position of indeter for the selected time step.

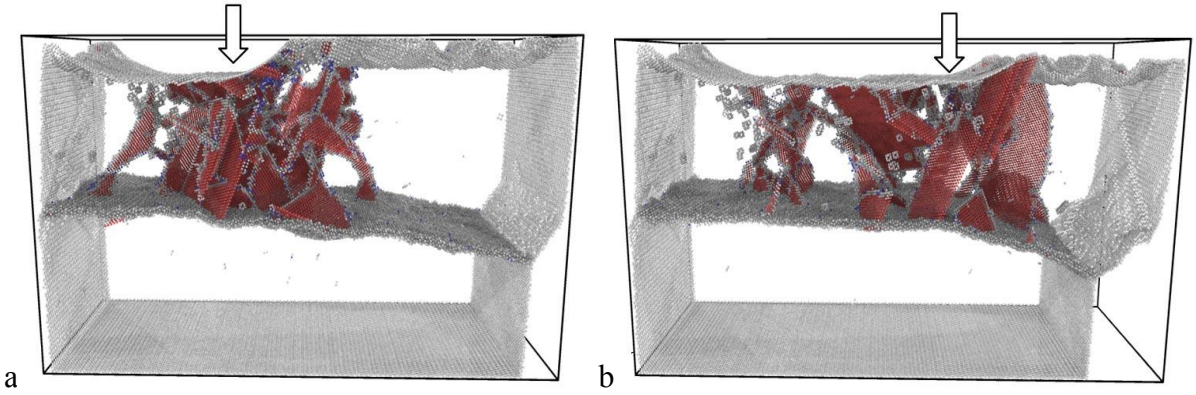

Figure 4: The structure of the modeled sample in which GB was mirrored relative to the plane of the defect as compared with the example shown in Fig. 2 at two consecutive time steps: a) 1.0 ns, b) 2.5 ns.

In order to verify the influence of the loading direction with respect to the boundary structure, we simulated a specimen with a grain boundary of special type Σ5 whose structure was mirrored relative to the plane of the defect as compared to the above example. Two variants were studied: 1) sample with the same geometry and 2) the sample where the bottom grain was increased twice to avoid the influence of substrate. Figure 4 shows the structure of the sample (1) 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). The similar conclusion can be done for the sample (2) shown in Figure 5.

Figure 3b illustrates the grain boundary position for this case at an initial and final time point. Unlike the previous case, the resultant displacement of the boundary towards the substrate from the free surface changes insignificantly on the first stage. The boundary

displacement increases with distance from this region with respect to the initial position of the indenter. This is related to specific stress and strain redistribution during the formation of a system of defects in the loaded grain. Subsequent motion of the boundary to the surface of the lower grain is impeded by the fixed substrate.

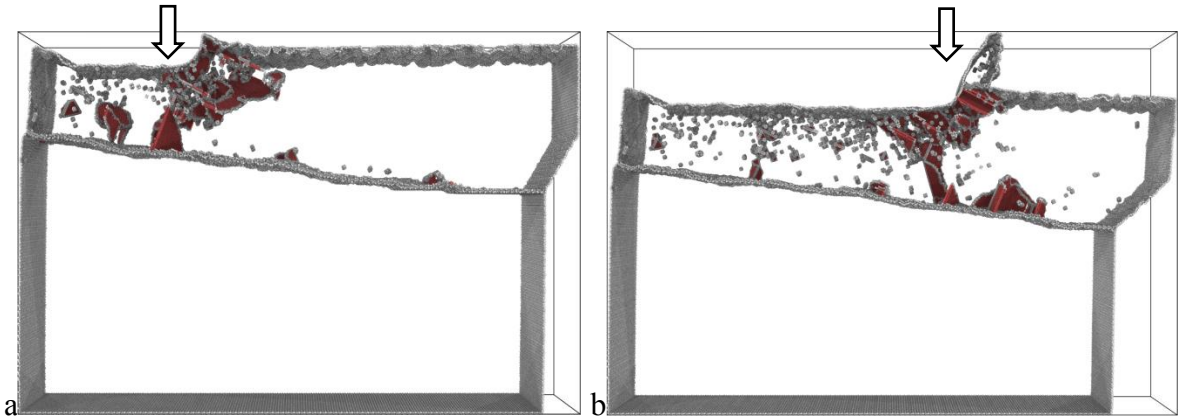

Figure 5: The structure of the modeled sample with increased bottom grain at two consecutive time steps: a) 2.0 ns, b) 5.0 ns.

