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MOLECULAR-DYNAMICS INVESTIGATION OF NANO-BURNISHING PROCESS

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Abstract. It is well known that the burnishing process affects the surface characteristic, namely: surface roughness, surface hardness, wear resistance, fatigue resistance and increased maximum residual stress in compression. Unfortunately we still far from full understanding what parameters and mechanisms are responsible for the certain surface modification. That is why methods of computer modeling can be considered as useful tool to investigate surface changing during contact interaction as well as burnishing process. It is more essential if we consider processes are taking place at atomic scale level.
In the paper we try to reproduce the details of burnishing process at nano-scale level. To investigate features of surface treatment we use the molecular dynamics simulation. Various pure crystalline materials were considered. Results of our modeling are very close to the experimental observation

1 INTRODUCTION

Performance of various assemblies and machine components are determined by the qualitative characteristics of the surface layer, resulting during the finishing treatment. One of the modern techniques of high surface finish of parts in mechanical engineering is a method of surface plastic deformation, which is called as burnishing. It was established that the burnishing improves wear resistance of parts by 20-40%, fatigue by 30-70%, resistance to contact fatigue by 20-40% [1]. Changing the properties of surfaces after burnishing is connected with the change in the structure of a thin surface layer due to plastic deformation. Under the influence of the indenter motion change of orientation and shape of grains, which are crushing, flattening and stretching, forming the texture of the surface layer [2] are taken place.

It is extremely difficult to investigate the structural changes occurring in the surface layer of material directly during the burnishing. In this regard, methods of computer simulation can

be an important complement to experimental studies. However, models based on the methods of continuum mechanics do not allow us to reveal the mechanisms of structural rearrangements in the surface layer of the material. Therefore, the purpose of this research was to study the origination and development of structural defects by modeling of nano-burnishing with help of molecular dynamics method [3, 4].

2 DESCRIPTION OF THE SETUP

A copper crystallite was chosen as a model material to investigate the result of nano-burnishing process. The interatomic interaction was constructed within the embedded-atom method [4, 5]. This potential with a high accuracy describes the elastic and surface properties as well as 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] of fcc lattice were corresponded to the X, Y and Z axis. Dimensions of the model sample in the direction of the coordinate axes were equal to 40.13 x 24.95 x 16.63 nm, respectively.

The scheme of the model sample is shown in Figure 1. The roughness of the surface layer with a maximum depth of 2.5 nm was specified directly in the simulated crystallite at the initial stage. The roughness was created by the removal of surface-layer atoms that fall within the sphere of radius, which ranged from 0 to 2.5 nm. Center of the sphere was located at the level of the surface layer, and its position in the plane XoZ was determined using random numbers. The periodic boundary conditions were simulated in the Z direction. Thus the replication of the simulated fragment allows one to simulate the length of the sample in a given direction. Surfaces along X and Y axis were simulated as free. The lower layer of atoms (dark bottom layer in Figure 1) was fixed, imitating the unmovable substrate. Thickness of the substrate was 0.73 nm. Over the substrate a special "damping" layer of atoms, which used the procedure to reduce the kinetic energy accumulated due to dynamic loading was added. Introducing of such layer with properties of heat transfer allows us to take into account the length of the sample depth of the material in Y direction. The thickness of the "damping" layer was 1.45 nm. Its kinetic temperature - the temperature obtained from the equality of thermal and kinetic energy, was maintained in the range from 125K do135K.

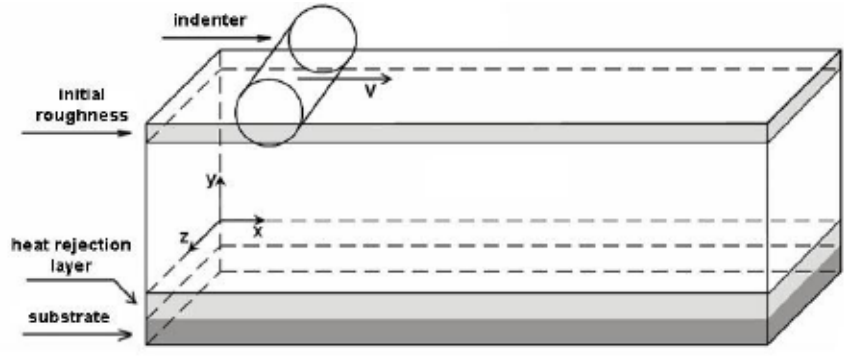

Figure 1: The scheme of the modeled sample

The burnishing was performed using an indenter, whose action has been realized through the force field in the shape of the cylinder with the axis along the axis Z and a certain radius. On the atoms that fall into this area, forces acting in the direction from 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 burnishing of the model sample was carried out using two indenters with radii differ by 4 times: 4 nm and 16 nm.

