Molecular dynamics simulations of the collapse of a hollow thick-walled cylinder

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Abstract

In the paper simulation of the deformation of copper single crystal under high-speed axisymmetric loading was carried out using the method of molecular dynamics. Sample in the form of a hollow thick-walled cylinder was simulated. It is found that the compressive deformation when reaching a certain value leads to the formation of stacking fault in the inner surface of the cylinder. It is shown that depending on the orientation of a single crystal lattice stacking fault formation comes in various planes. It was found that the order of the plane of motion of dislocations depends on the angle between the plane and the direction of loading. Agreement of the results with the experimental data allows the use of modeling techniques to the study of the basic laws of plastic deformation in single crystals. The observed regularities of formation of localized deformation bands can be used to understand the processes of deformation of pure single crystals.

1 Introduction

Despite some progress, associated with using, both modern experimental research methods and new theoretical approaches, It is attending to the issue of studying the characteristics of localization of plastic deformation in crystalline materials [1, 2]. Increased interest caused by the fact that an understanding of the basic mechanisms of plastic deformation of crystalline materials is directly related to the ability to control their strength and deformation characteristics.

It should be noted that the most common strain localization phenomenon is seen in the cases of high degrees, high speeds and temperatures of deformation. This is manifested as the forming of stationary bands, also known as the term shear bands and represents an area of the material in which the strain rate is much higher deformation rates in the other volumes [3, 4]. The formation of shear bands plays a crucial role in the further deformation, because in most cases they are the harbinger of destruction of the material. At the same time it is known that with increasing of the deformation the scale of manifestations of its localization varies from block to grain from grain to grain complex and further to the sample as a whole. Thus, this process is multi-layered. Therefore, the initial stage of the origin and development of the process of localization of deformation is inextricably linked with the features of material response to the load on the microscale [5, 6]. In the transition to microscale research conducted on single crystals become important.

In [7], devoted to high-speed axisymmetric loading of copper single crystals noted that the spatial position of the centers of localization of deformation is determined by crystallography of active slip systems. Thus, the order of connection of a close-packed direction of sliding is determined by the corresponding factor Schmid. Note that in the cited paper the method of explosive loading of a hollow thick-walled cylinder was used. The advantage of this approach is the possibility of combining in one experiment all possible orientations of the single crystal relative to the applied load in the plane defined by the base plane of the sample. Since for the experimental solution of the problem requires laborious preparation of the corresponding single-crystal samples, taking into account their small spatial scales the issue can be effectively studied using modern methods of computer simulation [8].

Thus, the aim of this work is a theoretical study of the origin and development of the process of deformation localization on the scale of individual atoms depending on the crystallographic orientation of the plane of the base of the hollow cylindrical sample under high speed axisymmetric loading.

2 The results of computer simulation

2.1 The results of sample loading with the base plane (001) and (111)

For research of high-speed loading of single-crystal sample of copper on the scale of individual atoms the method of molecular dynamics using the software package LAMMPS was chosen. The interaction between the particles is described by means of the embedded atom method [?, 9]. Simulated sample was a defect-free hollow copper cylinder whose axis of symmetry was directed along the Z-axis of the laboratory system of coordinates. The inner and outer radii of the cylinders is $36,15$ Å and $144,6$ Å. The height of the cylinder was set equal to $108,45$ Å. Initially two samples were considered. Orientation of their crystal lattice has been chosen so that the axis of the laboratory coordinate system X, Y and Z correspond to the crystallographic directions [100], [010] and [001] and $[11\bar{2}]$, $[\bar{1}10]$ and [111]. Axisymmetric loading was simulated by specifying an atom located on the outer surface of a cylinder of constant velocities. Velocities were directed toward the center of the cylinder in a plane parallel to the base sample, and velocity magnitudes are equal to 10 м/с. The thickness of the loaded layer was 5 Å. Periodic boundary conditions was modelling along the cylinder axis Z. The initial kinetic temperature of the simulated sample was 140 K. High-speed algorithm Werle was used for integrating the equations of motion. Total number of atoms exceeded 500000.

