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Calculation of the stress level in modeling the inter-dislocation interaction of aluminum bronze

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Abstract. The behavior of a polycrystal during deformation depends on the deformation of its constituent grains, their boundaries, and the degree of interaction. In this case, the deformation of a single grain is determined by its orientation and morphology. An urgent task is to estimate the stress level for individual grains of a polycrystalline aggregate of aluminum bronze. This problem can be solved by molecular dynamics simulation of crystallites with different crystallographic and geometric characteristics. Based on the results of the active plastic deformation simulation, the main types of dislocations are identified and their role in plastic deformation and hardening is determined. It has been established that the orientation of the lateral faces under moderate deformations has little effect on the fraction of dislocations of various types and the stress. A noticeable effect is exerted by the compression axis crystallographic orientation and the sample height.
Keywords: aluminum bronze, molecular dynamics method, deformation, stress, dislocation interaction

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1. Introduction

The density of defects capable of resisting shear determines the hardening of a crystalline material during deformation. These are defects whose motion determines the possibility of plastic deformation itself. Such defects at moderate degrees of deformation include point defects, dislocations, twins, and, under certain conditions, grain boundaries. Active plastic deformation at low and moderate temperatures leads to an increase in the number of dislocations and deformation twins, which, in turn, will resist shear to gliding dislocations. The possibility of shear in an individual slip system will be determined by the shear stress. The magnitude of the stress depends on the Schmid factor and the local stress in the region of the shear system. Accounting for substructural strain hardening is a complex problem. From the results of studying the structure by transmission electron microscopy, the moments of the processes of motion and interaction of dislocations remain unclear. This gap can be filled, in particular, by molecular dynamics simulation. Naturally obtaining the distribution of stresses with a well-chosen potential of the interaction of atoms and setting the boundary conditions, we have the opportunity to study in detail the processes in a small volume of material.

Using atomic simulation, it is possible to track changes in homogeneous nucleation of dislocations in single crystals under uniaxial loadings changes as a function of crystallographic orientation. In copper studies at 10 and 300 K along with the dislocation nucleation factor determined by the conventional Schmid factor (shear stress in the direction of slip), the influence of the stress normal to the slip plane (Schmid and non-Schmid terms) is taken into account [1,2]. Molecular dynamics simulation of the loadings of TiAl alloys in the <001> direction at temperatures 10 and 300 K made it possible to determine the dependence of tensile and compressive strength on temperature and the reasons for this effect [3]. The strengthening structural element is stacking-fault tetrahedra (SFT). The modeling of their formation mechanisms and the dependence of the formation on the stacking fault energy and the crystallographic orientation of loading are the subject of works [4,5]. The influence of the stacking fault energy of FCC metal grains with different morphology on stress-strain curves has been studied. The influence of grain morphology on the mechanical characteristics and the relationship between the formation of sessile dislocations and hardening has been established [6]. The nucleation of dislocations, formation of twins, the interaction of dislocations and twins, and the relationship of these processes with the mechanical behavior of FCC metals are studied in the works [7,8].

In the manufacture of products using the 3D surfacing method, a mixed grain structure is formed. One of the characteristic features of which are the formations of large grains elongated in the direction of the surfacing plane. In this regard, the question of the behavior of individual grains with different crystallographic orientations and morphology under loading becomes topical. This will make it possible to predict mechanical properties and obtain products with an optimal grain structure.

Using aluminum bronze as a model material and data on the crystallographic and morphological characteristics of the product obtained by 3D electron-beam surfacing [9], the following problem was posed. Establish for individual grains (single crystals) the influence of the compression axis crystallographic orientation and lateral faces and their morphology on structural changes during deformation and their relation to stress by molecular dynamics simulation.

