Diffusion mechanism at grain boundaries in two-dimensional metals

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Abstract

The present paper is concerned with the research of diffusion mechanism at grain boundaries in two-dimensional metals by the method of molecular dynamics. It is found that the fundamental diffusion mechanism at low-angle grain boundaries of two-dimensional metals is the result of interaction of grain boundary dislocation pairs. The creep of dislocation pairs in the opposite sides is observed in the experiments. The chains of the displaced atoms can be seen in the directions connecting the cores of two dislocations. In high-angle boundaries, the chains of the displaced atoms form between the areas of local pressure and tension.

Keywords: Molecular dynamics; Diffusion; Grain boundaries; 2D metals; Diffusion mechanism

1. Introduction

The process of diffusion at grain boundaries takes a prominent place among different aspects of diffusion. This research concentrates in particular on the problem concerning the diffusion at grain boundaries, because it proceeds more intensively than over the volume. The relation of the diffusion coefficients at the boundary and volume usually has the values $D_b/D > 10^5$ at $T < 0.6 \cdot T_m$ (where T = temperature, T_m = melting temperature) [1]. As many researches show [2], the relation D_b/D depends on mutual orientation of grains. In this connection, the relation D_b/D is less when the density of coinciding sites is higher, in other words, when the boundary contains less density of structural irregularities. There are typical defects of grain boundaries: vacancies, interstitial atoms, and dislocations [2,3]. The diffusion mechanisms at grain boundaries are often connected with grain boundaries defects, which are more structurally 'washed' than in the volume of a crystal [2,3]. The most obscure mechanism is diffusion mechanism across the axis of grains tilt, in low-angle grain boundaries – across the cores of grain boundary dislocations. The present paper is devoted to the research of diffusion mechanism at grain boundaries in two-dimensional metals Ni, Cu and Al by the method of molecular dynamics. Diffusion at grain boundaries in a two-dimensional model proceeds only across the axes of the tilt of grains. The study of diffusion mechanisms in a three-dimensional system is connected with the difficulty of visualization of atomic displacements inside the calculated block. That is why a two-dimensional model is used in the present study. A two-dimensional model allows studying the trajectories of the displacements of atoms evidently by special visualizators in a diffusion process.

2. Method description

The packing of atoms of two-dimensional metals was corresponded to the plane (111) of FCC lattice. Interatomic interactions were described by pair central Morse potentials. The parameters of the potentials were chosen by the energy of sublimation of pure metals, the volume module of elasticity, and lattice's parameter. In addition, the given potentials were approved if they corresponded with the values of the temperature coefficient of a linear expansion, energy of vacancy formation, energy of vacancy migration and other values.

The relaxation of the systems under study was held by the method of molecular dynamics. The atomic displacement was calculated by the solving of the system of ordinary differential equations of Newton's movement. The interactions of atoms were limited by the distance

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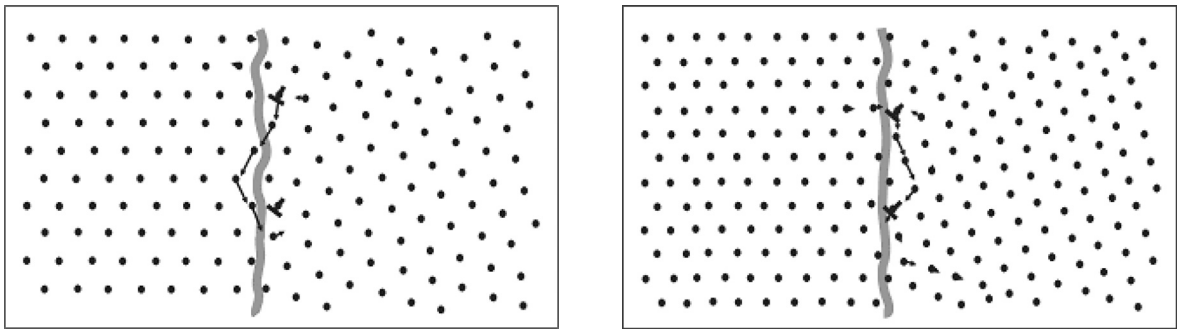


(a) (b)

Fig. 1. Atomic displacements (shown by black arrows in the scale 1:1) at the grain boundary with the angle of disorientation $\Theta = 16^{\circ}$: (a) at the moment of time 13.4 ps in two-dimensional Al at a temperature of 700 K; (b) at the moment of time 48.0 ps in two-dimensional Cu at a temperature of 910 K. The state of the grain boundary is marked by the grey line.

8 Å. The temporal step of recalculation of the movement equations system was equal to 10^{-14} seconds. The temperature was given by the initial velocities of atoms: every atom of the calculated block had the initial velocity equal to root-mean-square velocity in correspondence with Maxwell distribution multiplied by $\sqrt{2}$. The directions of the velocities were given as accidental ones, but on condition that total impulse of atoms in the calculated block was to be equal to zero.

Intergrain boundary was made by the turn of two crystal blocks relative to each other and the following conjugation. The conjugation included the procedure of the removing of excess atoms, dynamical relaxation, and cooling. An atom was removed in the case when the distance between two neighbouring atoms was less than $0.7 \cdot r_0$, where r_0 = minimal interatomic distance in an ideal crystal. The dynamical relaxation was then studied. During the relaxation, the atoms were displaced to the equilibrium positions. In this connection, the temperature of the calculated block increased to some small value. Cooling to 0 K was the final stage of preparation of the calculated block. The obtained configurations of the calculated block were used as starting points in the main experiments.