In this paper the evolution of the structure of the sample as a result of the applied axisymmetric compression was analyzed using a search algorithm of changes of the local topology of the atomic bonds [10]. It is found that the compressive deformation when reaching a certain value leads to the formation of defects in the inner surface of the cylinder structure. Fig. 1 shows the evolution of the structure of two simulated crystallites, which shows only the atoms with the local topology of atomic bonds differs from the original fcc lattice. On Figure 1 gray color mark atoms that locate on the inner and outer free surfaces. Red color indicates atoms with hcp a local topology

of atomic bonds. It is clearly seen that the bands of localized atomic displacements that are formed on the inner surface of a hollow cylinder, formed mainly by atoms with a local topology of the atomic bonds are close to the hcp lattice. Thus, the obtained structural defects correspond to the stacking fault. With further loading of the simulated sample the number of stacking faults increases, and they extend from the inner free surface where the strain reaches a maximum value in the volume of the material.

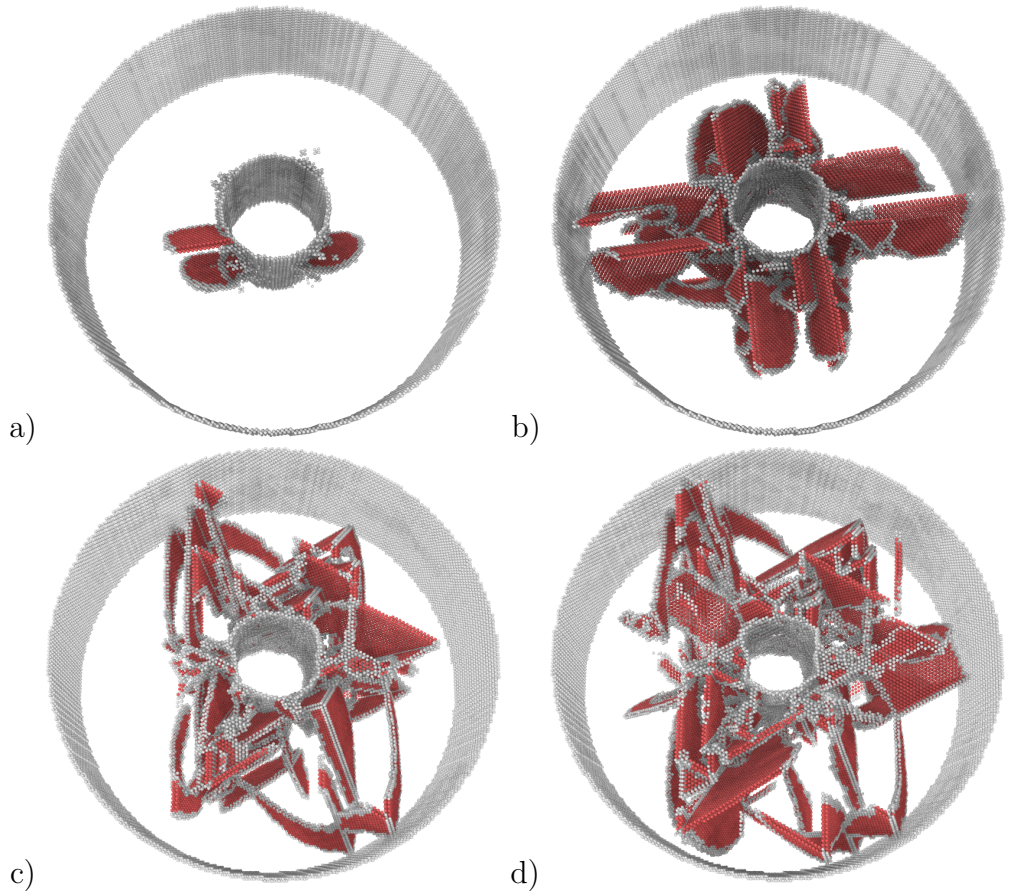


Figure 1: A three-dimensional image of the structure of the simulated crystallites at the stage of strain localization at different times. For a cylinder with the orientation of the base (001): a) $t = 39$ ps, b) $t = 45$ ps. For a cylinder with the orientation of the base (111): c) $t = 39$ ps, d) $t = 45$ ps.

Note that the generation of defects in the structure of the sample with orientation of the base (001) begins at time $t = 38$ ps, whereas for the sample with orientation (111), this process occurs at $t = 27$ ps. The difference between the behaviour of both of loaded crystallites is also the angle between the slip planes and the axis of the cylinder. Thus, for the sample with the crystallographic orientation of the base plane (001), the angle $\phi \approx 54,74°$, a sample with a base (111) $\phi \approx 70,53°$. This leads to difference in the start time of defect formation. Thus, the order of priority activity of slip systems in the considered samples are not observed, and the bands of localized atomic displacements are formed simultaneously on all possible slip planes.