3 RESULTS OF MODELING

3.1 Burnishing using the indenter with a radius of 4 nm

Results of simulation showed that the nano-burnishing by cylindrical indenter with radius of 4 nm on a small spatial interval resembles the process of cutting or scratching. When the indenter moves horizontally a "bead" forms before it from the atoms of the upper layer. As it moves, the height of "bead" is growing. This is clearly seen in Fig. 2, which shows the topography at different times of a single central layer of atoms arranged in parallel planes XoY. Arrow indicates the position of the axis of the cylindrical indenter at a given time. If we compare the surface profile before and after the passing 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 one order as for given sizes of the modeled object may be interpreted as a modeling of burnishing. Indeed, after the passage of the indenter the surface roughness does not disappear completely, but it is decreasing. Indenter geometry (small size or large curvature radius) leads to generation of a “bead” in front of its motion from the atoms of the surface layer. This should further increase the resistance force of the indenter movement. We should expect that at a certain magnitude of the resistance force the indenter starts to move in the Y direction over the surface of the crystallite, thereby creating an induced periodic roughness due to the peculiarities of the process. Such behavior can be compared with the results of nano-burnishing within the dynamic instability of the process.

Figure 3 shows the structure of the simulated crystallite at time t = 2 ns. The position of surface atoms along the axis Y is marked by color: from blue to red. The layer which location corresponds to a penetration depth of the indenter (y = -3 nm) is selected as a basic level

To analyze the peculiarities of structural transformations during the nano-burnishing process the special algorithm to search the local structural changes was used. This algorithm allows one to identify the generation of defects such as dislocations and stacking faults in the fcc lattice. Description of the algorithm is given in [7]. According to the results during the treatment of the modeled sample there are numerous structural defects are nucleated in the bulk of the material. Movement of the indenter leads to growing of its number, 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 to form nano-fragment structure with misoriented nano-grains.

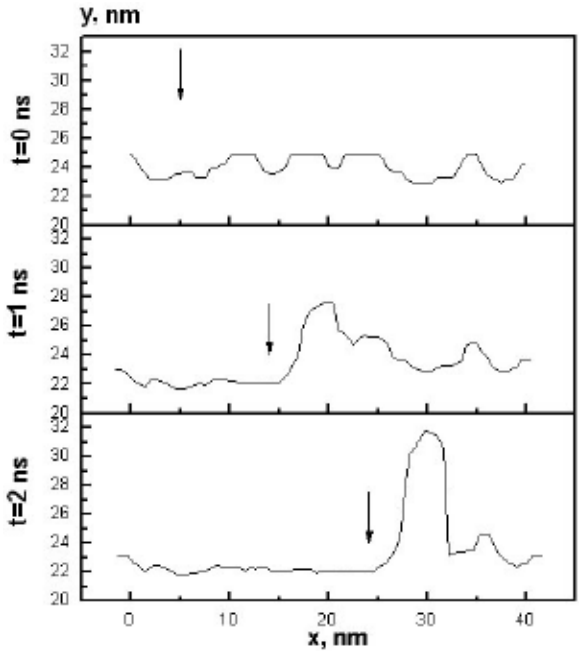

Figure 2: The surface profile of the modeled crystallite at different times. By arrow the position of center of the indenter is shown. At time t=0 the indenter was located over the surface of the crystallite.

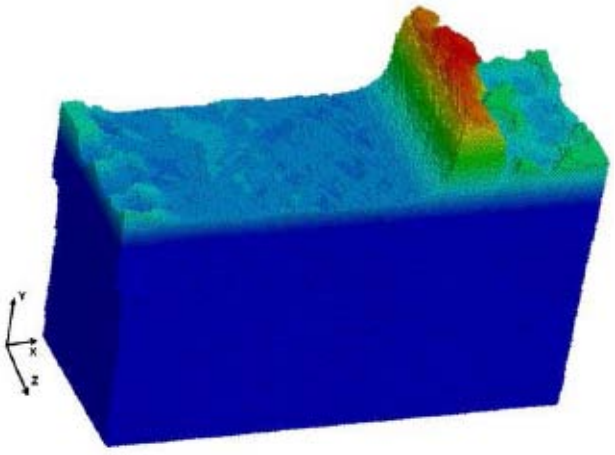

Figure 3: The structure of the modeled crystallite at time t=2 ns.

