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Molecular dynamics study of migration mechanism of triple junctions of tilt boundaries in fcc metals

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ABSTRACT

The study of migration mechanism of triple junctions of tilt boundaries with misorientation axes ⟨1 1 1⟩ and ⟨1 0 0⟩ on the example of nickel was performed by the method of molecular dynamics. It was found that migration and elongation of low-angle ⟨1 0 0⟩ boundaries is realized through slipping of pair grain-boundary dislocations with the subsequent change of dislocations-partners. During the changing of dislocation-partners, the decomposed dislocations slipped, the climb of the dislocations was not observed. The migration of ⟨1 1 1⟩ tilt boundary occurred as a result of the combined action of two mechanisms: the mechanism described above and the mechanism consisting in the joint slipping of pair grain-boundary dislocations, which, in contrast to grain-boundary dislocations in ⟨1 0 0⟩ boundaries, have common slip planes. The second mechanism has relatively low activation energy, as a result of which ⟨1 1 1⟩ boundaries are much more mobile than ⟨1 0 0⟩ boundaries.

During the triple junction migration, at an elongation of the low-angle boundary, a new geometrically necessary dislocation appeared, as a rule, from the migrating triple junction, after which the dislocation-partners are redistributed at the elongating boundary near the junction as a result of their split and subsequent merging with the formation of zigzag atomic displacements.

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 classical theories of grain growth in ordinary coarse-grained polycrystals generally assume that the triple junctions have infinite mobility and grain growth is realized by the migration of grain boundaries [1]. However, the experiments [2–4] and the results of computer simulation of grain growth [5–8] have shown that the mobility of triple junctions of grain boundaries is a finite value. The finite mobility is due to the fact that the movement of the triple junction is accompanied by transformations of the defect structure at the grain boundaries near the junction. Works [2–8] made a significant contribution to the development of ideas about the mobility of triple junctions of grain boundaries in metals. Nevertheless, there are a number of open questions at present. First of all, it is an accumulation of numerical data associated with the structural and energy characteristics of the migration of triple junctions for different metals depending on various external and internal factors; investigation of the effect of impurities, crystal lattice defects (especially vacancies and dislocations) and free volume on the mobility of the junctions. In addition, an important issue is to elucidate the atomic mechanisms of the processes of structure transformation and migration of triple junctions of boundaries of different types.

The mechanism of migration of triple junctions is connected with the migration mechanism of grain boundaries and before talking about the atomic mechanism of junctions' migration it is necessary to understand the mechanism of boundary migration. Despite the long-standing interest in this problem, at present there are still disagreements and unresolved issues related to the migration mechanism of grain boundaries. It is considered that the low-angle tilt boundaries migrate through the combined action of two mechanisms: slip and climb of grain-boundary dislocations [9]. In [10,11], for example, the authors came to the conclusion that the main mechanism of migration of tilt boundaries is the climb of grain-boundary dislocations. But, on the other hand, it is known that ⟨1 1 1⟩ tilt boundaries have the highest mobility, while ⟨1 0 0⟩ tilt boundaries, for example, migrate much more slowly [9,11–13], although the density of jogs at grain-boundary dislocations in ⟨1 0 0⟩ boundaries is higher, i.e. the climb of dislocations must

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pass more intensively in these boundaries than in ⟨1 1 1⟩ ones. The reason for the significant difference in the mobility of ⟨1 1 1⟩ and ⟨1 0 0⟩ boundaries, as the migration mechanism, are not fully understood.

It is known that low-angle boundaries migrate more slowly than high-angle boundaries [9,14]. However, there are still disagreements regarding the activation energy of migration. For example, in [14,15] it is said that the activation energy decreases almost monotonically with an increase in the misorientation angle in the range of low-angle boundaries. But in [11,16] the results of experiments of tilt boundaries migration have shown that low-angle boundaries with the same misorientation axis have almost the same activation energy of migration, which indirectly indicates an identical elementary mechanism of migration of such boundaries.

Our work is devoted to the investigation of the atomic mechanism of migration of triple junctions of tilt boundaries with misorientation axes ⟨1 1 1⟩ and ⟨1 0 0⟩ on the example of nickel using the molecular dynamics method.