2. Materials and methods

Simulation of plastic deformation by compression of single crystals aluminum bronze (Cu-13at.% Al) was carried out by molecular dynamics. The crystal has the form of a tetragonal prism with dimensions 30a×60a×30a (h/d=2) and 30a×30a×30a (*h/d*=1) along X, Y, and Z axes (a is the lattice constant of the aluminum bronze). The deformation was determined by moving at a constant speed of 5 m/s with two rigid 5A-thick atomic layers in the plane X0Z above and below the sample. The LAMMPS software package and the interparticle potential constructed using the embedded atom method were used for simulating. The equations of motion of atoms were integrated by the Verlet high-speed method. The OVITO [10] program allows consideration of movement and interaction of locations in crystal structures. This is achieved by applications of the program. The common neighbor analysis [11] was used to determine the structural location of each atom and to determine the type of crystal lattice (BCC, FCC, HCP). The dislocation extraction algorithm [12] converted the initial atomistic representation into a linear representation of dislocations and the determination of their Burgers vectors. The analysis made it possible to systematize dislocation complexes that carry out sliding along with Shockley dislocations or are barriers to sliding [13].

3 The relationship between the structural changes and the deformation curve

The results of molecular dynamic simulation showed that plastic deformation of single crystals of aluminum bronze is carried out by the generation of Shockley dislocations from the places of stress concentration. Originating at the vertices of the sample, they slip in the octahedral plane through the crystal. In single crystals oriented for sliding along three (orientation of the load axis Y – [111]) and four (orientation of the load axis Y – [100]) equally loaded planes, it becomes possible to interact with dislocations in adjacent planes. As a result, slip is performed by complex defects consisting of Shockley dislocations and dislocations of other types [13,14]. Areas with a higher dislocation density are formed in these crystals. When simulating, they are observed near the loaded layers. The lateral surfaces of the crystal are set free. The interacting dislocations in the thickenings carry out oscillations. After some time, the dislocation or dislocation complex breaks away from the thickening and goes through the crystal.

Consideration of the deformation of Ni and Cu-13at.% Al single crystals with the compression axis orientation [111] showed that, regardless of the magnitude of the stacking fault energy (SFE), their stress-strain curves consist of areas of increase and decrease in the values of the acting stress [13]. These curves characterize the process at the micro-level and describe elementary slip events (Fig. 1). The highlighted section of the stress-strain curve can be compared with the processes of changes in the dislocation structure in the simulated volume. The stress reduction section coincides with the sliding of the dislocation complex from one cluster to another dislocation cluster (A in Fig. 1 and Fig. 2a). No displacements are observed in stress-strain curve areas (B in Fig. 1 and Fig. 2b). Shockley partial dislocations take an active part in the formation of dislocation complexes. Thus, the areas of softening on the stress-strain curve are due to relaxation (decrease) of stress because of sliding of dislocations. If the increase in load is not accompanied by sliding, then an increase in stress is observed on the curve.