Figure 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 dots (non-defected areas). Centers of the atoms with a local topology of the structural links which is different from the fcc lattice are marked by large dots. For better visualization centers of surface atoms are marked by small red dots.

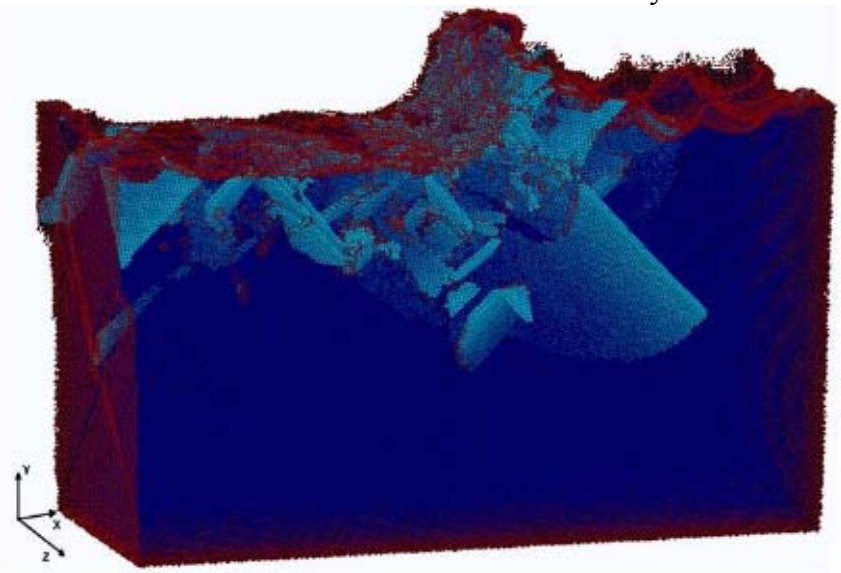

Figure 4: 3D visualization of local structure transformations in the modeled crystallite at time t=1.8ns

3.1 Burnishing using the indenter with a radius of 16 nm

Due to the size of the indenter with a radius of 16 nm were comparable to the size of the modeled crystallite, the algorithm of loading to imitate the burnishing process was differed from the previous case. Thus, the initial position of the center of the indenter was set outside of the modeled fragment. Then, as in the first case, the load was specified in two stages: indentation and phase of horizontal movement of the indenter. As a result of indentation the left edge of the modeled fragment was exposed to the forces from the force field of the indenter, which, as in the previous case, was pressed into a depth of 3 nm, comparable to the maximum surface roughness.

After reaching a certain depth of the indenter penetration a relaxation stage during 5 ps was modeled. In the second stage of loading the motion of the indenter alone X-axis (Fig. 5) with a constant velocity 10 m / sec was simulated. During all calculation the indenter moves along the X axis on the distance of 56nm.

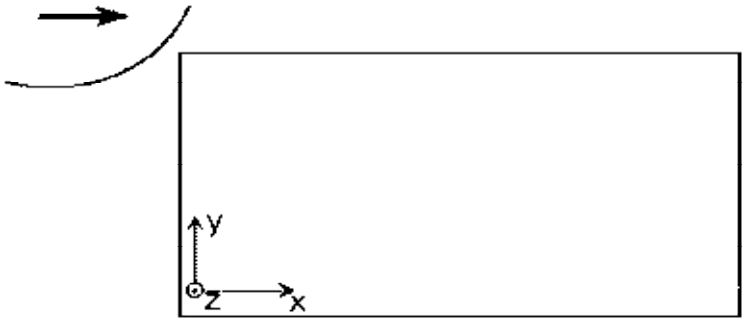

Figure 5: The scheme of nano-burnishing process. Radius of indenter 16 nm.

According to the results of calculation treatment of the modeled crystallite with bigger indenter as a process closer to the real technological burnishing, because of small curvature of the indenter less contributes to a "bead" formation of the atoms of the surface layer. The indentation of individual rough surface in the volume of material that gives rise to both plastic and a large part of the elastic components of deformation in surface layer. In the central part of the modeled fragment smoothing of initial roughness of the surface layer within one order of magnitude (from 2 nm to 0.5 nm) is taking place. However, a significant part of stored elastic strain conditional by small curvature of the indenter, leads to the fact that during unloading (after passing of the indenter), the level of the surface restore by an average of 0.5 nm to a value of y = 22.5nm (Fig. 6).

