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THE FEATURES OF STRUCTURE TRANSFORMATION CAUSED BY NANO-BURNISHING PROCESS

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In the paper the method of molecular dynamics is used to investigate the features of structure transformation, which are taking place during the process of surface treatment. The force field of a cylindrical shape was used to imitate the motion with constant velocity of hard indenter. The following parameters of tasks were varied: the radius of indenter, initial immersion depths, surface roughness, number of passes and the initial position of the indenter. Calculations were performed for the pure crystallites of copper and iron. According to the modeling the treatment of the surface layer can leads to formation of numerous structural defects, which can provide effect of nano-fragmentation of material near the surface. A comparison of surface topography before and after treatment was analyzed also. Results of our study are in good agreement with experimental data.

Keywords: molecular dynamics, structure transformation, nano-burnishing.

1. Introduction

Performance properties of various assemblies and machine components are determined by the qualitative characteristics of the surface layer, obtained during the finishing processing. One of the modern efficient techniques of finishing processing surface of parts in mechanical engineering is a method of surface plastic deformation, which is called burnishing. Established that processing of surfaces by the burnishing can improve the wear resistance of parts by 20-40%, fatigue resistance by 30-70%, resistance to contact fatigue by 20-40% [1]. Changing the properties burnished surfaces is connected with the change in the structure of a thin surface layer owing to plastic deformation. Under the influence of the indenter of burnishing tool a change of orientation and shape of grains, which are crushed, flattened and stretched, forming the texture of the surface layer is occur [2].

Investigation of the structural changes occurring in the surface layer of material directly in the process of burnishing, it is extremely difficult. In this regard, methods for the numerical simulation can be an important complement to experimental studies. However, models based on the methods of continuum mechanics do not allow us to completely reveal the mechanisms of structural rearrangements in the surface layer of the material. Therefore, the purpose of this research was to study the origin and development of structural defects in the modeling of nano-burnishing process by molecular dynamics method [3, 4].

2. The object under simulation

As a model material for studying features of the process nano-burnishing was chosen a copper crystal. Selecting an object of investigation is caused by available expertise of simulation of such material and using previously verified the interatomic potential constructed within the embedded-atom method [4, 5]. This potential describes with a high degree of accuracy the

elastic and surface properties, and energy parameters of the defects of the modeled system. The equations of motion were integrated with time step Δt = $0,001$ ps. The calculations were performed on a multiprocessor cluster Skif Cyberia using a software package LAMMPS [6]. The total number of atoms exceeds 1.5 million. The simulated crystal was oriented in such a way that the crystallographic directions [100] [010] and [001] fcc lattice match the X, Y and Z. Dimensions of the model sample in the direction of the coordinate axes were equal to $40.13 \times 24.95 \times 16.63$ nm, respectively.

Schematic representation of the model sample is shown in Figure 1. At the initial stage in the simulated crystallite the roughness of the surface layer with a maximum depth of 2.5 nm is explicitly specified. The initial roughness was created by the removal of surface-layer atoms that situated within the sphere of radius, which ranged from 0 to 2.5 nm. Center of the sphere was located at the level of initial surface layer, and its position in the plane XoZ determined using random numbers. In the Z direction were simulated periodic boundary conditions, repetitive simulated fragment and, thus, allowing to simulate the length of the sample in a given direction. The rest of the surfaces (along the X and Y) were simulated as free. The lower layer of atoms (dark bottom layer in Figure 1) was fixed, simulating the substrate. Thickness of the substrate was 0.73 nm. Over a layer of substrate was set a special "damping" layer of atoms, where the procedure to reduce the kinetic energy accumulated due to dynamic loading was used. Using the layer with the properties removing of heat simulates the length of the model sample in depth of the material in the direction of the axis Y. The thickness of the "damping" layer was 1.45 nm. His kinetic temperature - the temperature obtained from the equality of thermal and kinetic energy, was maintained in the range from 125K to 135K.

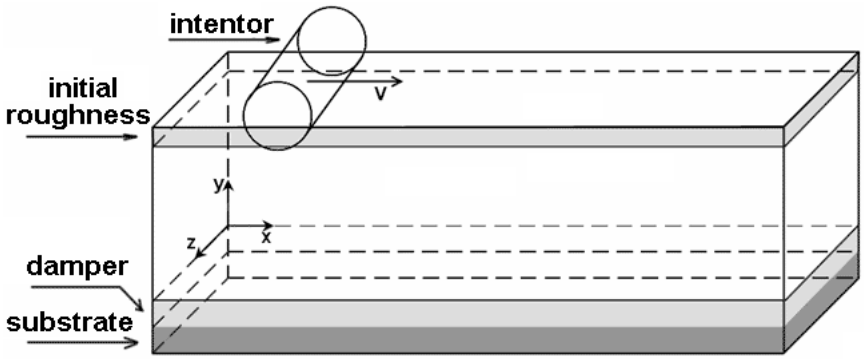


Fig. 1. Schematic presentation of the simulated sample.