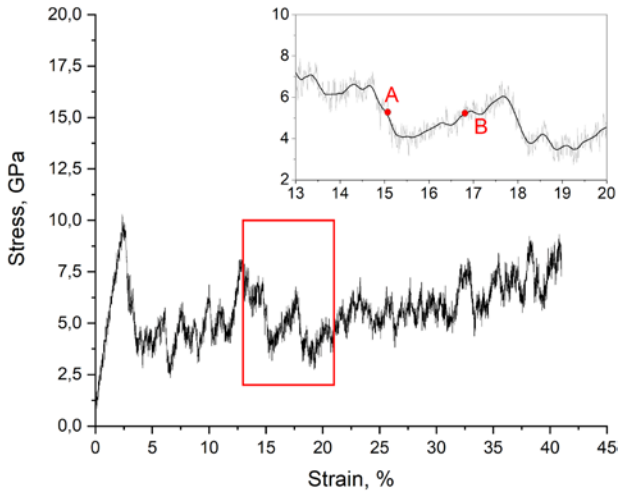
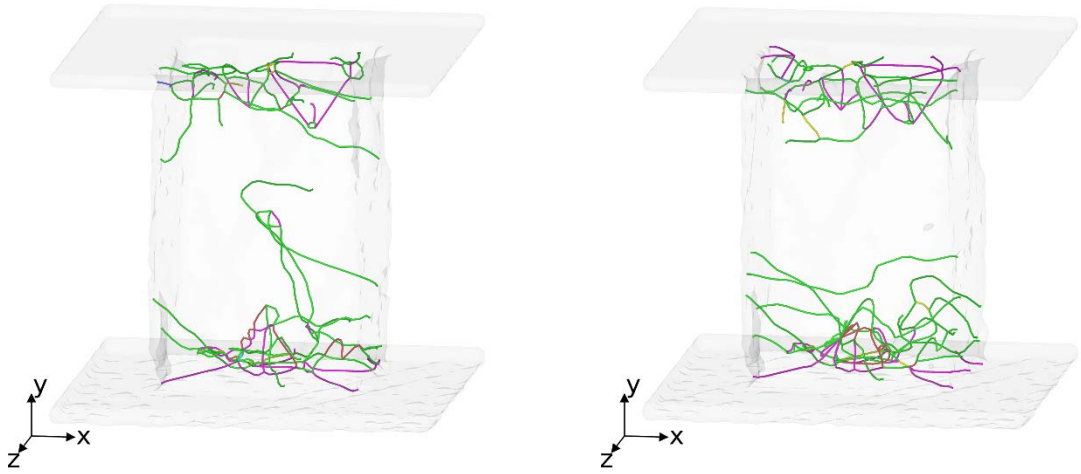


Fig. 1. The stress-strain curve of Cu-Al alloy single crystal with a highlighted fragment, that shows areas of hardening and softening



a) b)

Fig. 2. The evolution of the dislocation structure of Cu-Al alloy single crystal at strain: (a) 15%; (b) 16.8%

It can be assumed that the stress level that the dislocation structure withstands under load is related to the strength of dislocation configurations from interacting dislocations. In this case, it speaks of a substructural hardening mechanism. The contribution to the resistance to dislocation motion associated with a dislocation structure without sub boundaries depends on the density of dislocations. The empirical formula gives a proportional relationship with the square root of the average dislocation density for a uniform distribution of dislocations [15]. In the formation of dislocation clusters, the inversely proportional relationship between the stress and the distance between dislocation clusters is usually considered. Nickel has a high SFE, and dislocation clusters are observed in it from the very beginning of plastic deformation. Therefore, the stress level at the second stage of the deformation curves is associated with the distance between these clusters [15]. Alloy Cu-13at.% Al has a low SFE value. The dislocation clusters are formed already at developed deformation during the transition to the third stage of the strain hardening curves. Deformation can also occur by twinning. The tendency to form clusters or deformation by twinning depends on the crystallographic orientation, temperature, and strain rate.

The molecular dynamics method provides a unique opportunity to isolate dislocations of different types and makes it possible to determine the fraction of the length of each of them in the volume of the simulated crystal. The fraction of the length of each type of dislocation and calculated stress depending on the strain is shown in Fig. 3. The most mobiles are complete perfect dislocations $\frac{a}{2}\langle 110\rangle$ (blue) and Shockley partial dislocations $\frac{a}{6}\langle 112\rangle$ (green). The detailed mechanism of sliding of a complete dislocation in an FCC crystal by splitting into partial ones is considered in [13]. Partial dislocations make up the bulk of dislocations and provide the main deformation of the crystal. Other types of dislocations are observed in the simulated crystal. Stair-rod dislocations $\frac{a}{6}\langle 110\rangle$ (magenta), Hirsch $\frac{a}{3}\langle 001\rangle$ (yellow), and Frank partial dislocation $\frac{a}{3}\langle 111\rangle$ (cyan) are highlighted separately. Dislocations of other types $\frac{a}{3}\langle 110\rangle$, $\frac{a}{3}\langle 112\rangle$, $\frac{a}{6}\langle 013\rangle$, $\frac{a}{6}\langle 114\rangle$, and some others are combined into one group (red). These dislocations form stationary configurations or low-mobility dislocation complexes [14]. Slow dislocation complexes provide sliding simultaneously along two adjacent planes. This option is realized only for the orientations of the deformation axes [100] and [111]. According to the simulation results, upon deformation of single crystals with the [110] compression axis,

dislocations of different slip systems practically do not interact. This orientation has the lowest stress level. The main dislocation type is Stair-rod dislocations.

