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MOLECULAR DYNAMICS INVESTIGATION OF GRAIN BOUNDARIES TENSIONS IN TRIPLE JUNCTIONS IN NICKEL

G.M. Poletaev[1*], D.V. Novoselova[2], V.V. Kovalenko[3], D.V. Kokhanenko[4], M.A. Iliina[4]

[1]Altai State Technical University, Lenin str. 46, Barnaul, 656038, Russia

[2]Kuzbass Institute of the Federal Penitentiary Service of Russia,

Oktyabrsky pr. 49, Novokuznetsk, 654066, Russia

[3]Siberian State Industrial University, Kirova Str. 42, Novokuznetsk, 654007, Russia

[4]Financial University under the Government of the Russian Federation, Barnaul brunch,

Lenin Str. 54, Barnaul, 656036, Russia

*e-mail: gmpoletaev@mail.ru

Abstract. In the work, the mutual tension of tilt grain boundaries with disorientation axes <111> and <100> in a triple junction on the example of nickel is investigated by the molecular dynamics method. The ratio of the boundary tensions found in the molecular dynamics model is compared with the ratio calculated using the Yang relation through the ratio of grain boundary energies. It is shown that both methods give close values. In addition, it was found that the elongation or contraction of low-angle tilt boundary at the triple junction motion is accompanied by the formation of zigzag displacements of atoms, which apparently appear due to the splitting and sliding of grain-boundary dislocations. The formation of new geometrically necessary dislocation during the boundary elongation occurred, as a rule, in the triple junction or in an already existing grain-boundary dislocation.

Keywords: molecular dynamics; triple junction; grain boundary; boundary migration; triple junction migration; boundary energy; boundary tension; tilt boundary.

1. Introduction

The triple junction (or triple line) of grain boundaries is a linear defect, along which three variously oriented grains or three grain boundary surfaces are conjugated. The mutual angles under which the grain boundaries are located in the triple junction are determined, as a rule, by the energy of the boundaries and their relative tension [1]. In most cases, the angles between the boundaries at the junctions are close to 120°, which indicates an approximately equal tension (and energy) of many boundaries [1, 2]. Nevertheless, for low-angle or special boundaries, the tension is much smaller than for the high-angle boundaries − the angles between the boundaries in triple junctions with the participation of such boundaries can differ significantly from 120° [1, 3, 4]. The connection between the energy of the boundaries and the angles between them in the triple junction describes the Herring equation [5]:

$$\sum_{i=1}^{3}\left(\sigma_i\vec{b}_i+\left(\frac{\partial\sigma_i}{\partial\varphi_i}\right)\vec{n}_i\right)=0, \quad (1)$$

where σ_i is energy of the *i*-th grain boundary; $\vec{n}_i$ is unit vector normal to the *i*-th boundary; $\vec{b}_i$ is unit vector directed from the junction along the *i*-th boundary; ϕ_i is angle characterizing the orientation of the *i*-th boundary in space (Fig. 1).

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The first term in equation (1) describes the mutual arrangement of the grain boundaries corresponding to the equilibrium state. The second − the equilibrium with respect to the rotation around the axis along the junction line. Rotation of the junction can occur not only at the stage of its formation, but also in the process of recrystallization and deformation [1].

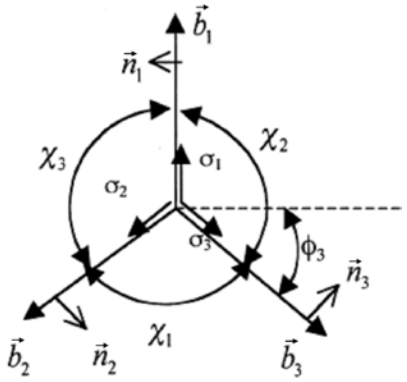

Fig. 1. Geometric parameters of the triple junction to the Herring equation. The figure is taken from [5].