Process of burnishing was performed using an indenter, whose action has been realized through the force field in the shape of the cylinder with certain radius and the axis along the axis Z. Forces acted on the atoms that situated into this area in the direction of the axis of the cylinder. The direction and magnitude of the force is described by $F(r) = -K(r - R)^2$ where K – constant, r – distance from the center of the cylinder to the atom, and R – radius of the cylinder, while at r $>$ R $F(r) = 0$. The process of burnishing the model material was carried out using two indenters with radii differ by 4 times: 4 nm and 16 nm.

3. Burnishing by the indenter with a radius of 4 nm

The simulation results showed that the process nano-burnishing with a radius of cylindrical indenter 4 nm on a small spatial interval resembles the process of cutting or scratching. When the horizontal movement of the indenter in front of it the bulge of the atoms of the upper

layer formed. As it moves, the height of the bulge is growing. This is clearly seen in Fig. 2 and Fig. 3, which show the topography at different times of a single central layer of atoms arranged in parallel planes XoY and the structure of the simulated crystallite with at time t = 2 ns. Arrows indicate the position of the axis of the cylindrical indenter at a given time. If we compare the surface profile before and after the passage of the indenter (for example, in Fig. 2 profiles at t = 0 and t = 2 ns), we can see that the characteristic size of the roughness of the surface layer decrease markedly. The difference in the scale reaches the same order as that for data sizes of the simulated pattern may be interpreted as an imitation of burnishing. Indeed, after the passage of the indenter the surface roughness does not disappear completely, but it is burnished. Features of the indenter (its small size or large radius of curvature) will lead to what generated in the course of the movement bulge of the atoms of the surface layer should further increase the resistance force to the movement of indenter. We should expect that at a certain magnitude of the force of resistance to tangential movement the indenter starts to move in the Y direction over the surface of the crystallite, thereby creating an induced periodic roughness due to the features of the process. Such behavior can be compared with the results nano-burnishing within framework of the dynamic instability of the process.

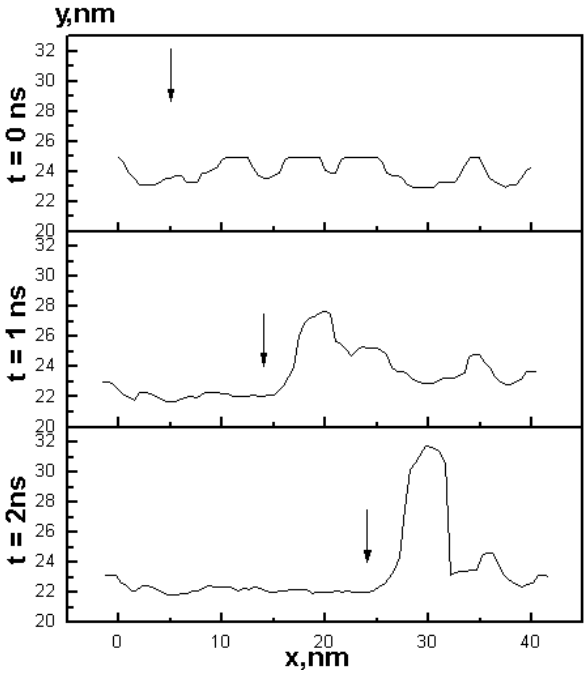


Fig. 2. The surface profile of model crystal at different times. The arrow shows the position of the indenter. At time t = 0 the indenter is over the surface of the crystallite.

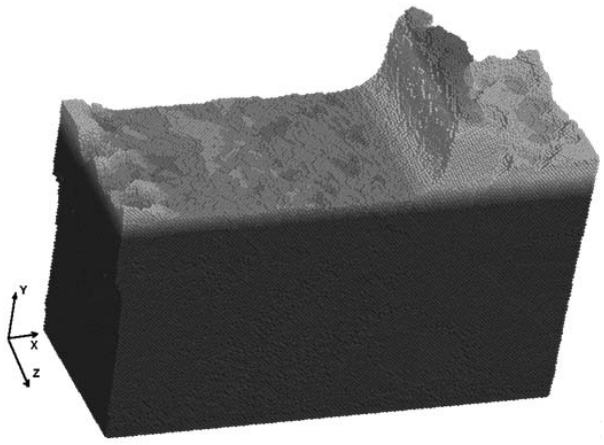


Fig. 3. The structure of the model crystal at time t = 2 ns. Indenter radius r = 4 nm.