Fig. 7 shows the structure of the model crystal at time t = 4ns. The position of surface atoms along the axis Y is marked by color: from blue to red. The layer which location corresponds to a penetration depth of the indenter (y = -3 nm) is selected as a basic level.

Analysis of structure of the modeled crystallite showed that larger number of different structural defects appears bulk in the sample than in case of the indenter with a radius of 4 nm. This difference is due to the greater area of contact and a greater degree of deformation.

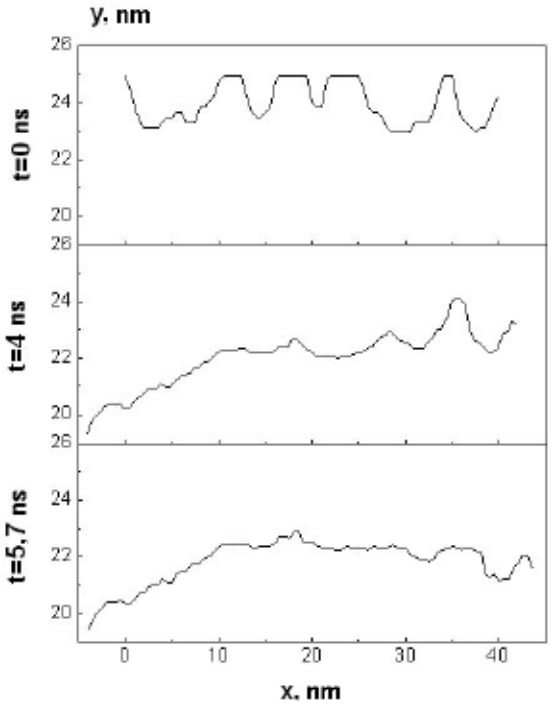

Figure 6: The surface profile of the modeled crystallite at different times. By arrow the position of center of the indenter is shown. At time t=0 the indenter was located on the left and over the surface of the crystallite.

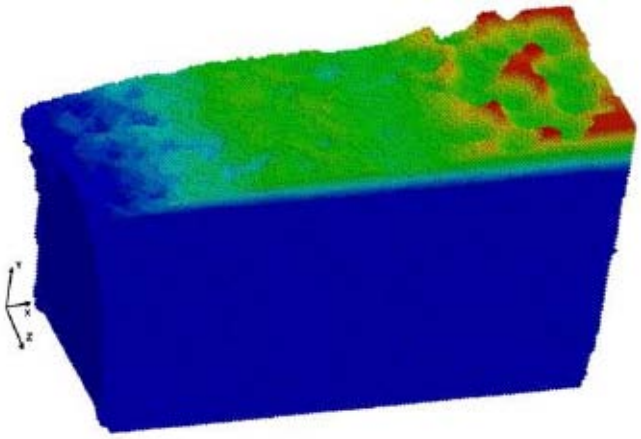

Figure 7: The structure of the modeled crystallite at time t=4 ns By color the vertical position of surface atoms is indicated.

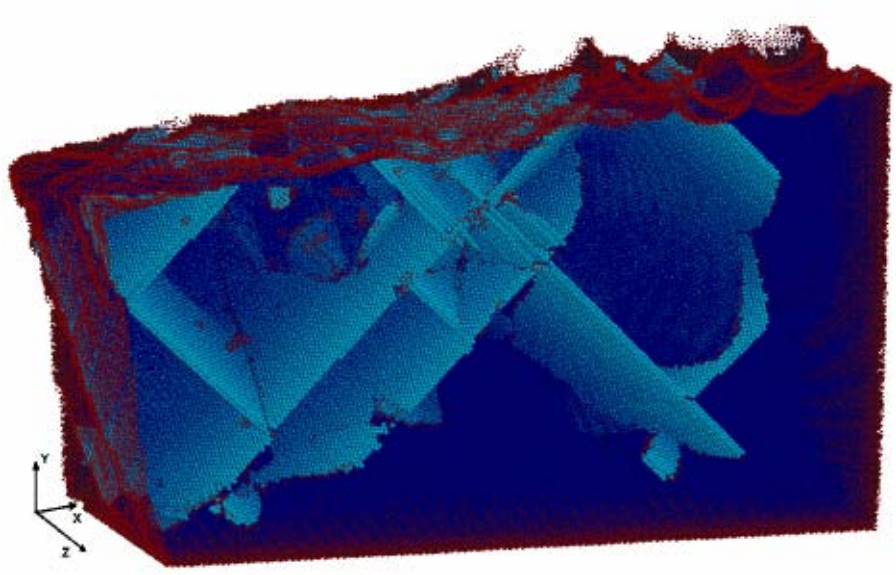

Figure 8: 3D visualization of local structure transformations in the modeled crystallite at time t=3.5ns.