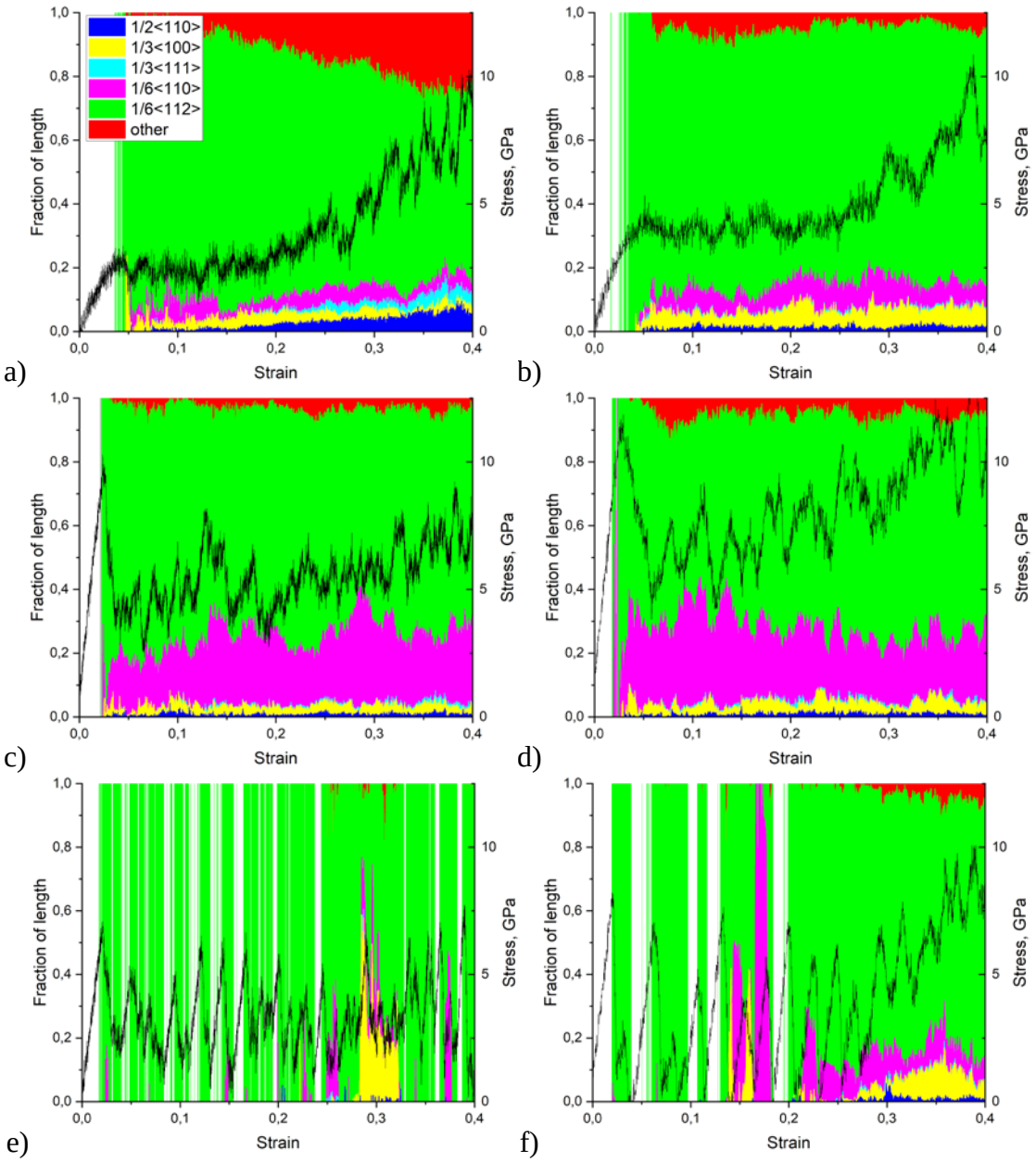


Fig. 3. The fraction of the length of each type of dislocation (P) depending on the strain in [100] single crystal with {001} lateral faces (a, b), [111] single crystal with {111}/{112} lateral faces (c, d) and [110] single crystal with {110}/{001} lateral faces (e, f). The black line is the stress-strain curve. Samples with an h/d ratio equal to 2 (a, c, e) and 1 (b, d, f)

The ratio of the share of Stair-rod dislocations to Shockley dislocation differs for materials with different SFE. For [111] nickel single crystals, this ratio is 0.67, and for the Cu-13at.% Al alloy one is 0.25. The ratio of these values is 2.7, which corresponds to the ratio of the operating stress levels of these materials. An analysis of the dislocation structure of these materials showed that a higher SFE favors the formation of tetrahedral complexes from Stair-rod dislocations. These complexes are stable dislocation configurations in a noticeable range of increasing stresses, making it difficult for dislocations to slip. These data show the important role of Stair-rod dislocations in deformation resistance and their contribution to

hardening, as well as tetrahedral complexes from these dislocations. However, the formation of tetrahedral complexes depends on the number of equally loaded slip systems. Their formation is observed for the orientations [100] and [111]. Tetrahedral complexes are not formed when the deformation axis is oriented [110]. The difference in dislocation formation for orientations at the corners of the stereographic triangle causes different stress levels (Fig. 3 a, c, e). The stress comparison is carried out using the approximated average of stress fluctuations for deformation of 0.4. A comparison of the stress values for samples with *h/d* = 2 gives a value of 7.5 ... 