2. Description of the model

The model in the present work was based on the proposed and developed in [2–8] model of triple junction migration. In [6,7], the two-dimensional molecular dynamics model was used, but with respect to the mechanism of grain boundaries migration, especially low-angle boundaries, two-dimensional and three-dimensional models have a fundamental difference. In the two-dimensional model, grain-boundary edge dislocations do not have periodically located jogs along the dislocations nuclei, which play an important role in grain boundary processes, especially diffusion [17]. Therefore, it was decided to create the three-dimensional calculation block in the molecular dynamics model in the form of a plate with a thickness of 6 atomic planes (Fig. 1). This thickness is sufficient for the appearance of effects associated with jogs of grain boundary dislocations. The calculation block had a height of 25.9 nm, a width of 17.2 nm and a thickness of 1.2 nm in the case of junctions of ⟨1 1 1⟩ tilt boundaries. For junctions of ⟨1 0 0⟩ boundaries, the dimensions were 26.4 nm, 17.6 nm and 1.1 nm respectively. The blocks contained about 50,000 atoms. Along the Z-axis (Fig. 1), an infinite repetition of the structure was simulated, i.e. periodic boundary conditions were imposed. The grain boundaries must be fixed at the border of the calculation block, which implies the preservation of the crystal lattice orientation of three different grains at the border of the block. In this connection, the block borders were rigidly fixed along the X and Y axes.

The force leading to the junction migration is created by the tension of boundaries 1 and 2, which stretch and pull down boundary 3, resulting in an increase its length, and the lengths of boundaries 1 and 2 are reduced (Fig. 1). The tension of the grain boundaries is due, similarly to a surface tension, to the proportionality of the total energy of the boundary and its area. In the case when the specific energy of the boundaries 1 and 2 is greater than the energy of the boundary 3 (for example, if the boundaries 1 and 2 are high-angle and the boundary 3 is low-angle), the tension of the boundary 3 is weaker and it is lengthened under the action of the tensions of the boundaries 1 and 2, and the triple junction is migrated. Migration of the triple junction occurs until the establishment of equilibrium values of the lengths of the boundaries and the angles between them corresponding to the minimum energy of the calculation block. Up to this point, due to the relatively large length of the calculation block along the Y axis (Fig. 1), the triple junction is managed to pass a significant distance in the considered model (more than 2/3 of the length of the calculation block), which allows to study the velocity and mechanism of its migration.

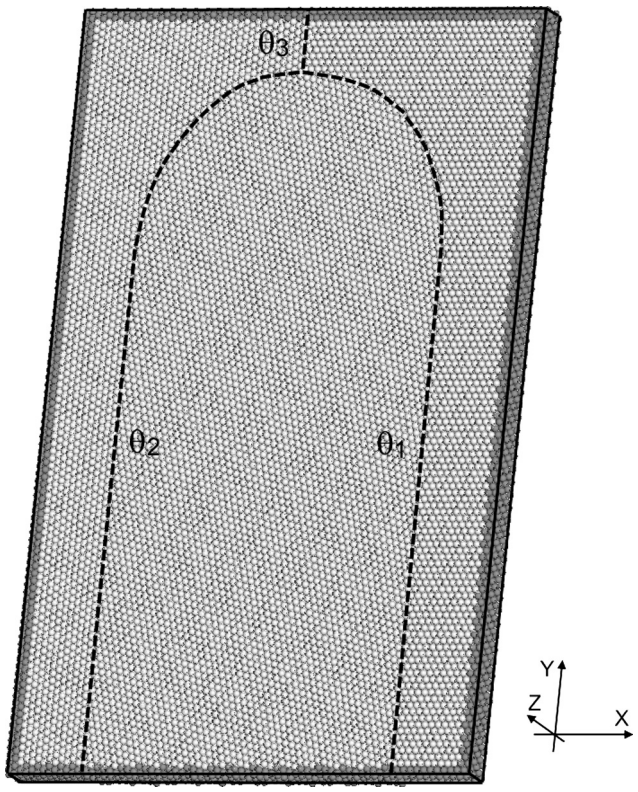

Fig. 1. Calculation block for modeling the migration of ⟨1 1 1⟩ 15°/15°/30° triple junction. Dark-gray atoms at the edge of the calculation block remained motionless during the computer experiment (rigid boundary conditions). θ_1, θ_2, θ_3 are misorientation angles of grains.

Various combinations of grain misorientation angles were considered, but most of the results were obtained for junctions with three sets of misorientation angles: $\theta_1 = 30°$, $\theta_2 = 25°$, $\theta_3 = 5°$ (for brevity, the designation 30°/25°/5° was used in the work); 30°/20°/10° and 15°/15°/30°. Special boundaries were not considered.

