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MOLECULAR-DYNAMIC INVESTIGATION OF CONTACT INTERACTION OF PURE METALS

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In using the method of molecular dynamics simulation of contact interaction between the copper crystallite and the various pure metals under shear loading was carried out. Shown that the structure of the boundary layer obtained during the shear deformation is determined by the loading conditions and materials of contact pair. In particular, in the interaction of copper with aluminum, soft aluminum material begins to be introduced into the lattice of copper, and in the interaction of copper with iron, this process is not observed. The effect of loading conditions and mode of heat transfer was studied. The research results can be useful for controlling strength properties of interfacial layer coated material, as well as to control the properties of the surface layer in contact problems.

Keywords: molecular dynamics, contact interaction of pure metals.

1. Introduction

A large variety of realized micromechanisms interaction under conditions of frictional contact and multilevel nature of the processes of friction and wear leads to the need to develop new tools explicitly take into account features of the studied phenomena [1–3]. This leads to considerable interest in development, including computational methods to study and analyze a wide range of processes in the surface layers of the solid [3–5]. The results obtained during the simulation allow better understand the mechanisms of contact interaction, which enable targeted impact on the structure and composition of the surface layers of frictional materials to enhance and improve their performance.

Because the friction and wear processes are accompanied by intensive formation and accumulation of damage in the contact area, mixing the material, cleavage and other processes related to the continuity violation use of computational methods based on the concept of particles [5, 6] is the predominant. Gained by the authors experience in the development and application of particle method for solving various tribological problems on mesoscopic scales [7–10] allows us to speak about the effectiveness of using of this approach. In particular, the formation in a contact patch ”quasi-liquid” layer in which structure differs from the structure in the bulk of both interacting bodies was shown in [8]. The structure and composition of the layer significantly affect on sliding mode of interacting bodies and determine the macroscopic characteristics of friction. Were suggested possible ways to reduce or increase the calculated value of the coefficient of friction by introducing appropriate inclusions in the surface layer of material contacting pair [9], as well as methods of stabilizing a given friction coefficient during the whole process of friction [10], which is particularly important from a practical point of view.

In this study, we attempted to analyze the features of the development processes of deformation and fracture of thin surface layers which are implemented under of conditions of frictional contact at the nanoscopic scale. For this purpose, the method of particles on the atomic scale - a method of molecular dynamics [11] was selected.

2. Influence of crystallographic orientation

For calculations within the molecular dynamics method was used the software package LAMMPS [12], which has the possibility of parallel computing. Originally considered frictional contact between two crystalline materials with properties of Cu and Al, whose atomic lattice were oriented so that the axis of the X, Y and Z coincide with the crystallographic directions [100] [010] and [001] for the aluminum crystallite (Fig. 1a). In some calculations, a copper crystal was oriented so that the X, Y and Z coincide with the directions [130], [$\overline{3}$10] and [001], in others it was the same direction as the atomic lattice of the crystallite aluminum. Relative slippage of the crystallites at a speed of 20 m/s along the X axis was simulated by setting the extra velocity to the boundary atoms of crystallites, external to the contact plane. The thickness of the loaded layers for each of the grains correspond to two radii of cutoff of the interatomic potential (R_{cut} = 0, 501 nm for copper), which was described in framework of the embedded-atom method [13]. The choice of potential was determined by the possibility with a high degree of accuracy to describe the elastic and surface properties, and energy parameters of defects of the system. The equations of motion were integrated with time step Δt = 0, 001 ps. The total number of atoms exceeds 200000. In the direction of X and Y axes periodic boundary conditions were simulated, and in the Z direction the load is not set. In the calculations the following characteristics of the contact have changed: the conditions of loading and the crystallographic orientations of the atomic lattices. In addition, by varying the profile of the contacting surfaces have changed the conditions of conjugation implemented at the junction.