In the case of equilibrium of the triple junction, when its configuration remains unchanged, the second term in the Herring equation (1) can be neglected. Then for the angles between the grain boundaries, we can write the Yang [5]:

$$\frac{\sigma_1}{sin\chi_1} = \frac{\sigma_2}{sin\chi_2} = \frac{\sigma_3}{sin\chi_3}, \quad (2)$$

The Herring and Yang equations are used to determine the relative energy of the grain boundaries by the angles between them in triple junctions. It was shown in [3, 4], for example, that special boundaries, possessing a relatively small energy, can adjoin to the junction even at an angle close to 90°. In addition, in work [3] it is said that the tension of the high-angle boundaries and the boundaries of the mixed type is approximately the same.

Triple junctions, as grain boundaries, can migrate. Migration of triple junctions and a change in their configuration play an important role in the deformation of polycrystals with a small grain size, so at the present time, much attention is paid to the mobility of triple junctions. However, the assumptions underlying the classical theories of grain growth are debatable, especially for the case of nanocrystalline materials [6]. For instance, experiments [7-9] and the results of computer simulation of grain growth [10, 11] have shown that the mobility of ternary joints of grain boundaries is a finite value. It is noted in [7-11] that there are two temperature sections of the motion of the system of boundaries with a triple junction in metals: at low temperatures the junction has a retarding effect on the mobility of the system (junction kinetics) − its mobility is less than the grain boundaries; at high temperatures the mobility of the system is determined by the mobility of grain boundaries (boundary kinetics), that is at high temperatures the junction becomes more mobile than the boundaries. For different materials and types of grain boundaries, there is a different transition temperature from the junction to the boundary kinetics.

In the model of L.S. Shvindlerman et al [7, 8] it is considered the migration of the triple junction due to the tension of the boundaries 1 and 2 (having approximately equal tension), which "pull" the boundary 3 on themselves. The motion of the triple junction occurs along the line of boundary 3, while the boundary 3 itself lengthens during the migration process. According to the works of L.S. Shvindlerman with co-authors [7, 8], the criterion for the transition from the boundary kinetics to the junction kinetics during the triple junction migration is the parameter Λ:

$$\Lambda = \frac{2\varphi}{2\cos\varphi - \sigma_3/\sigma}, \quad (3)$$

where φ is the dihedral angle at the vertex of the triple junction (half the angle between boundaries 1 and 2), σ is the surface tension of boundaries 1 and 2 (in the Shvindlerman model it is assumed that the boundaries 1 and 2 have equal tension), σ_3 is the surface tension of the boundary 3. At $\Lambda<<1$ the angle $\varphi \rightarrow 0$ and the velocity of motion of the system is controlled by the mobility of the triple junction (junction kinetics regime). For $\Lambda>>1$ the angle φ tends to its equilibrium value, which is typical for a fixed boundary system. The velocity of the system of grain boundaries with the triple junction in this case does not depend on the mobility of the triple junction and is determined only by the properties of the boundaries (boundary kinetics regime). At the junction kinetics, the reduced mobility of the triple junction according to [7, 8] is determined by the formula

$$A_{tj} = \frac{\upsilon a}{2\cos\varphi - \sigma_3/\sigma} = A_{0tj} \exp\left(-\frac{H_{tj}}{kT}\right), \quad (4)$$

where υ is the migration velocity of the triple junction, a is the distance between boundaries 1 and 2 in the Shvindlerman model, A_{0tj} is pre-exponential factor, H_{tj} is the activation energy of the junction migration, k is the Boltzmann constant, T is the temperature.

As can be seen, in formulas (3) and (4), needed for determining the relative mobility of triple junctions, the ratio of the boundary tension at the joint σ_3/σ is used. To apply the mathematical model of triple junction migration in computer simulation, it becomes necessary to conduct additional studies to determine the ratio σ_3/σ. The present paper is devoted to calculating the ratio σ_3/σ using the molecular dynamics method.

2. Description of the model

The study was carried out using the example of triple junctions of tilt boundaries with misorientation axes <111> and <100> in nickel. The ratio of the boundaries tensions at the junction σ_3/σ was found by two methods: using the Yang's equation (2) and by the energy values of the joining boundaries.