Interactions between atoms in the computer model were described by the many-body Cleri-Rosato potentials [18], built within the tight-binding model. Parameters of the potential for Ni were taken from [18]. This potential has been repeatedly used in molecular dynamics models and has been tested for a large number of characteristics [19–21]. The experience of its application shows that with its help it is possible to describe the various properties of metals and alloys.

The time step of integration of atomic motion in the method of molecular dynamics was equal to 2 fs. The temperature of the calculation blocks was set via the initial atomic velocities in accordance with the Maxwell-Boltzmann distribution (wherein the total momentum and the angular momentum of atoms in the calculation block were equal to zero). To keep the temperature constant during the simulation, the Nose-Hoover thermostat was used.

3. Results and discussion

During the computer experiments, it was noted that triple junctions of tilt boundaries with the misalignment axis ⟨1 1 1⟩, in fact, migrate much faster than the junctions of ⟨1 0 0⟩ boundaries. The velocity of their migration differed, as a rule, in several times at the same temperature.

Triple junctions with misorientation angles of grains 15°/15°/30° migrated much more slowly in the model than, for

example, 30°/25°/5° or 30°/20°/10° junctions. This was due to two reasons. Firstly, this was connected with the ratio of the boundaries tensions in the junction. Obviously, the lower the tension of the boundary 3, which is prolonged as a result of the junction migration, in comparison with the tensions of the boundaries 1 and 2 (Fig. 1), the faster the triple junction should migrate. Secondly, the mobility of the triple junction is affected by the mobility of the boundaries themselves.

Interesting features related to the atomic mechanism of the change in the length of low-angle boundary 3 during the junction migration were found. The emergence of new grain-boundary dislocations was accompanied by the formation of zigzag displacements of atoms. The examples of such displacements during the migration of ⟨1 1 1⟩ 30°/25°/5° and ⟨1 0 0⟩ 30°/20°/10° triple junctions are depicted in Fig. 2. The displacements are shown by segments connecting the initial and final positions of atoms (only displacements greater than 0.1 nm are shown).

When the boundaries with a high disorientation angle elongated, the ordered atomic displacements were not observed. However, at the transverse migration of the high-angle (even at a misorientation angle of 30°) boundaries, the ordered displacements of atoms in the form of a grid with square cells in the case of the ⟨1 0 0⟩ boundaries (Fig. 3) or hexagonal cells in the case of the ⟨1 1 1⟩ boundaries (Fig. 4) were clearly observed. The size of the cells was inversely proportional to the angle of misorientation. Despite the large misorientation angles (30°, 20° and 15°) corresponding to high-angle boundaries (i.e. the boundaries in which individual grain-boundary dislocations do not separate), the displacements of atoms during the migration looked the same as for low-angle boundaries.

The obtained similarities in the mechanisms of migration of low and high-angle tilt boundaries with misorientation axes ⟨1 1 1⟩ and ⟨1 0 0⟩ indicate an interesting fact of a uniform structure of low and high-angle boundaries.

In order to understand the mechanism of the appearance of zigzag atomic displacements during the elongation of boundary 3 and the displacements in the form of a square or hexagonal grid during the migration of boundaries 1 and 2, let's consider grain-boundary dislocations in such boundaries. Edge grain-boundary dislocations differ from ordinary intra-grain dislocations. First, they are, as a minimum, paired (Fig. 5). The atomic planes of both grains break off at low-angle boundary. It is usually energetically advantageous for such broken atomic half-planes, belonging to different grains, to combine into one defect, which is a grain-boundary dislocation. Some of them have relatively high Burgers vectors. Second, grain boundary dislocations, in contrast to ordinary ones, have a high density of jogs, which depends on the orientation of the boundary plane and the direction of the misorientation axis [17].

In our case, the first circumstance is important, and also the fact that these pair dislocations can split. At ⟨1 1 1⟩ boundaries, for example, dislocations can split with the reaction $1/2[1\,\bar{1}\,0] \rightarrow 1/6[2\,\bar{1}\,\bar{1}] + 1/6[1\,\bar{2}\,1]$, at ⟨1 0 0⟩ boundaries – $1[0\,\bar{1}\,0] \rightarrow 1/2[0\,\bar{1}\,1] + 1/2[0\,\bar{1}\,\bar{1}]$ [17].