During the tangential motion of the indenter number of structural defects is also growing, and they extend from the surface into the bulk material. Thus the result of plastic deformation is the formation of a modified surface layer with properties different from properties of the material in bulk. Analyzing the structure formed by many intersecting planes of stacking faults it is possible to say about generation of nano-fragmentation structure in the surface layer of the modeled fragment. Figure 8 shows the simulated fragment at 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 dots (non-defected areas). Centers of the atoms with a local topology of the structural links which is different from the fcc lattice are marked by large dots. For better visualization centers of surface atoms are marked by small red dots.

4 CONCLUSIONS

In conclusion, we note that the results of computer simulations agree well with experimental data, obtained using scanning electron microscope Tescan Mira 3 LMU [8]. So, fig. 9 shows the structure of the surface layer of steel 20X13 at the initial state and subjected to burnishing processing of diamond spherical indenter with a radius of sharpening R = 4 mm. Applied force P = 230 N, feed S = 0,08 mm / rev, speed burnishing V = 100 m / min. It was established that nano-burnishing leads to structure changing in a thin surface layer, namely, as a result of plastic deformation is the formation of fine-grained structure, which increases the microhardness, elastic limit and yield strength of the surface layer [1].

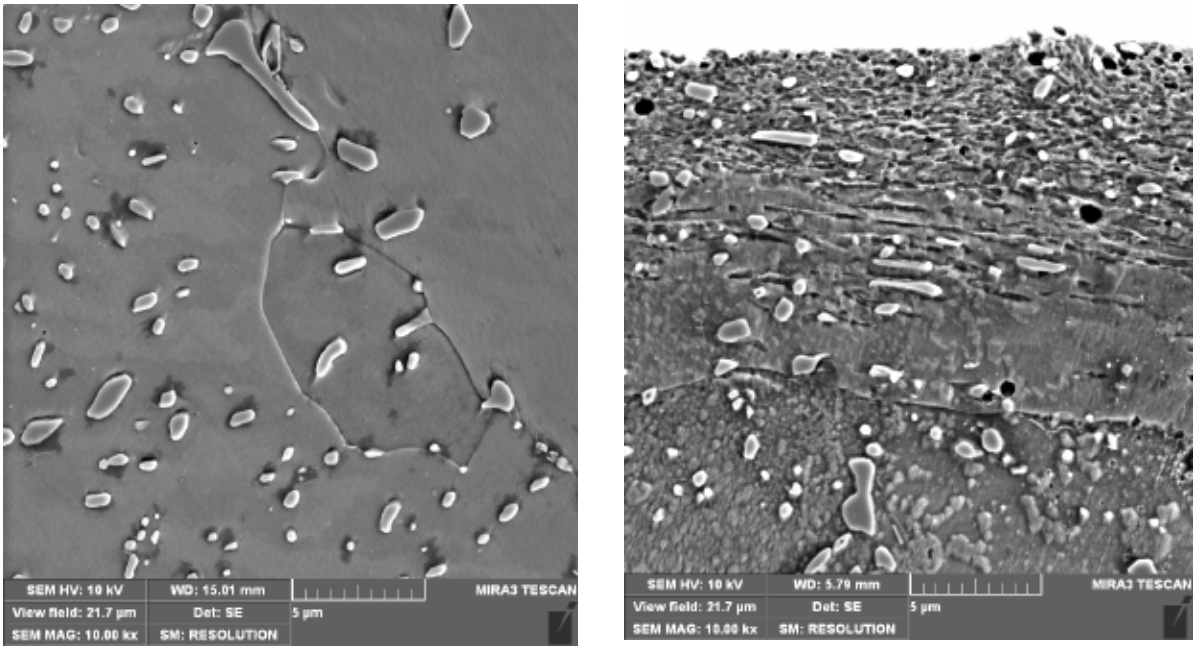

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Figure 9: Structure of surface layer of steel 20X13: a) initial state and b) after nano-burnishing with diamond indenter.

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