The simulation results showed that for the both considered specimen configurations numerous structural defects are generated in the grain bulk under local shear loading. These are mostly stacking faults. The formation of numerous defects in the surface layer can also be indicative of possible surface nanofragmentation and nanoblock structure formation. 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. Atomic displacements in the middle layer of the bicrystal in the time interval 50 ps close to t = 0.5 ns are represented in Fig. 6. One can clearly see the structure of formed blocks in the upper grain deformed by the indenter.

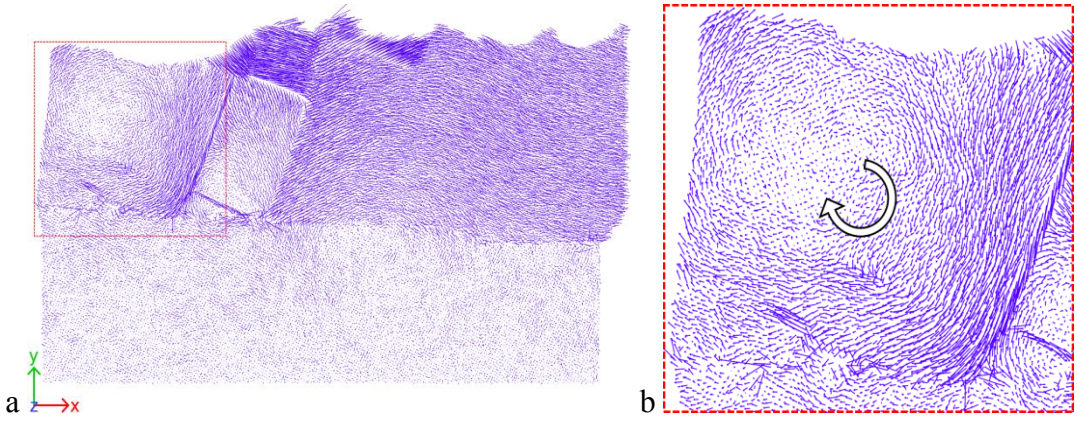

Figure 6: The map of displacements at the time interval (0.50 - 0.55) ns for the atoms of the central cutting of the modeled bicrystal with the thickness of 3 atomic layers. Hereafter the size of segments is increased up to 5 times for the better visualization. The arrow in zoomed fragment indicates the direction of rotation.

A detailed analysis of atomic displacements in the formed blocks showed that they can be rotational. Figure 6 gives a magnified image of a formed structural block. The block is seen to rotate as a whole about the axis parallel to the Z direction. Further calculations revealed that the angle of rotation along different directions for formed blocks 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 as depicted in Figure 7.