9 GPa for the [100] and [111] orientations, and for the [110] orientation this value is lower and amounts to 5 GPa. An important feature is the lack of hardening for the latter orientation. This corresponds to the case of weak interdislocation interaction. The increased stress is caused not only by the density of the barriers to slip dislocations, but also determined by crystallographic and geometric factors. They determine the initial conditions for shear in a slip system.

Therefore, when considering the influence of the compression axis on the density of the barriers and the stress level, take into account the influence of the crystallographic orientation of the lateral faces and the height of the sample. Changes in these parameters reveal the role of the geometric (morphological) factor in the development of the shift. A comparison of the influence of the crystallographic orientation of the lateral faces was made for the orientations [100] and [110]. [100]-monocrystals are modeled with lateral faces {001} and {110}. For this orientation, 8 shear systems (4 planes, 2 directions in each plane) are equally loaded. As noted in [14], sliding, in this case, is accomplished by complex defects in adjacent planes. The difference in the orientation of the lateral faces has little impact on the fraction of the types of dislocations formed. This seems to be associated with a slightly higher stress value for [100]-single-crystal lateral faces: {001} – 9 GPa and {110} – 7.5 GPa. The general development patterns of the dislocation structure in both single crystals are identical. In [110]-monocrystals were examined with two sets of lateral faces: {110}/{001} and {111}/{112}. In both cases, there is a weak interaction of gliding dislocations and a change in the local stress near the same average level of 5 GPa. A short-term increase in stress is associated with the formation of Stair-rods or Hirsch dislocations, and a decrease with their disappearance.