In the first case, it was held the simulation using the molecular dynamics method for establishing an equilibrium correlation of the angles between the boundaries in the junction. The ratio σ_3/σ was determined through the Yang relation [5]:

$$\frac{\sigma_3}{\sigma} = \frac{sin\chi_3}{sin\chi}, \quad (5)$$

where χ_3 is the angle between boundaries 1 and 2 ($\chi_3=2\varphi$), χ is the arithmetic average of the angles χ_1 and χ_2 (in the Shvindlerman model it is assumed that the angles χ_1 and χ_2 are equal).

The calculation block was created in the form of a cylinder (Fig. 2) of a sufficiently large diameter to establish the equilibrium angles between the boundaries. The diameter of the calculation blocks was approximately 260 Å. The blocks contained from 55000 to 59000 atoms. The thickness of the cylindrical blocks, on the contrary, was chosen to be small − 6 atomic planes, which made it possible to select blocks of larger diameter with the same number of atoms. The thickness was 12.2 Å for <111> tilt boundaries and 10.6 Å for <100> boundaries. In total, 8 triple junctions were considered: 4 different sets of joining boundaries for the misorientation axes <111> and <100>: 15°/15°/30°, 30°/25°/5°, 30°/20°/10°, 5°/5°/10°. The lateral surface of the cylindrical blocks during the computer experiment was rigidly fixed (rigid boundary conditions). Along the Z axis, periodic boundary conditions were imposed.

The interactions of nickel atoms with each other were described by the Cleri-Rosato potential [12]. This potential has proved itself well in a number of calculations of the structural and energy characteristics of metals performed by molecular dynamics [13-16]. The

time integration step in the molecular dynamics method was equal 5 fs. Temperature in the model was set by changing the velocity of atoms in accordance with the Maxwell-Boltzmann distribution. To keep the temperature constant during the simulation, the Nose-Hoover thermostat was used.

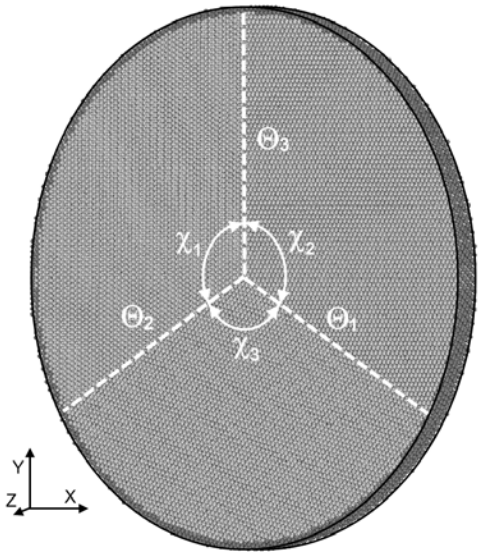

Fig. 2. The calculation block with the initial configuration of the boundaries at the junction. Θ_1, Θ_2, Θ_3 – misorientation angles of the grains.

The simulation was carried out at the temperature of 1700 K for 2000 ps. This duration of the computer experiment, as a rule, was sufficient to establish an equilibrium configuration of the boundaries in the triple junction at the given temperature. At the end of each experiment, the calculation block was cooled to 0 K to study the final structure and displacements of atoms during the grain boundaries migration.