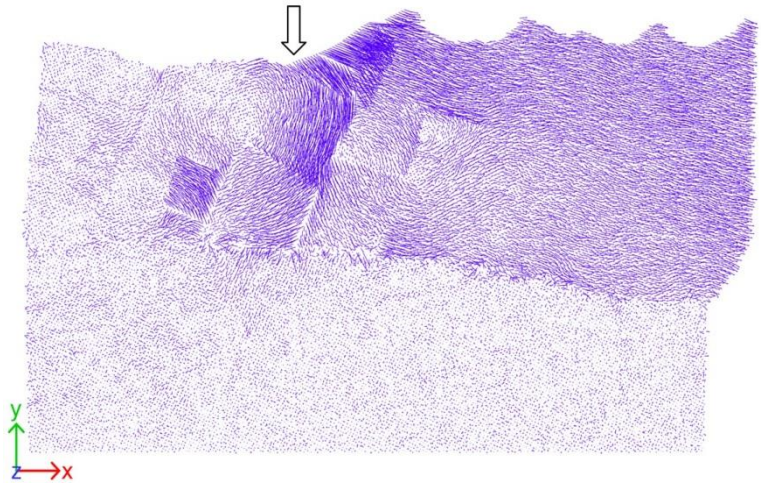

Figure 7: The map of displacements at the time interval (1.0 - 1.05) ns for the atoms of the central cutting layer of the modeled bicrystal with the thickness of 3 atomic layers. The size of segments is increased up to 5 times for the better visualization.

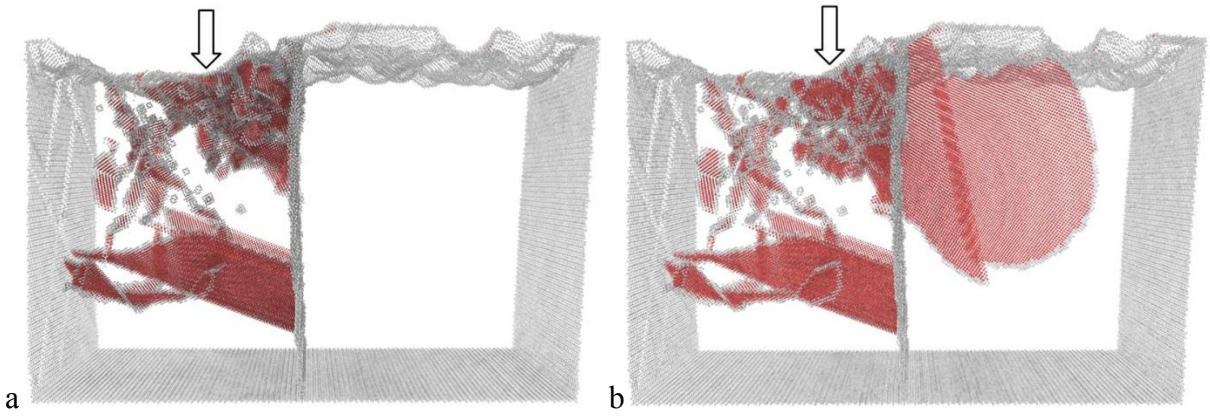

Figure 8: The structure of the modeled fragment with vertical orientation of the GB at different time steps: a) 0.8 ns, b) 0.9 ns. Red spheres indicate position of atoms with hcp local topology of atoms relation; gray spheres depict atoms located at the border and close to grain boundary.

On the next stage we simulated a specimen with a grain boundary oriented parallel to the Y0Z plane (position 2 in Fig. 1). In this case, no grain boundary displacement along the X axis was observed under the action of the counterbody microasperity. The presence of the grain boundary, like in the previous cease, inhibits the propagation of structural defects, but only until the indenter is at a sufficient distance from the boundary plane. When the indenter

approaches the grain boundary, stacking faults are also formed in the distant (relative to the loaded) grain. The structures of the modeled fragment for the respective time steps are shown in Figure 8.

5 CONCLUSION

The computer simulation performed on the scale of single atoms revealed plastic deformation mechanisms in a material with internal structure under local shear loading. According to the obtained results, plastic deformation can occur through the formation of a system of numerous intersecting planar defects such as stacking faults. This leads to the formation of individual material nanofragments divided by an interfacial layer. Atomic displacements in the formed fragments can be rotational. The resultant structure of the modified surface layer is a system of misoriented nanoblocks.

Simulation showed that the presence of a grain boundary in the crystallite inhibits defect propagation to the specimen bulk under shear loading and can induce recrystallization of individual grains only. Despite only two limiting cases of grain boundary orientation were considered, it can be suggested that the behavior of a crystallite with a defect oriented at an arbitrary angle to the free surface is a combination of processes occurring in the studied cases.

Additionally, the obtained results can be used to explain features of surface layer nanostructuring in final burnishing.

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