One of the parameters describing grain morphology is their shape. It can be described by the shape factor, which characterizes the degree of deviation of the shape from the equiaxial one. Three main axes of the ellipse inscribed in the grain can be taken as the shape parameters. In axially symmetric form, the degree of inequality is described by the ratio of the longest axis of the ellipse to the shortest axis. As a variable parameter when simulating single crystals in the form of the tetragonal prism, we took the ratio of the sample height to its width. We used the ratios of these parameters equal to two and one. In these cases, we also have a difference in the scheme of principal stresses in such samples in the presence of end face friction. The geometric position of the main stress concentrators, which are the tops of the sample and the end face ribs, changes as well. Their position relative to the deformed volume for single crystals with different h/d ratios will differ. Reducing the height of the sample increases the probability of interaction between dislocations of different slip systems. This is reflected in the simulation results. If we compare orientations with different ratios of specimen height to width (Fig. 3), then the following conclusions can be drawn:

1. The strain stress of a single crystal with h/d = 1 is equal to or slightly higher than in single crystals with h/d = 2.
2. A change in the sample height leads to a redistribution of the fraction of low-mobility dislocations, which play the role of barriers to the development of shear.

In fact, by reducing the height of the sample at a constant width, we increase the volume fraction of stress concentrators, activate a large volume fraction of dislocation sources, and, therefore, increase the rate of accumulation of dislocations per unit volume, the probability of

interaction of dislocations and the formation of low-mobility dislocations that prevent slip. As a result, the formed dislocation structure provides a higher level of stress. This effect illustrates a somewhat different understanding of the action of the Hall-Petch equation. In this case, it is not the limitation of the path of dislocations by grain boundaries that are taken as a basis, but a higher probability of barrier-breaking by dislocations inside the grain. Although, technically, as the height of the sample decreases, the average grain size decreases.

In addition, for a more complete analysis of the influence of the shear geometry on the stress level, it is important to consider the orientation of the shear directions and planes relative to the lateral faces. For the loading scheme between two punches with free lateral faces, the shear planes are in different conditions. In the deformed volume, depending on the crystallographic orientation of the faces, one can distinguish a volume in which there are no reverse stresses from the opposite punch and the shift is freely carried out towards the free surfaces [6-8]. The deformation is higher in this area. The presence of these areas somewhat reduces the amount of stress required for deformation. This causes a lower stress in [100] single crystals (h/d=2) with {110} lateral faces as compared to {001}. Dislocations in this volume reach the surface more easily without accumulating in the crystal. If the shear planes are limited by the punches of the testing machine, then thickening of dislocations occurs near them. We also note that as the height of the sample decreases, the rate of accumulation increases.

4 Conclusion

The results of simulating single crystals of aluminum bronze made it possible to establish a relationship between dislocations of a certain type, dislocation complexes, their mobility, and deformation curves. The fraction of the main types of dislocations, which determines the magnitude of the stress, has been identified. The leading role in shear resistance, in the formation of mobile and stable dislocation complexes (tetrahedral), belongs to Stair-rod dislocations. It is shown that the decrease in stress is associated with the process of dislocation slip. The rise in stress corresponds to the period of no-slip, and the hardening value is determined by the dislocation interactions.

The influence of crystallographic and geometric (morphological) factors on the type of dislocations and their role in strengthening is considered. The shear in adjacent slip planes is realized by complex defects, and it is observed for the [100] and [111] orientations. For all orientations, there is a connection between the formation of the Stair-rod and other sedentary dislocations and the level of the acting stress. The orientation of the lateral faces has little effect on the formation of dislocations and stress. The main influence is exerted by the geometric arrangement of the planes relative to the base stress concentrators and lateral faces, as well as the volume fraction of the stress concentrators. These changes are manifested largely with a decrease in the height of the sample compared to the orientation of the lateral faces.

The simulation results make it possible to establish the texture and morphological parameters of the grain structure, which provide the greatest value of substructural hardening. The grain orientation relative to the applied load should be grouped near the <100> and <111> poles. The shape of the grains should be closer to the equiaxed. The increase in the Hall-Petch contribution is achieved by reducing the grain size. These results can be extended to FCC materials and used as criteria for obtaining the optimal structure of products.

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