2.2 The loading of the sample with the base plane (134)

To study the effect of crystallographic orientation of the base plane of cylindrical sample at its deformation properties, we modelled the axisymmetric high-speed loading of copper single crystal, the shape and dimensions of which were similar to the cases described above.

The crystallographic orientation of the lattice in the sample was as follows: along the cylinder axis (axis Z) direction [134] along the X and Y axes – $[11\bar{1}]$ and $[\bar{7}5\bar{2}]$, respectively. As before, the formation of stacking faults was observed near its inner free surface at certain degree of deformation of sample. Fig. 2 shows the structure at consecutive sample instant of time. It is possible to select a sequence in the formation of bands of localized atomic displacements in the sample under loading. Initially bands arise in a plane , which extends at an angle $90°$ to the axis of the cylinder (Fig. 2a). Then, stacking fault begin to form in the plane ($\phi = 76,9°$ to the cylinder axis) (Fig. 2b). The plane with a misorientation angle $\phi = 47,2°$ becomes the third slip plane (Figure 2c). The latter stacking faults appear in the (111) plane (misorientation angle $\phi = 25,1°$) (Figure 2d). Thus, in sequence of formed atomic displacements localized bands order was observed and associated with a decrease of the misorientation angle between the cylinder axis and corresponding slip plane. This result is fully consistent with the physics of the phenomenon under study and is in good agreement with data of experimental studies [7].

2.3 Influence of crystallographic orientation on the magnitude of deformation.

In this study we evaluated the strain under which the localized atomic displacements appear in the crystallites. The deformation amount was calculated by the following formula:

$$\varepsilon = \ln(r_0/r) \tag{1}$$

where r and r_0 the current and the initial distance from the center of the cylinder to the selected atoms. The calculation results of deformation depending on the time of loading in case of the cylinder with the orientation of the base (001) was shown in Fig. 3. The position of selected atoms in the sample for which the value of the deformation calculated, observed in Fig. 3 in the upper left corner. Along the Z-axis atoms were selected in the atomic plane situated in the middle of the sample.

According to these results, the deformation of different parts of the cylinder before the inception of the bands of concerted atomic displacements is predominantly homogeneous character. The small difference to the velocity of the atoms 1 and 2 caused by their proximity to the free surface. Beginning at time ≈ 40 ps a sharp increase of the deformation rate observed in crystallite areas located on the inner surface.

The observed difference in the magnitude of the displacement of various groups of atoms caused by formation of structural defects near the inner free surface of the crystallite. Fig. 4 shows the trajectories of motion of atoms in the central

