Interaction of edge dislocation with copper atoms in an aluminum crystal

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Abstract. In this work, the interaction of the moving edge dislocation with obstacles in form of copper atoms is studied using the molecular dynamics simulations. The samples are aluminum monocrystals of $52 \times 60 \times 15 \text{ nm}^3$ with axes oriented along directions $[\bar{1}10]$, $[111]$, $[11\bar{2}]$. The structure of copper solid solution is reproduced with following procedure: aluminum atoms are randomly selected and replaced by copper atoms. The concentration of copper atoms varies from 0.25% to 1%. The dislocation movement occurs under action of shear deformation. It is found that zones with a low concentration of copper atoms only slow down dislocation in an aluminum matrix, and the zones with a high local concentration of copper atoms not only produces stronger resistance to dislocation movement, but also they cause the change in the slip plane of the dislocation segment. When a significant part of a dislocation line moves to a neighboring slip plane, the complete transition of the dislocation to this slip plane can occur. It is also noted that such transitions of dislocation segments from one slip plane to another are accompanied by the formation of vacancies. Also the maximum value of the shear stress $\sigma_{xy}$ is estimated–its value is approximately 250 MPa.

1. Introduction
The interaction of dislocations with obstacles of various types is a very important problem in connection with the practical use of metal alloys. For example, the hardening of metals by heat treatment or plastic deformation can lead to slip dislocations and they can meet various obstacles or inclusions. At the moment, the internal processes occurring as a result of the interaction of the edge dislocation with various obstacles are not completely understood and require further study. Molecular dynamics (MD) method is one of the most powerful tools for studying processes at the atomic scale which is used to study the aforementioned problem. For example, the paper [1] describes the need for calculating the energy of a dislocation core using first-principles calculations to examine interactions of dislocations in solid solutions. Besides, the general nature of the dislocations behavior can be described via MD method, because it is possible to carry out a lot of simulations with different temperatures, loads, etc. The study [2] also uses this method to compare the existing theory of dislocation interaction and simulation data and shows that the theory does not always describe the interaction well, and there is a need to verify the results of the theory using MD method. Today, research on the interaction of dislocations and foreign inclusions is actively conducted: part of such works is devoted to hardening of alloys by impurity atoms [1–3], others concentrate on the interaction of dislocations and nanoscale inclusions [4–9]. The data obtained at the atomistic level are then used in continuum or discrete dislocation dynamics models of plastic deformation of metals [5, 10–13].
In the present work, a solid solution of copper in aluminum is studied, since copper is the main additional component of aluminum alloys widely used in technical applications stimulating both experimental and theoretical studies. The general behavior of an edge dislocation is studied in its interaction with atoms of a copper solid solution.

2. MD simulation setup
The movement of dislocations in metals happens during plastic deformation. In this work, the MD method is used to simulate the plastic deformation in the aluminum crystal [14]. The method of classical MD is a powerful tool for modeling the plastic deformation of metals, and the results of simulations agree with experimental data, as, for example, in [5, 15, 16]. The atomic interactions are determined by the angular dependent potential (ADP) for aluminum and copper [17]. The description of Al–Al and Cu–Cu interactions in this potential was previously formulated by authors for embedded atom method (EAM) formalism and it was shown that these two potentials well reproduce elastic constants and energy of various defects for both aluminum and copper [18, 19]. Angular dependent potential additionally accounts the energy of noncentral atomic interactions that are introduced through the dipole and quadrupole summands into the total energy. These terms take into account lattice distortions from a cubic structure, which can occur locally when an aluminum atom is replaced by a copper atom, or when hardening phases are formed in aluminum–copper system. The authors [17] demonstrated that ADP well reproduces lattice parameters, formation energies, and elastic constants of the main hardening phases in Al–Cu system such $\theta$ and $\theta'$ phases. This potential was previously used in MD study of hardening of Al–Cu alloy in case of Guinier–Preston zones [5] and in case $\theta'$ phase [9], where some comparison with experimental data on dynamical loading of aluminum–copper alloys was performed. The first step is creating samples: the atoms in the monocrystal of aluminum with volume of $52 \times 60 \times 15$ nm$^3$ with the axes of system oriented along [110], [111], [112] crystallographic directions are randomly selected, then they are removed and the copper atoms are inserted at their positions. This scheme of axes orientation in an MD system is typically used in research of dislocations motion [20]. In this work, the samples with a concentration of copper atoms in the aluminum matrix of 0.25%, 0.5%, 1% are studied. After that the edge dislocation is created by an insertion of atomic half-plane to the system [21]. Initially, dislocation is located in the center of the system.