With a detailed examination of the atomic mechanism of elongation of ⟨1 0 0⟩ and ⟨1 1 1⟩ low-angle boundaries during the triple junction migration, it was found that in the process of changing the length of the boundary, some paired grain-boundary dislocations decomposed and changed the dislocations-partners. As a result, zigzag displacements of atoms appeared (Fig. 5). Wherein the split dislocations slipped, the climb was not noticed. A new, geometrically necessary, dislocation with an elongation of the boundary appeared mainly from the migrating triple junction. As a rule, one dislocation appeared from the pair. Then a redistribution of the dislocations-partners occurred at the elongating boundary near the junction, which led to the formation of zigzag atomic displacements (Fig. 2).

The migration of boundaries 1 and 2 during the triple junction movement also proceeded by the mechanism described above, i.e. by splitting and changing the dislocations-partners. Fig. 5a shows that, as a result of this mechanism, during the migration of ⟨1 0 0⟩ low-angle tilt boundaries, the displacements of atoms form a grid with square cells (as in Fig. 3). In the case of migration of ⟨1 1 1⟩ boundaries, in addition to this mechanism, a mechanism of joint sliding of pair grain-boundary dislocations is added (2 in Fig. 5b). In contrast to grain-boundary dislocations of ⟨1 0 0⟩

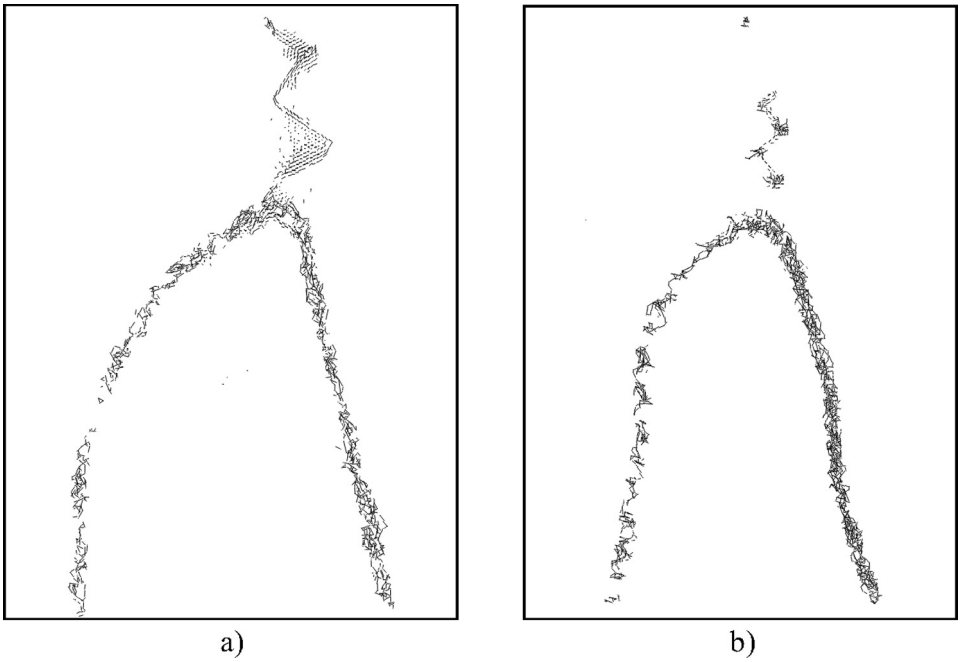

Fig. 2. Atomic displacements during migration of the triple junctions at the temperature of 1700 K: (a) ⟨1 1 1⟩ 30°/25°/5° (from 750 to 800 ps from the start of the simulation); (b) ⟨1 0 0⟩ 30°/20°/10° (from 1200 to 1330 ps). Displacements greater than 0.1 nm are shown.