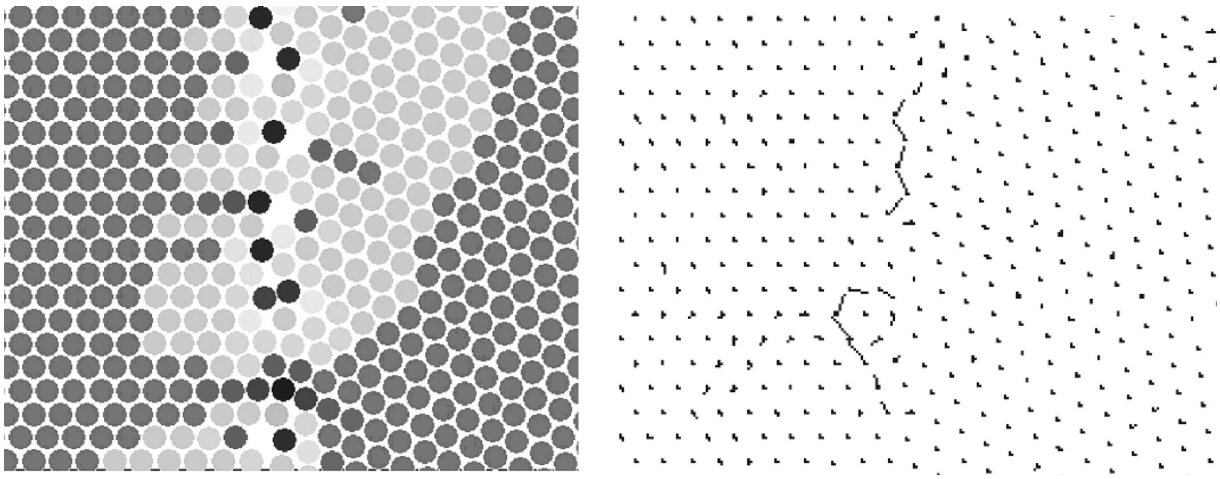
The calculated block contained about 5000 atoms. Rigid boundary conditions were applied on the block boundaries to avoid the migration of intergrain boundary outside the calculated block.

3. Results and discussion

The mechanism of grain boundary diffusion in two-dimensional metals was studied by the visualizator of the trajectories of atomic displacements. It was found that the fundamental diffusion mechanism at the low-angle grain boundaries of two-dimensional metals was the result of interaction of grain boundary dislocation pairs. The creep of dislocation pairs in opposite sides was observed in the experiments. The broken atomic row of one dislocation was lengthened at the expense of shortening of the other dislocation atomic row. In this connection, the chain of the displaced atoms was observed in the directions connecting the cores of two dislocations. The inverse displacements of atoms – the return of atoms to the initial positions – were observed. One of the important elements of a similar mechanism is the appearance of the vacancy in the chains of the displaced atoms. The trajectory of the vacancy migration from one dislocation core to the other can have ring reserved elements. These cause the appearance of ring exchange displacements of atoms at the boundary. Figure 1 shows the examples of the creep of grain boundary dislocations.

For high-angle grain boundaries, the diffusion mechanism is actually the same. However, the notion of grain boundary dislocations in this case loses its meaning. The mechanism can be interpreted as the interaction of point defects pairs: grain boundary vacancies, and interstitial atoms. The chains of the displaced atoms appear in the process of thermal movements of atoms (as in the case of low-angle boundaries) from pressure areas (interstitial atoms) to the tension area (vacancies). Figure 2(a) shows the areas of tension and pressure at the boundary with the angle of grains disorientation $\Theta = 24^{\circ}$ at the start of the experiment by different shades of grey colour. As it is seen from the figure, the areas of pressure and tension periodically alternate along the boundary. Figure 2(b) shows the displacements of atoms at the same segment of the boundary after 15 ps.

As in the case of low-angle boundaries, the important



(a) (b)

Fig. 2. The diffusion at the high-angle intergrain boundary ($\Theta = 24^{\circ}$) in two-dimensional Ni: (a) areas of pressure (dark areas) and tension (light areas) along the boundary at the start of the experiment; (b) the displacements of atoms at the same segment of the boundary after 15 ps at a temperature of 1400 K.

element of diffusion mechanism is the appearance of cyclic displacements of atoms. Non-closed chains of the displaced atoms, shown in Fig. 2(b), are less stable than the closed chains. They can have the reverse 'recoil' – the return of atoms to the previous positions. The closed chains appeared as the result of the filling of a vacancy formed in the initial chain of the displaced atoms by the atom which was not belonging to this chain.

4. Conclusion

The diffusion at the grain boundaries in two-dimensional metals Ni, Cu and Al was studied by the method of molecular dynamics. It was found that the fundamental diffusion mechanism at the low-angle grain boundaries of two-dimensional metals was the result of interaction of grain boundary dislocation pairs. The creep of dislocation pairs in opposite sides was observed in the experiments. The chains of the displaced atoms were found in the directions connecting the cores of two dislocations. In high-angle boundaries, the chains of the displaced atoms formed between the areas of local pressure (grain boundary interstitial atoms) and tension (grain boundary vacancies). The most stable were the displacements of atoms along the closed trajectories. The closed chains formed as the result of migration of a vacancy outside the initial chain of the displaced atoms.

References

[1] Bokshtein BS. Diffusion in Metals. Moscow: Metallurgiya, 1978.
[2] Glater G, Chalmers B. High-angle Grain Boundaries. Moscow: Mir, 1975.
[3] Kaybishev OA, Valiev RZ. Grain Boundaries and Properties of Metals. Moscow: Metallurgiya, 1987.