3. Results and discussion

During the computer experiments, interesting features related to the atomic mechanism of changing the length of the low-angle boundary 3, boundary which is prolonged as a result of migration of the triple junction (the vertical boundary at the top in Fig. 2), were found. The nucleation and disappearance of grain-boundary dislocations was accompanied by the formation of zigzag displacements of atoms. Fig. 3a shows an example of the formation of new grain-boundary dislocation at elongation of <100> 5° low-angle boundary as a result of migration of <100> 30° (right) and <100> 25° (left) high-angle boundaries. The appearance of new dislocation is geometrically necessary. With gradual elongation of the boundary (due to the reduction of the high-angle boundaries 1 and 2), the appearance of new torn atomic half-plane, i.e. edge dislocation, occurs not in the pure crystal, but in the region of another defect: another dislocation or high-angle boundary. In the example shown in Fig. 3a, the doubling of the Burgers vector occurred in the existing grain boundary dislocation. After this, the dislocations pushed away from each other and dispersed along the slip planes with the formation of zigzag atomic displacements (Fig. 3a). The increase in the Burgers vector occurred spasmodically, in connection with which the migration rate of the junction and the lengthening of the boundary 3 changed abruptly. Migration slowed down before the formation of a new grain-boundary dislocation and acceleration after.

When modeling the migration of the junction of <111> tilt boundaries, it was noted that the boundaries with such misorientation axis migrate much faster than <100> boundaries, which is apparently connected with the difference in the formation energy of grain-boundary

dislocations in the considered boundaries. At the same time, the mechanism of elongation of <111> low-angle boundary was analogous to the mechanism of elongation of <100> boundary. Moreover, this mechanism turned out to be reversible − with the shortening of the length of the low-angle boundary, the reverse process took place: two dislocations merged into one with a subsequent abrupt decrease in the Burgers vector. Fig. 3b shows an example of zigzag atomic displacements when <111> 10° low-angle boundary reduced during <111> 5°/5°/10° triple junction migration.

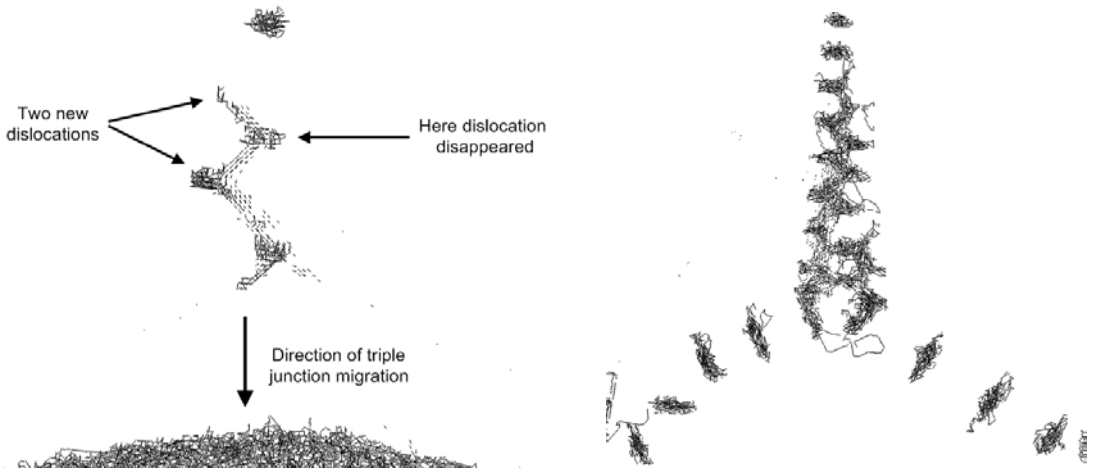

Fig. 3. The formation of zigzag atomic displacements during the migration of the triple junction: a) when <100> 5° low-angle tilt boundary elongated as a result of migration of <100> 30° (right) and <100> 25° (left) high-angle boundaries; b) when <111> 10° low-angle boundary reduced (the vertical boundary from above) during migration of <111> 5°/5°/10° triple junction.

The second method for determining the ratio of the boundary tensions in the triple junction σ_3/σ was to find the ratio of grain-boundary energies. It was assumed that the tension of the boundary is proportional to its energy. The values of the boundaries energy were taken from [17], where they were calculated using the same interatomic interaction potential as in the present paper. Figure 4 shows graphs of the dependences of the energy of <111> (a) and <100> (b) tilt boundaries for metals Ni, Cu, Al, taken from [17].