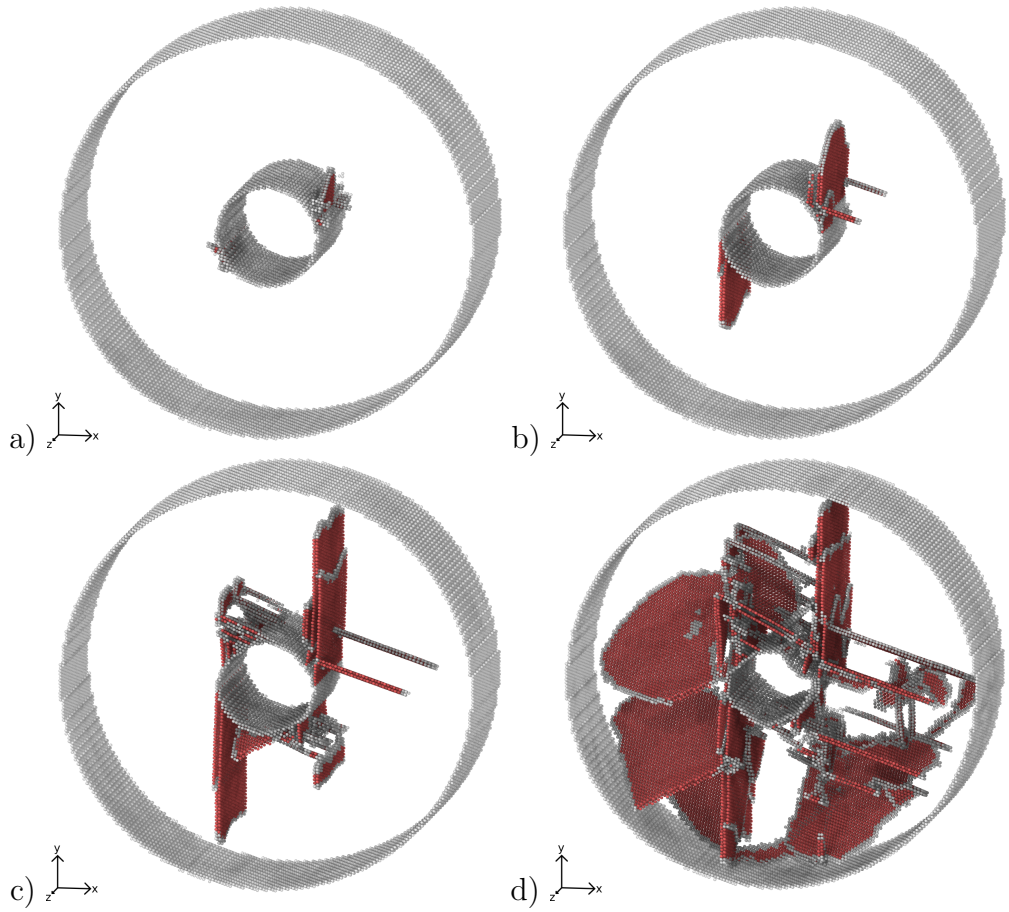


Figure 2: A three-dimensional image of the structure of the simulated crystallite at the stage of strain localization at different times: a) 26 ps, b) 28 ps, c) 33 ps, d) 47 ps.

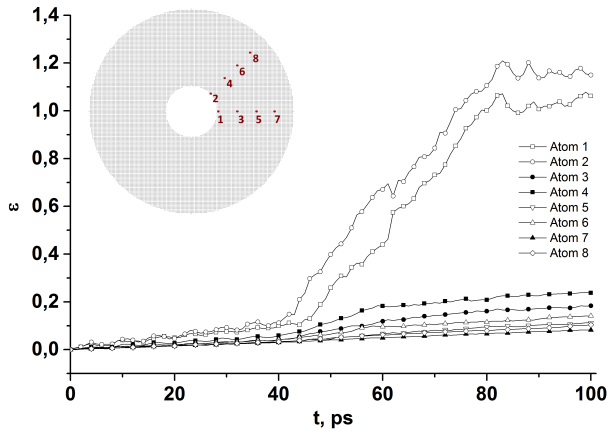
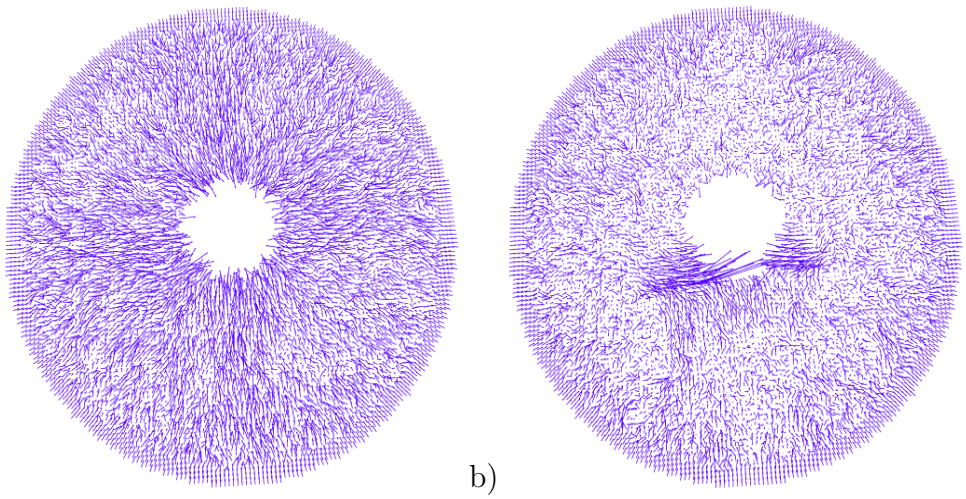


Figure 3: The time dependence of the calculated amount of deformation for selected atoms.

layer of the cylinder at successive times. The time of formation of localized bands displacements of atoms is clearly seen in the time interval from 37 ps to 39 ps (Fig.

4b), despite the fact that at the previous time interval inhomogeneous distribution of the displacement is not observed (Fig. 4a).



a) b)

Figure 4: Displacements of the atoms of the central layer of the cylinder in the intervals: a) from $t = 34$ ps to $t = 36$ ps and b) from $t = 37$ ps to $t = 39$ ps.

A comparison of the localization zones of atomic displacements with the local topology of atomic bonds showed that the atomic displacements are realized in the areas of formed structural defects - stacking faults. This is evident from a comparison of the trajectories of the atoms shown in Figure 4b with Figure 5, which shows the local topology of atomic bonds to atoms of the same dedicated central layer of the crystallite. Figure 5 atoms with an fcc topology atomic bonds (defect-free part of the crystallite) was marked by greem color and red represents the atoms with the local topology of the gpu interatomic bonds.

