Modeling of Behavior of Crystallite with Interface under 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 $\Sigma 5$ (oriented along and perpendicular to the loading direction) and with interface between different materials. 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. It was shown that the presence of grain boundary prevents extension of defects in sample. In case of modelling of interface between Cu and Fe processes are taken place near the interface were analyzed.

1 Introduction

Problems of description of the behavior of the material near the interface have always attracted the attention of engineers, materials scientists, experts in the field of physics and chemistry. This is not only the importance of enhancing fundamental knowledge regarding this complex interdisciplinary field of research, but the significance of their practical applications, especially in the various branches of engineering. In this paper a study in the framework of molecular dynamics of processes occurring near the free surface with the initial roughness during contact of the sample with microasperity of counter-body was carry out. Previously, similar studies have been performed for single crystals of copper and α-iron [1]. It was shown that in the surface layer material under conditions of simulated types of load numerous surface defects developed. It has been established that the depth distribution and the concentration of defects associated with the size of the loaded part of the microasperity. Furthermore, it was shown that the formation of defects in the surface layer leads, furthermore, to generate individual grains, misoriented with respect to each other. Obvious that in reality, the internal structure of the material is far from the ideal structure of a defect-free single crystals. It contains both multiple local structural defects and a large number of interfaces. It is especially actual near the free surface, where there is a possibility of restructuring of the atomic lattice due to redistribution of the excess volume [2]. In this paper, using molecular dynamics simulations we investigate the influence of internal interfaces (grain boundaries and the interface of dissimilar materials) on the development of structural defects in the bulk of the sample near the free surface with an initial roughness under frictional contact of sample with microasperity of counter-body. We consider various options for the location of the grain boundary and interface.

2 Numerical model

Research was conducted in the framework of molecular dynamics method using the software package LAMMPS [3]. The copper crystal containing planar inner interface, which in the first series of calculations was a tilt grain boundaries $\Sigma 5$, was considered as the simulated sample. The tilt grain boundary was modelled using Coincidence Site Lattice (CSL) principle. The structure of the defect created by setting the specific orientations of the crystal lattices of each of the grains. In the second part of the computing the interface is an interface of contacting metals Cu-Fe. Initial roughness is in both cases the depth of 2nm was set by removing part of the atoms of the surface layer. Periodic boundary conditions were along the Z-direction The bottom layer of atoms (Fig. 1) was fixed. Over the substrate layer a special heat dissipation layer was modeled to simulate a length of the sample in the direction of the axis Y. The interaction between atoms was described within the embedded atom method [4]. The total number of atoms was about 880000 in case of modelling interface between Cu and Fe and 1300000 in case of modelling copper crystal with grain boundary. 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 $\Delta t = 0.001ps$.

Field indenter of cylindrical shape with radius $4nm$ and the axis along the axis Z was used as a counter-body microasperity. The force acting in the direction from the cylinder axis on the atoms falling within the area indenter. Value of the force is described by $F(r) = -K(r-R)^2$, where K - constant, r - distance from center of cylinder to the atom, and R - the radius of the cylinder, and at $r > R$ $F(r) = 0$. The speed of movement of the indenter in the X direction was $10m/s$. Indenter was immersed in the sample to a depth of $3nm$.