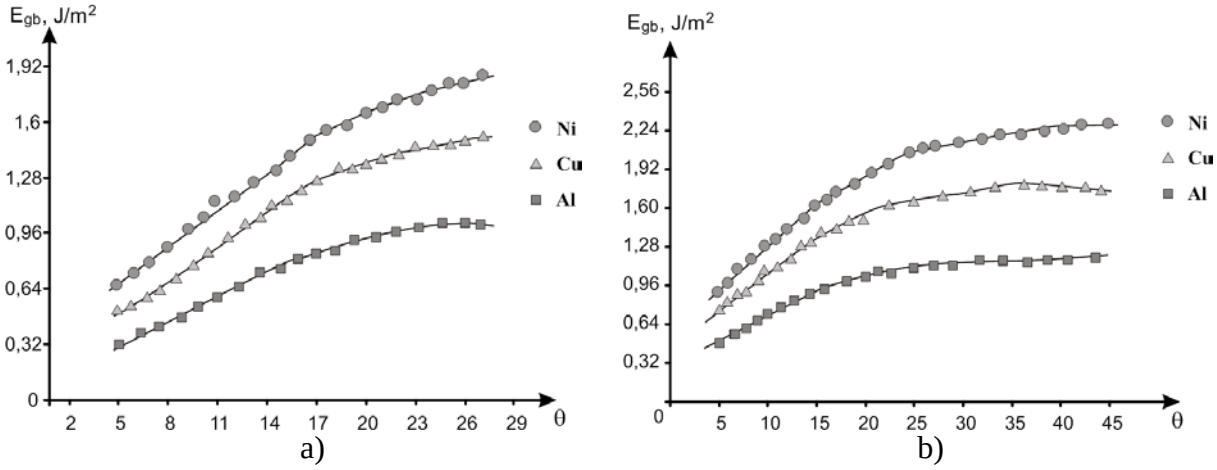

Fig. 4. Dependences of the energy of <111> (a) and <100> (b) tilt boundaries on the misorientation angle for metals Ni, Cu, Al, taken from [17].

This method of determining the ratio σ_3/σ, from our point of view, is more accurate, since potentially more errors are possible in the first method. Nevertheless, as it turned out, the agreement between the two methods is quite good. Table 1 shows the values of the ratio σ_3/σ obtained by both methods for the considered triple junctions.

Table 1. Values of the ratio σ_3/σ for the considered triple junctions.

The axis and misorientation angles of the joining boundaries	$\frac{\chi_3}{\chi}$, Model (I)	$\frac{\sigma_3}{\sigma}$, Model (I)	$\frac{\sigma_3}{\sigma}$, Theory (II)
<111> 15°/15°/30°	94 / 133	1.36	1.32
<100> 15°/15°/30°	112 / 124	1.12	1.29
<111> 30°/25°/5°	155 / 102,5	0.43	0.37
<100> 30°/25°/5°	161 / 99,5	0.33	0.44
<111> 30°/20°/10°	138 / 111	0.71	0.67
<100> 30°/20°/10°	144 / 108	0.62	0.64
<111> 5°/5°/10°	112 / 124	1.12	1.53
<100> 5°/5°/10°	114 / 123	1.09	1.37

4. Conclusion

In the work, the mutual tension of tilt grain boundaries with disorientation axes <111> and <100> in a triple junction on the example of nickel is investigated by the molecular dynamics method. The ratio of the boundary tensions found in the molecular dynamics model is compared with the ratio calculated using the Yang relation through the ratio of grain boundary energies. It is shown that both methods give close values.

Triple junctions of <111> boundaries migrated faster than junctions of <100> boundaries, but the mechanism of elongation or reduction of the boundaries at the junction motion had similarities. It was found that the elongation or contraction of low-angle tilt boundary is accompanied by the formation of zigzag displacements of atoms, which apparently appear due to the splitting and sliding of grain-boundary dislocations. The formation of new geometrically necessary dislocation during the boundary elongation occurred, as a rule, in the triple junction or in an already existing grain-boundary dislocation.

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