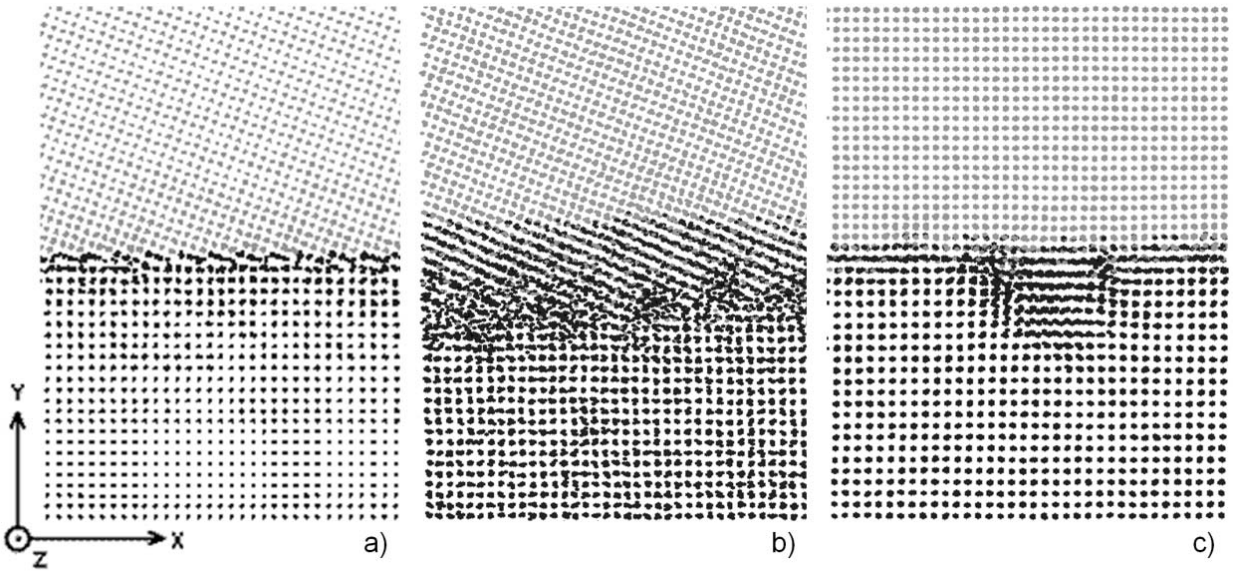

Fig. 1. a) The initial structure of interacting crystallites, b) and c) structure of modeled crystallites after 500 ps with different initial relative orientation of the crystal lattices

According to the results of molecular dynamic study the features of the behavior of crystalline materials strongly depend on the conditions implemented at the junction. In particular, in the area of tribological contact may occur effects associated with the loss of crystalline order of the interacting materials. This is followed by formation of a layer in which interdiffusion of atoms belonging to both the crystallites is occurred (Fig. 1b). And this process is mechanically activated, which can significantly improve its dynamic characteristics. Likewise, in the conditions of mechanical activation can be increasing of speed, for example, processes such as oxidation of

the materials pair friction pairs. It should be noted that this result was indirectly mentioned in [9], where based on a comparison of the values of coefficient of friction for various contacts was concluded about the rate of formation of oxide films on surface of pure metals. By comparing the simulation results at different scales, also it should be noted analogy of the effect of the formation of the mixed layer that was observed in [8,9] on the scale of individual grains of nanocrystalline materials obtained by the simulation by movable cellular automata. This suggests a multiscale of studied processes and a commonality of the nature of the observed phenomena.

However, an explicit account of the atomic structure of interacting materials enable identifies and some features of the behavior of crystalline materials during their interaction. In particular, during such interaction, it is possible the formation of disoriented nanoblock structure in aluminum near the interface area, which is clearly seen in Fig. 1c. Individual blocks are nanocrystalline grains. These effects contribute to increase the resistance of the relative sliding surfaces of contacting bodies. It should be noted that the formation of block structure observed experimentally near the surface under conditions of tribological contact. The results of molecular dynamics simulations show that under conditions of straitened shear deformation may occur the growth of one of the contacting grains of nanocrystalline materials at the expense of the structure of the neighboring grain. In this case, the movement of intergrain area is determined by the loading conditions. In addition, the contact area of two interacting bodies could be the place of nucleation of defects such as dislocations, stacking faults, etc., which are distributed from the zone of the interface into the bulk of material (Fig. 2). The intersection of multiple dislocations can also lead to fragmentation of the material.