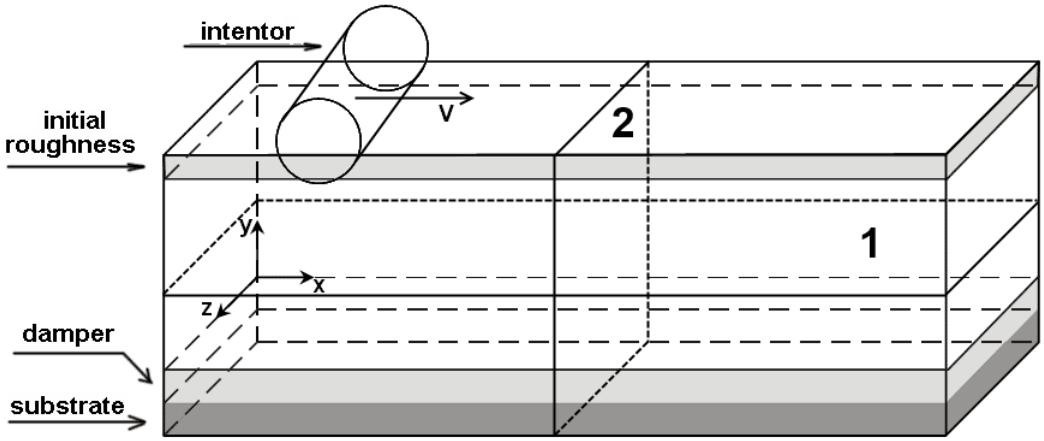


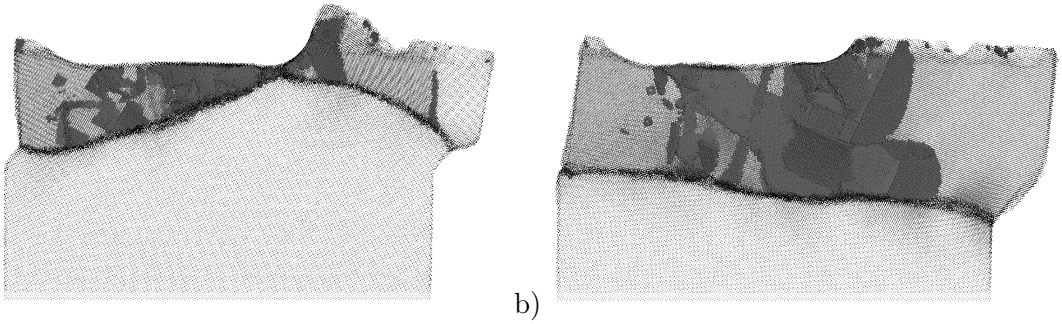
Figure 1: Schematic representation of the simulated sample

3 Behavior of the sample with the tilt grain boundary

Originally a sample with grain boundary type $\Sigma 5$, located in plane XoZ in the center of crystallite (position 1 in Figure 1) was considered. The simulation results showed that due to movement of microasperity counter-body a plurality of stacking faults formed in volume of the grain. The presence of grain boundary leads to contain the spread of a defect in the neighboring grain. It was also found that as a result the external shear load

grain boundary starts moving in the direction perpendicular to the plane of the defect. This effect has been studied and described previously [5]. The essence of the effect is the following. In conditions of the shear deformation occurs heightening of atomic layers of a grain, due to the involvement of atoms in contact with the plane of the boundary and initially owned the opposite grain. This leads to the growth of one of the grain and the displacement of boundary. Analysis of the structure at different times showed that the movement of boundary does not occur at the same time. Only the part of the boundary is moving, which is in front of the indenter. This leads to a curvature of the plane of the defect and its outlet at the free surface. Fig. 2a shows the structure of the sample on the projection plane XoY at the time when the grain boundary under the influence of an external load rises to the surface. It can be seen that the defects are concentrated in the upper structure portion of the sample that was formerly a single grain.

To test the effect of loading direction with respect to the structure of boundary in the work sample containing grain boundaries of a special type $\Sigma 5$, whose structure was mirrored relative to the plane of the defect as compared with the example described above was modeled. Fig.2b shows the structure the sample at the same time as shown in Fig.2a. It can be seen that the plane of the defect in this case is less deformed, and the movement of a grain boundary in a direction perpendicular to the applied load is limited by the influence of atoms on the substrate of sample.



a) b)

Figure 2: Projection of atoms onto the plane XoY. Large gray dots indicate atoms with fcc structure, black - atoms at the surface and at the grain boundary

At the next stage of the research sample in which grain boundary was located parallel to the plane YoZ (position 2 in Figure 1) was generated. The simulation results showed that under the action of microasperity displacement of the boundary along the Y axis is not observed. The boundary, as in the previous case, prevent the spread of the defects, but until the microasperity is at a distance from the boundary (Fig. 3). At the approach of the indenter to grain boundary stacking faults arise in both grains of sample.

Thus, via computer simulation, it was shown that the presence of grain boundary in the crystallite limits the spread of defects in the sample volume under shear loading conditions, and can lead to recrystallization of the individual grains. Although it has been studied only the two limiting cases arrangement of grain boundaries in the material, it can be assumed that the behavior of the defect located at an arbitrary angle to the free surface is a combination of processes that occur in these cases.

4 Behavior of the sample with the interface Cu-Fe

The next stage of research was to model the behavior of the sample consisting of metals of different sorts under conditions of shear loading caused by the motion a microasperity of

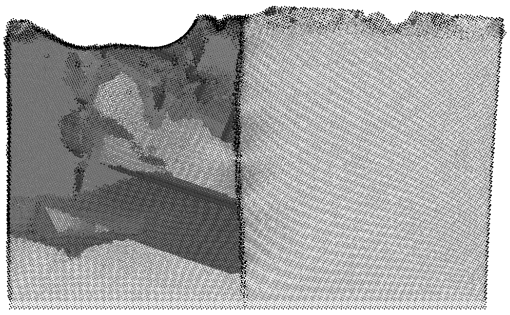
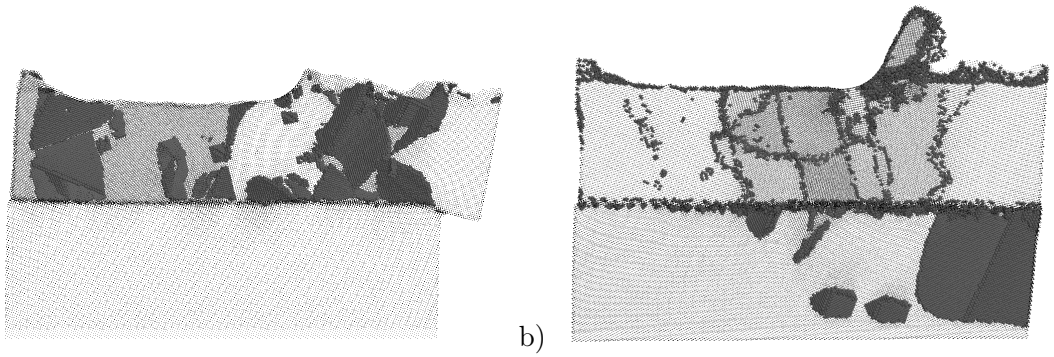


Figure 3: The projection of atoms of the structure with a vertical grain boundary on the plane XoY

counter-body. We consider the planar conjugation initially defect-free crystallites of copper and alpha-iron. The structure of copper part of the sample coincides with the structure of copper crystallite discussed in earlier, when the grain boundaries was oriented parallel to the plane XoZ (position 1 in Figure 1). Crystallographic orientation of bcc crystallite was a mirror image of orientation of the copper fragment with respect to the interface.