To analyze the features of structural transformations in the process nano-burnishing algorithm of the search of the local structural changes was used, which allows you to identify the occurrence of defects such as dislocations and stacking faults in the fcc lattice. Description of the algorithm is given in [7]. The results of research showed that in the bulk of the sample at modeling process of burnishing numerous structural defects are appearing. There are dislocation, walls of dislocations and stacking faults. During the movement of the indenter their numbers are

growing, and they extend from the surface into the bulk material. Thus, as a result of plastic deformation formed a modified surface layer with properties different from properties of the material in bulk. Formation of numerous defects in the surface layer also means the possibility of surface nanofragmentation and forming nanograin structure.

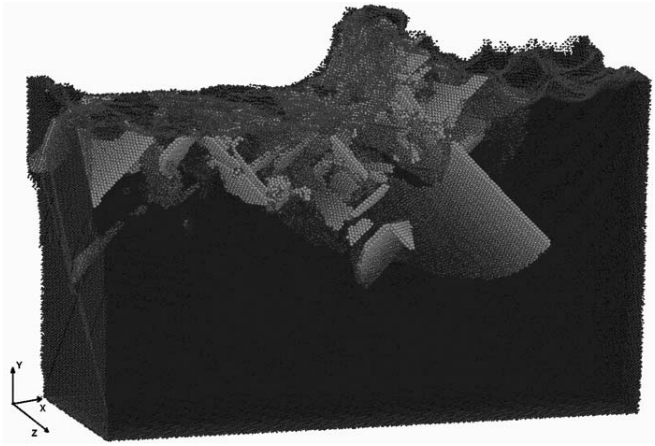


Fig. 4. 3D image of the local structural changes in the simulated crystallite at time t = 1.8 ps.

Fig. 4 shows the simulated fragment at the time when the structure of surface defects was formed. Centers of the atoms with a local topology of the structural bonds of the fcc lattice, marked with small spheres (defect-free areas). Centers of the atoms with a local topology of the structural links is different from the fcc lattice are marked by large spheres. For better visualization centers of surface atoms are marked by small dots.

4. Burnishing by the indenter with a radius of 16nm

Since the size of the indenter with a radius of 16 nm was comparable to the size of the modeled fragment, the loading procedure to simulate the nano-burnishing process was differed from the previous task. Thus, the initial position of the center of the indenter was set outside of the modeled fragment. Then, as in the first case, the loading was divided in two stages: indentation phase and horizontal motion of the indenter. Initially indenter was pressed into a depth of 3 nm, comparable to the maximum surface roughness. As a result of interaction with force field of indenter atoms start pressed out from the surface. After reaching a given depth the procedure of so-called relaxation of the sample began. At this stage during the time interval of 5 ps no additional external loading was applied on the modeled specimen, indenter was unmovable and the system reaches the equilibrium state. In the second stage of loading the motion of indenter alone the direction of X-axis (Fig. 5) with a constant velocity 10 m/s was simulated. During the complete calculation the indenter moves along the X axis on the distance of 56 nm.

According to the results of calculations in case of the indenter with radius of 16nm behavior of the system are more close to the technological process of nano-burnishing. It is because of smaller indenter curvature does not promote the formation of the bulge from surface atoms in front of the indenter (Fig. 7). There are deformation and indentation of individual roughs of the surface into bulk of the material. That gives rise to both plastic and a large part of the elastic components of deformation of the surface layer. In the central part of the modeled fragment burnishing of the initial roughness of the surface within the same order of magnitude (from 2 nm to 0.5 nm) is taking place. However, a significant part of stored elastic strain due to

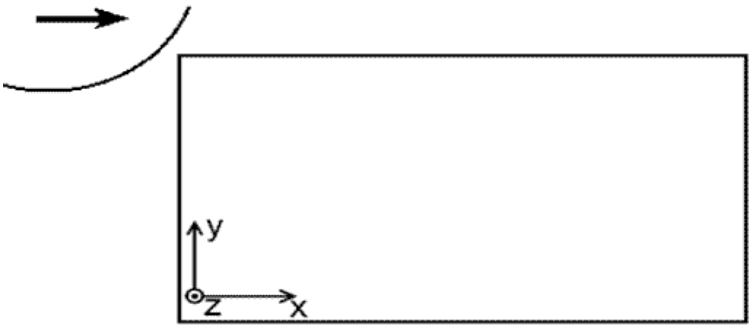


Fig. 5. Schematic presentation of nano-burnishing. Indenter radius is 16 nm.

the influence of the indenter with small curvature, leads to the fact that after the loading (since the passage of the indenter), the level of the surface increased by an average of 0.5 nm up to a value of y = 22.5 nm (Fig. 6).