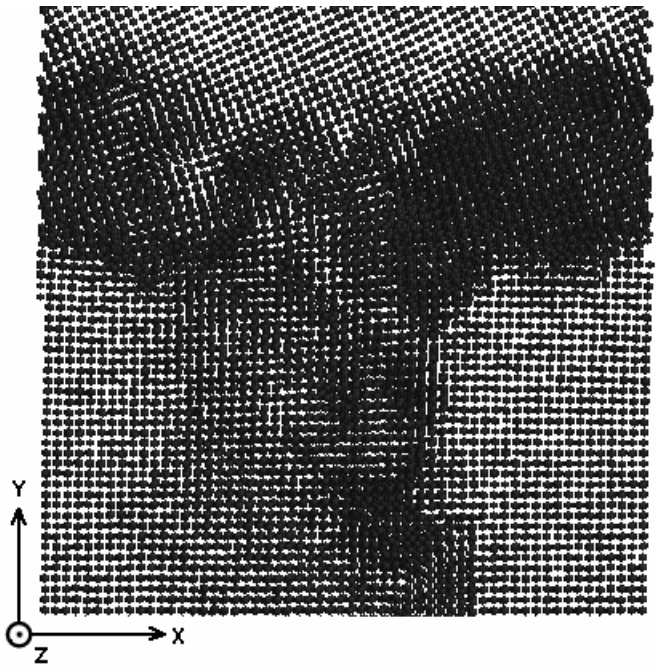

Fig. 2. The structure of simulated crystallites after 450 ps, characterized by the movement of grain boundaries with the formation of structural defects

In spite of the mentioned diversity of results of computer simulation, obtained by the molecular dynamic studies, in all cases may be noted that formation of interface layer with a composition and structure differed from the structure in the bulk material takes place. Features of this layer observed before, but on a different scale level. Formation of interfacial layer at the

atomic level changes surface properties of interacting materials, lowers energy barriers to form new phases (including metastable) and the initiation of chemical reactions.

3. Accounting for the effects of frictional heating

It is obvious that the intensive shear strain realized in conditions of contact interaction can lead to significant heating of material near the surface. So the next step of studying the features of contact interaction at the atomic scale is the explicit account of the effect of termofrictional influence upon changes in physical and mechanical properties and structure of the surface layers of contacting crystallites. In view of the smallness of the time intervals considered in the computer simulation, the steady stage of friction was investigated. the interaction of model materials with the properties of Cu and Ag, the atomic lattice of which were oriented so that the axis of the X, Y and Z corresponded to the crystallographic directions [100], [010] and [001] for the copper crystallite and the [120], [$\bar{2}$10] and [001] for the silver crystal (Fig. 3a), was simulated. Relative slippage of the crystallites at a speed of 20 m/s along the X axis was simulated by setting the extra velocity to the boundary atoms of crystallites, external to the contact plane. In the direction of X and Y axes periodic boundary conditions were simulated, and in the Z direction the load is not set. Here we consider two options for loading. In the first case, all energy imparted to the system due to external shear, redistributed within the simulated pair. In the second case, near of the loaded areas a special layer of atoms was simulated, within which was set additional dissipation of kinetic energy, thereby simulated the removal of heat from the contact area into the inner layers of extended contacting materials. Thus, the first option corresponds to the interaction of two thin films, and the second version can be viewed as a local contact of two bulk crystalline materials.