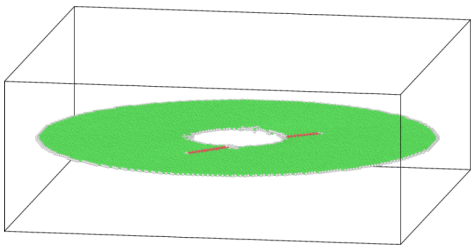


Figure 5: The central layer of the modeled cylinder at time $t = 39$ ps.

According to the results the behavior of the crystallite regions near the inner free surface is largely determined by the peculiarities of the restructuring of the crystal lattice due to the axisymmetric compression. Thus, further reduction of magnitude of the strain rate for the atoms 1 and 2 at time ≈ 80 ps (see. Fig. 3) caused by the collapse of the inner cavity of the cylinder. Character of displacement of atoms 3 and 4 also differs from the other groups of selected atoms. So, areas of cylinder remote from its axis by an amount not less than the half of the wall can be considered for evaluate the deformation properties of the simulated single crystal.

For comparison of deformation properties of cylindrical samples with different crystallographic orientation of their base in the paper average value of strain in

8 atoms in the layer lying remote from the cylinder axis by the same distance as the atoms 5 and 6 in Figure 3 was calculated. The position of the atoms used to estimate the value of the average strain differs by 45° with respect to the axis of the cylinder. The resulting time dependence of the average strain for the three considered crystallites with different crystallographic orientations of base shown in Fig. 6. Schematic representation of the positions of the atoms used for averaging the strain is shown in the upper left corner.

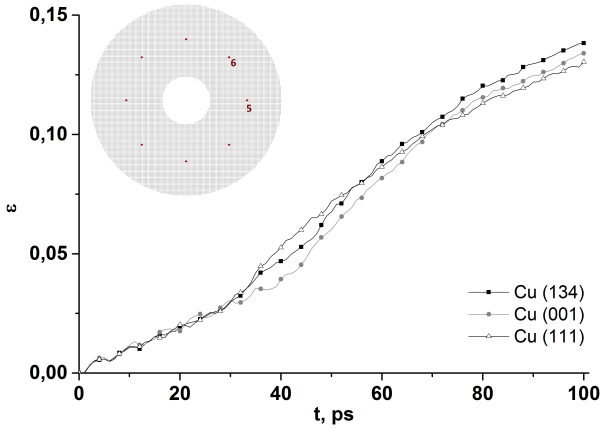


Figure 6: Averaged value of strain for copper samples with different crystallographic orientations their base.

The simulation results showed that the elastic deformation stage for all considered variants identical to the strain 0.03. Further loading causes the deformation rate of the samples that the base (111) and (134) increases as compared with the sample orientation with the base (001) for which this stage of deformation continues until 0.04. At high degrees of loading the rate of deformation of the sample with a base (111) slows down and becomes the minimum of all the considered variants. This dependence, apparently due to the relatively early formation of large number of stacking faults at the simultaneous activation of all possible slip planes. The presence of numerous structural defects leads to a further hardening of the sample. As for the samples with the orientations of a base (001) and (134), then over the entire active phase of loading the calculated average value of deformation for the variant (134) is located above a similar magnitude to case (001).

3 Conclusion

– A computer model of axisymmetric dynamic loading of copper crystallite on the scale of individual atoms showed good agreement between the simulation results and experimental data of explosive loading of copper single crystals. Both in the experiment and in the computer model the order of the activation of slip systems, which is determined by the corresponding value of Schmid factor, was noted. Thus, the proposed numerical model may be used for research of features of origin and development of plastic deformation in crystalline materials.

– It is shown using a computer model the influence of the chosen crystallographic plane of the base of the cylindrical sample on order of connection slip systems and

the resulting deformation properties of the simulated object. Thus in a sample with the base parallel to the crystallographic plane (111) slip system activation sequence is not observed, and the generated localized band of atomic displacements formed simultaneously in all possible slip planes. This nature of the response to external loading crystallite leads to the fact that its speed of deformation is maximum of the three modelled variants of sample in the initial stages of the plastic behaviour. During the further loading a relatively early activation of all possible slip planes leads to a slowing of the rate of deformation of the sample and in the final stages of loading, it becomes the minimum of all the considered configurations.

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