The second step is heating and relaxation of the crystal. The sample is heated to $T = 300$ K using the Nose–Hoover thermostat, and the system stresses are relaxed using the Nose–Hoover barostat during 10 ps with independent relaxation of $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$ components of stress tensor. After relaxation, the system is subjected to shear deformation: top layer of the crystal with 3 nm thickness is moved with a constant velocity of 3 m/s, while bottom layer of the same thickness is immobile. The temperature of system is maintained during the deformation at $T = 300$ K using a Nose–Hoover thermostat. Periodic boundary conditions along the X, Z axes are used to eliminate boundary effects during the simulation. Visualization and analysis of atomic structures are performed with the OVITO package [22].

3. Interaction of the moving edge dislocation with copper atoms
The edge dislocation begins to move in the aluminum crystal along the X axis during plastic deformation and interacts with many copper atoms on its way. The copper atoms are randomly located in the aluminum matrix. This means there are zones with high and low concentrations of copper atoms in solid solution. The zones with a high concentration (ZHC) of copper atoms are the main obstacles for the moving edge dislocation and further this study concentrated on them. If the dislocation stops at a meeting with ZHC, then the segment of this dislocation will go on the neighbor slip plane to bypass an obstacle. Then the dislocation passes the obstacle and
Figure 1. The vacancies formation during the interaction of the dislocation with the copper atoms. The dislocation segment leaves on the neighbor slip plane (a), the dislocation segment return on the main slip plane (b), the vacancy formation in the crystal (c).

Figure 2. The dependence of shear stress on time in the solid solution of aluminum and copper with the copper atom concentration of 0.5% (a) and in pure aluminum (b).

The dislocation segment goes back to the original slip plane. During the return of the segment to the initial slip plane, it emits vacancies lying on this plane. This process is shown in figure 1. The movement of a dislocation in the presence of many obstacles leads to a significant increase in the shear stresses acting in the system in comparison with pure aluminum. In pure aluminum, after initial acceleration, the dislocation moves at almost constant velocity, which makes small oscillations around the mean value [figure 2(b)]. Such oscillations can be explained by successive entering of a dislocation through periodic boundaries into the trace of another dislocation, as it was shown in work [23]. Average level of shear stress in the case of copper solid solution is about 250 MPa. Such a high value is related to the limitation of the dislocation velocity due to the constant interaction of the dislocation with impurity atoms.

The dislocation can completely transit to the neighbor slip plane of aluminum crystal in the case of high concentration of copper atoms in the aluminum matrix. Figure 3 shows the edge
dislocation, which is shifted to several neighbor slip planes from its initial slip plane in the sample with the highest concentration of copper atoms that is equal to 1%. In addition, there are many vacancies on each slip plane of dislocation. This mean that the dislocation does not immediately leave to another slip plane, but moves for some time on each plane and overcomes the obstacles.

Consider in more details the process of complete transition of dislocation to the neighbor slip plane. The time dependence of the shear stress component $\sigma_{xy}$ has two maxima corresponding to the simulation times of 600 ps and 1200 ps; this curve is shown in figure 2(a). These peaks correspond to the complete transition of the dislocation to the neighbor plane. Consider the first maximum: the dislocation is still in the initial slip plane while the shear stress begins to increase until reaching the peak (approximately 500 ps). At this moment, the dislocation interacts with the ZHC [figure 4(a)], which represents a strong resistance to the movement of the dislocation. This interaction immobilizes dislocation for a long time. Dislocation is located in approximately same position during 100 ps. The immobilization of dislocation for this time interval causes the increase in shear stress. Achieving a high level of shear stress stimulates the ejection of a dislocation segment into the neighbor slip plane that allows it to overcome an obstacle [figure 4(b)]. As mentioned above, the formation of vacancies is associated with the transition of the dislocation segment between close slip planes, and this fact shows that the dislocation experiences many transitions of this kind before it has completely gone to another slip plane. The dislocation completely passes to the neighbor plane by the time 720 ps. The similar situation occurs for the peak at time 1200 ps.