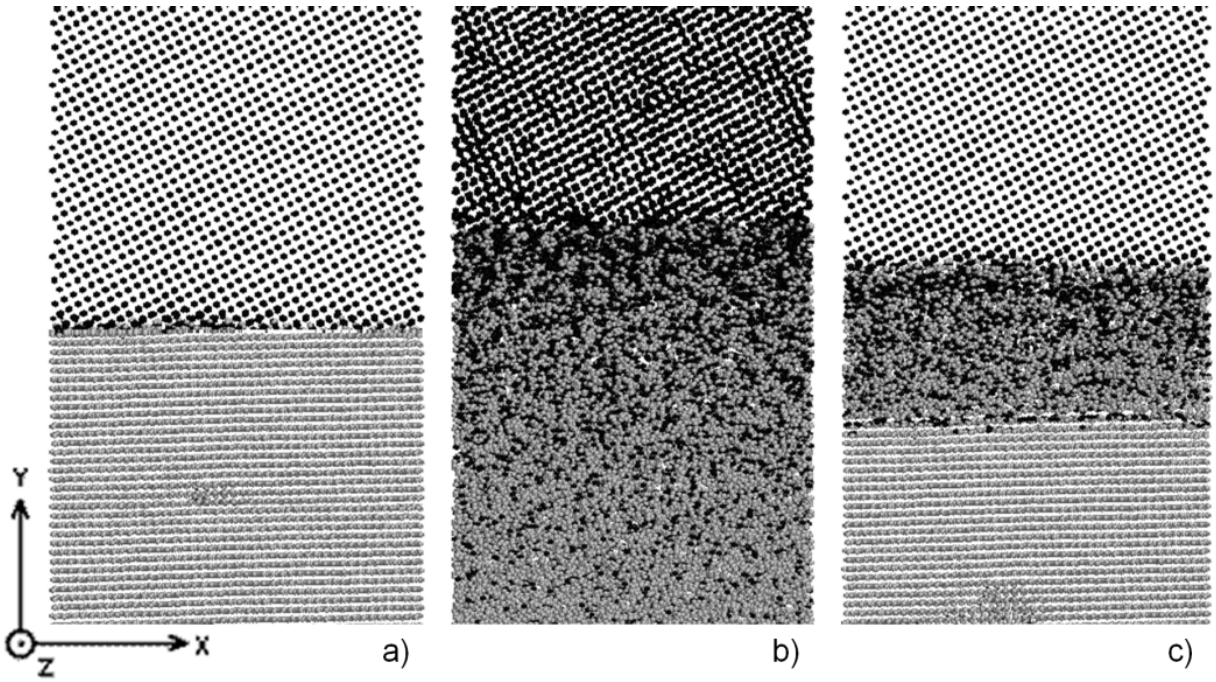

Fig. 3. The structure of simulated crystallites: a) original, b) the final structure in case without the heat removal and c) the final structure in case with the heat removal.

The results showed that the behavior of materials in the contact region for the options under consideration is markedly different. In the case of the interaction of two crystalline thin

films occurred heating the contact area with the achievement of the melting temperature of the copper crystallites. Fig. 3b clearly shows violation of the order of the atomic lattice in the bulk of simulated crystallite. In this case, a refractory material retained crystalline structure. Characteristically, the relative slippage of interacting material is accompanied by the mixing of atoms in the contact zone with a pronounced gradient nature of the implementation of the Ag atoms in the copper crystal is almost the entire depth of the modeled fragment. In the case of simulation of contact with the heat removal there is the preservation of crystal lattices of the two interacting materials under the same other conditions of loading, as in the first embodiment. Meanwhile zone of mixing of atoms of both substances is localized near the contact area, and the distribution of atoms in area of interface has uniform in character (Fig. 3c). The results of the simulation should take into account in various practical applications where the mechanisms are contact interactions are determining.

4. Accounting for the influence of type of material

It is obvious that not only the orientation and temperature, but the type of contacting materials affect on the features of contact interaction. This is primarily due to the difference between the phase diagrams of interacting agents. Thus, the next stage of the study was simulation of contact interaction of copper with different metals. The relative orientation of the crystals was selected so that the axes coincide with the directions [130], [$\bar{3}$10] and [001] for copper [100] [010] and [001] for the second crystallite (Fig. 1a). Loading conditions corresponded to the task of adapting frictional heating. Addressed the following metals: iron, nickel and lead.