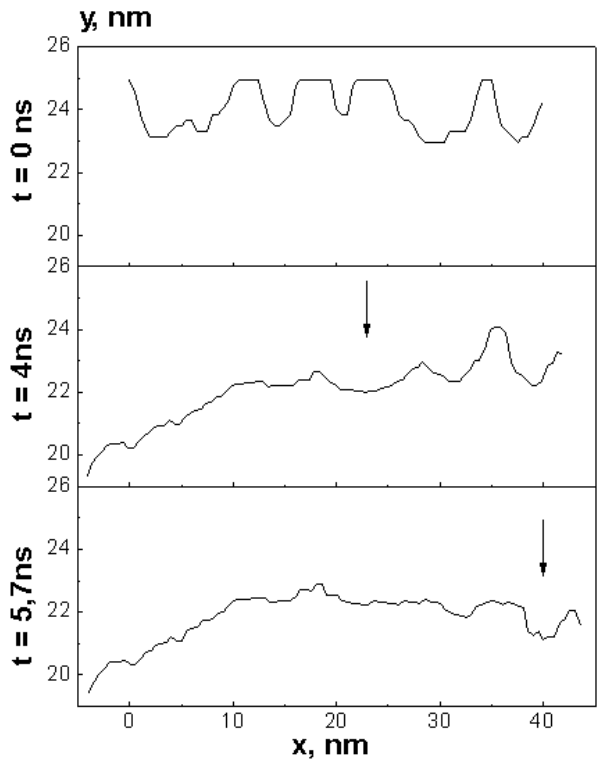


Fig. 6. The surface profile of model crystal at different times. The arrow shows the position of the indenter. At time t = 0 indentor is left and above the surface of the crystallite

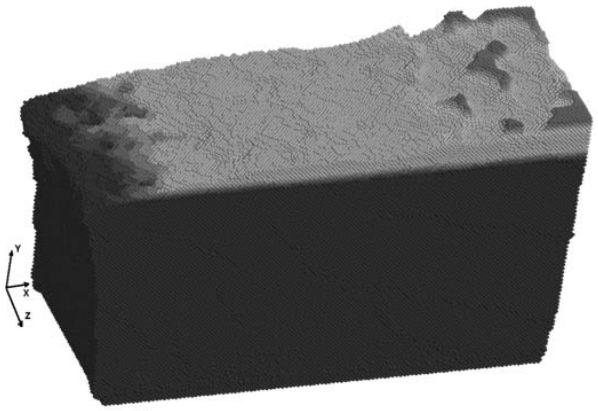


Fig. 7. The structure of the model crystal at time t = 4 ns. Indenter radius r = 16 nm

Structure analysis of the modeled fragment showed that much larger number of different structural defects appears in the bulk of the sample in case of the indenter with a radius of 16 nm. This difference is the result of greater contact area and greater deformation. During the movement of the indenter number of structural defects is also growing, and they extend from