4. Stress state of solid solution of aluminum and copper
As it was shown in work [23], the motion of dislocation occurs under the action of local shear stress. So we analyze the distribution of local stress near the dislocation line. The stress tensor per atom is calculated to estimate the local stresses in the crystal during simulation of plastic deformation [24]. The calculated $\sigma_{xy}$ value is averaged over a region representing a sphere with a diameter of 1 nm for constructing a map of local shear stresses in the sample.

The initial state of local shear stress is presented in 5(a): dislocation affects the distribution of local shear stresses in the crystal, because it has its own stress field. The development of plastic deformation leads to the formation of a local stress distribution close to the initial distribution of local shear stresses in crystal before and after the dislocation transition into the neighboring slip plane [figure 5(b)]. However, the total system stresses [figure 2(a)] have an interesting feature: initially, their value quickly increases, but after approximately 400 ps they fluctuate within 250–270 MPa (if large peaks are ignored in values of shear stress caused by the dislocation transition.

Figure 3. Motion of edge dislocation in solid solution of Al and Cu with a concentration of Cu atoms of 1%.
Figure 4. The edge dislocation before (a) and after (b) the complete transition to the neighbor slip plane in the aluminum and copper solid solution with the copper atom concentration of 0.5%.

Figure 5. The map of local shear stresses $\langle \sigma_{xy} \rangle$ at the beginning of deformation (a) and between complete dislocation transitions (b).

to another slip plane. This means that if the solid solute is deformed with a constant strain rate than this system will have a stationary state, at least for such simulation times. As noted previously in section 3, the shear stresses accumulate in the crystal when the edge dislocation leaves to close slip plane. Figure 6 shows that the value of local shear stresses
Figure 6. The map of local shear stresses $\langle \sigma_{xy} \rangle$ at the beginning of the dislocation transition to the neighbor slip plane (a) and at the time preceding the full transition (b).

increases in the crystal during the transition of dislocation: the large magnitude of local shear stresses in areas to the right of the dislocation is occurred when dislocation experiences inhibition after its interaction with ZHC. The edge dislocation starts moving again after about 60 ps and value of local shear stresses is relaxed [figure 5(b)]. It can be assumed that the complete transition of the edge dislocation to the neighbor plane is a threshold effect, which depends on a certain value of local shear stress in the zone near to the right of the dislocation.

5. Conclusions

In this paper, the interaction of edge dislocation with copper atoms in the solid solution of copper in aluminum matrix is investigated where copper atoms randomly located in the aluminum matrix. The crystal has volume of $52 \times 60 \times 15 \, \text{nm}^3$ and axes of system are oriented along $[\overline{1}10], [111], [11\overline{2}]$ crystallographic directions. The plastic deformation of crystal is performed using MD method for simulations of the motion of dislocation.

It is shown that zones with a high concentration of copper atoms in the solid solution are strong barrier to motion of edge dislocation, and dislocation can overcome them by ejection of segment to the neighbor slip plane. This effect is accompanied by the formation of the vacancies in the slip plane of the dislocation motion.

There are two peaks of the maximum on the dependence of shear stress and they correspond to the complete transition of the dislocation to the neighbor slip plane. The shear stresses $\sigma_{xy}$ reaches a maximum value of 350 MPa at the first peak of dislocation transition. Besides, the dependence of the shear stresses fluctuates in the range of 25–270 MPa after about 400 ps.

The map of local shear stress shows that the complete transition of the dislocation to the neighboring slip plane is a threshold effect and occurs after the accumulation of sufficiently large values of local shear stresses in the zones in the crystal close to the location of dislocation (value of local shear stress is approximately 1.6 GPa).
Acknowledgments
The work is supported by grant No. 18-71-10038 from the Russian Scientific Foundation.

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