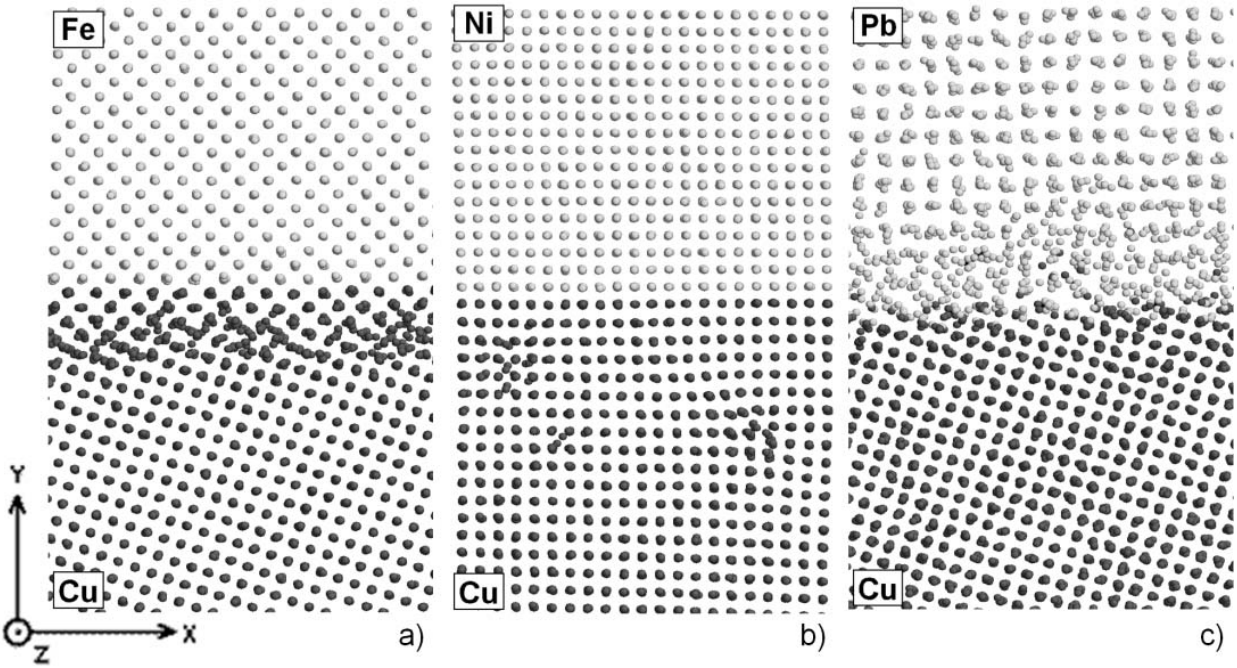

Fig. 4. Structure of sample in case of modeling the interaction of copper a) with iron, b) with nickel, a) with lead.

The simulation results showed that the behavior of metals in the contact area varies greatly. In the interaction of copper with iron a few atomic layers of copper transformed from the fcc structure into the bcc and incorporated into lattice of iron (Fig. 3a). Upon further loading, the restructuring does not occur, only region with disrupted structure at the interface between the bcc and fcc copper increases.

According to the results of modeling of copper with nickel the contact interaction reduces to a complete reorientation of the copper atoms and incorporating on the lattice of nickel (Fig. 3b). This is probably due to the fact that the lattice parameters for copper and nickel are very similar ($3,615$ Å and $3,524$ Å, respectively). High in comparison with other metals the rate of restructuring has suggested that the reorientation of the lattice will occur without an external load, but that has not been confirmed in the further study.

In the interaction of copper with lead, the simulation results are similar to the case of interaction between copper with aluminum. During the loading the atomic structure of lead near the interface starts to break down (Fig. 3c). With further load the width of the layer with structure similar to the irregular increases.

5. Conclusions

The main results can be formulated as follows. With the help of computer simulation revealed some features of contact interaction occurring at the level of individual atoms. It is shown that, during the relative sliding in the contact area a special interface layer formed, whose structure differs from the structure of the material in bulk. Conditions of formation of interfacial layer and its parameters are determined by various factors, such as: matter of contacting pairs, loading conditions, the degree of misorientation of atomic planes, conjugation conditions, etc. Thus, under certain conditions, atoms of one material can penetrate into the crystal lattice of another material, replacing the atoms in it basis. Because this process is a mechanically activated, then the rate of such diffusion is much higher traditional process. Change the crystallographic orientation of the contacting crystallite significantly affects the speed of the process of structural change.

The results of these studies can be used to understand the processes determining the strength properties of interfacial layer of the coated materials, as well as to control the properties of the surface layer in contact problems.

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