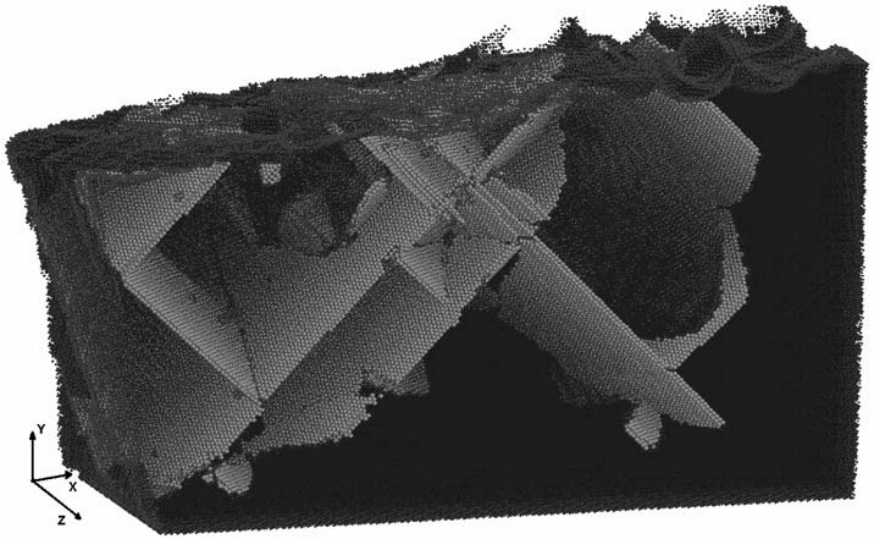
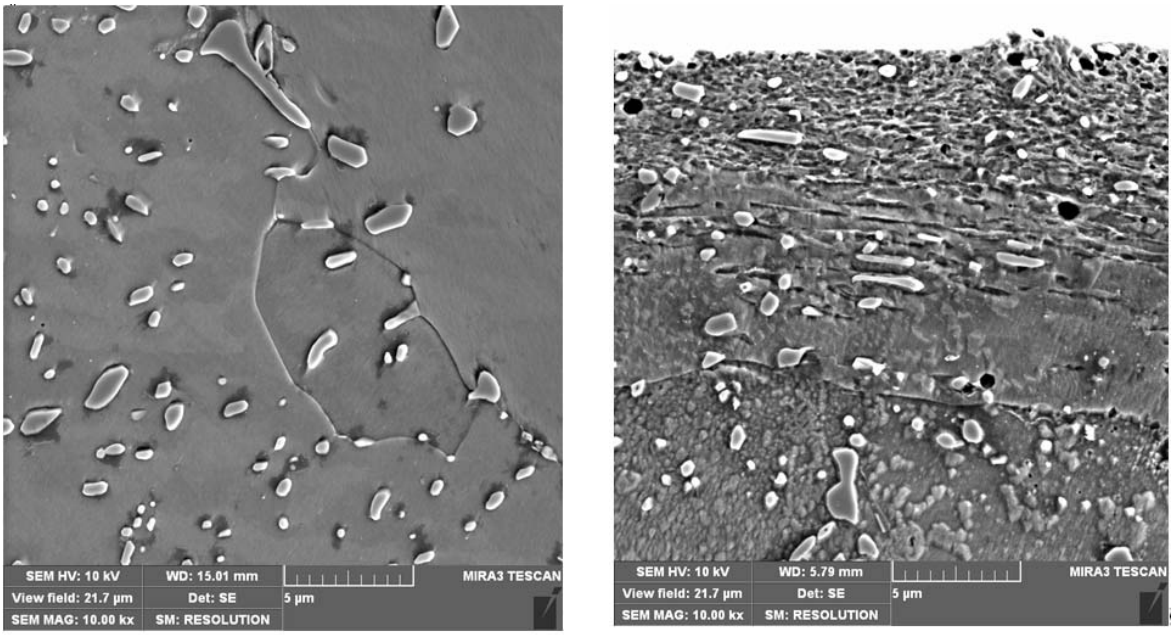


Fig. 8. 3D image of the local structural changes in the simulated crystallite at time t = 3.5 ps.



a) ×10000 b) ×10000

Fig. 9. Structure of the surface layer of steel 20X13: a) in the initial state and b) were subjected to the burnishing of diamond processing.

the surface into the bulk of the material. Thus the result of plastic deformation is the formation of a modified surface layer, which properties are differ from properties of the material in bulk. Analyzing the cellular structure formed by many intersecting planes of stacking faults can also talk about possible nano-fragmentation and grain structure formation in the surface layer of the modeled fragment. Fig. 8. depicts the simulated fragment at a time, which corresponds to a moment of structural defects formation near to surface area. Centers of the atoms with a local topology of the structural links of the fcc lattice, marked with small spheres (defect-free areas). Centers of the atoms with a local topology of the structural links is different from the fcc lattice

are marked by large spheres. For better visualization centers of surface atoms are marked by small dots.

In conclusion, we note that the results of simulations agree well with experimental studies, obtained using scanning electron microscope Tescan Mira 3 LMU [8]. Fig. 9 shows the structure of the surface layer of steel 20×13 in the initial state and subjected to burnishing procedure by diamond spherical indenter with a radius of sharpening R = 4 mm with a force smoothing P = 230 N, feed S = 0,08 mm/rev, speed burnishing V = 100 m/min. It was established that the nano-burnishing treatment changes the structure of a thin surface layer, namely, as a result of plastic deformation the formation of fine-grained structure, which increases the microhardness, elastic limit and yield strength of the surface layer [1] was observed.

Acknowledgements

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