Initially, the sample was considered in which the crystals of alpha-iron has been located near the substrate. The simulation results showed that due to the impact a microasperity counter-body structural defects are formed only in the copper crystals. Forming a plurality of defects leads to nanofragmentation of the copper fragment. Fig.4a shows the structure of the sample at time 2ns. In the illustration atoms with bcc and fcc structure marked with small dots. Atoms with local hcp structure — large gray dots. Other atoms вЂ“ black. It is seen that disturbances in the structure are formed only in the copper crystal. Displacement of part of the copper crystallite outside of iron crystallite due to the use of free boundary conditions along the direction of shear loading.

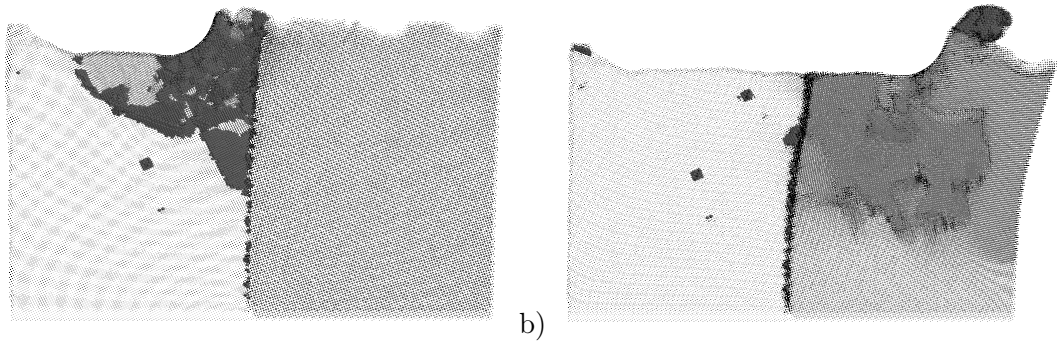
In the case where the sample surface is an iron crystal and copper crystal is located near the substrate defects is initially formed only in the iron crystal. However, stress caused in the structure by indenter passage leads to the formation of defects in crystals of copper. Fig.4b shows the structure of a modeled sample at time $2ns$. Here large dots marked not only atoms with hcp structure, but with a structure close to the bcc. Analysis of the crystal lattice near these atoms showed that this structure is observed near dislocations in bcc lattices. As in the case of copper, the occurrence of dislocation caused to the formation of fragments in which the orientation of the crystal lattice differs by $1-2$ degrees. Fig.4b this fragment visible in the upper center of the crystallite.



a) b)

Figure 4: The structure of the sample at a time $2ns$. The top crystal is a) copper; b) α-iron

Later the sample with an interface which is perpendicular to the free surface (position 2 in Figure 1) was simulated. Crystallites are arranged so that the initially indenter is passed on the copper surface and then the iron fragment. The results showed that, as in the case of the grain boundary in copper resulting structural defects do not pass through the interface. Fig.5a shows a sample at time $0.9ns$. Defects are observed only in the left part of the sample. At the approach of a microasperity of counter-body to the interface defects start to form in crystals of iron. It is interesting to note that after the removal of stress in the copper almost all of the defects have disappeared. This is clearly seen in Fig.5b. It is seen that in a copper crystal were only minor areas where atomic structure differs from fcc.



a) b)

Figure 5: The structure of the sample with a vertical interface at a time a) 0,9ns; b) 2,6ns

5 Conclusions

The main results are the following:

- behavior of copper crystallite with tilt grain boundaries Σ5 under conditions of localized shear loading generally identical to the previously described results [3]. When orientation of boundary parallel to the direction of loading rearrangement of the atomic structure can occur in the crystallite near the plane of the defect, followed by displacement of boundary position in the direction perpendicular to the loading. The difference is in the location of the shear load that causes curvature of the plane of the grain boundary. As shown by simulation results, a consequence of this behavior is the output of the grain boundary on the free surface.

- the presence of the grain boundary contain the spread of structural defects caused by localized shear deformation within the loaded grains. This is true for both the intergranular boundary arranged parallel to the loading direction and the perpendicular orientation of the boundary.

- in case of simulation interface of two different metals possibility of propagation defects in the neighboring crystallites depends on which material is exposed to shear strain. In the case of low-melting metal, structural defects are localized in its volume. In the case of refractory metal structural defects may also spread to the other side of the inner interface.

- research results can be used for understanding the development of plastic deformation near the surface of polycrystalline materials.

Acknowledgements

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