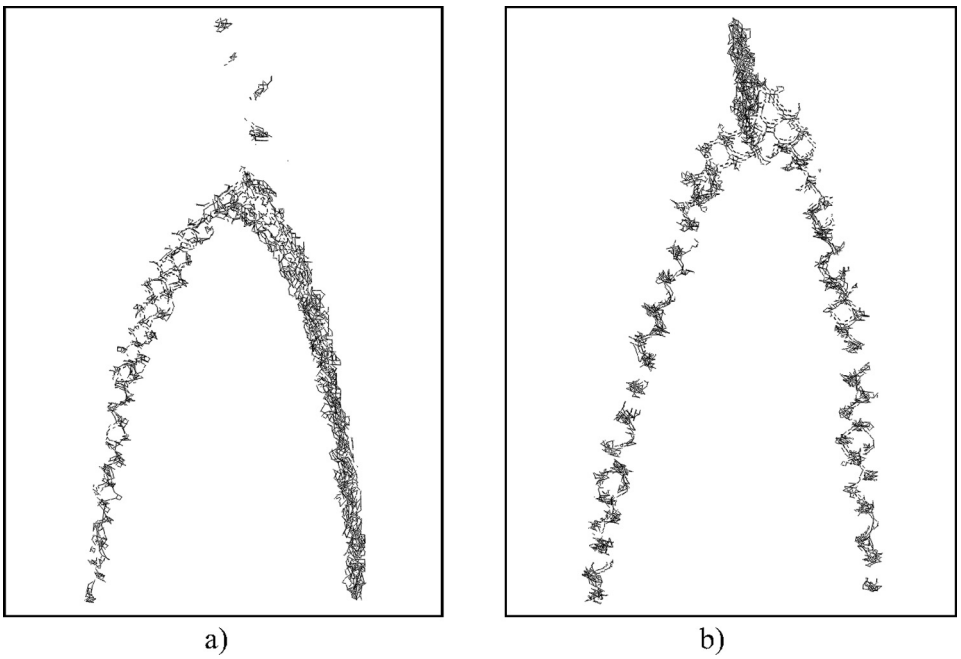

Fig. 3. Atomic displacements during migration of the triple junctions at the temperature of 1700 K: (a) ⟨1 0 0⟩ 30°/20°/10° (from 1700 to 2200 ps from the start of the simulation); (b) ⟨1 0 0⟩ 15°/15°/30° (from 3750 to 4500 ps). Displacements greater than 0.1 nm are shown.

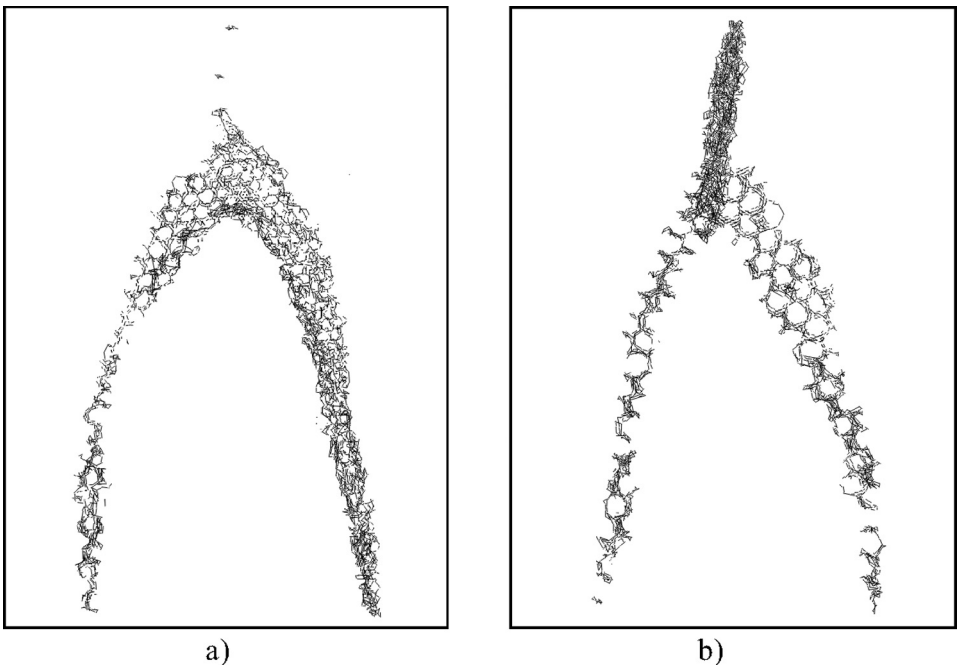

Fig. 4. Atomic displacements during migration of the triple junctions at the temperature of 1700 K: (a) ⟨1 1 1⟩ 30°/20°/10° (from 250 to 600 ps from the start of the simulation); (b) ⟨1 1 1⟩ 15°/15°/30° (from 3000 to 3750 ps). Displacements greater than 0.1 nm are shown.

boundaries, pair dislocations of ⟨1 1 1⟩ boundaries have common slip planes along which they can slide with a comparatively low activation energy. With simultaneous migration and reduction of the ⟨1 1 1⟩ boundary, as in the case of boundaries 1 and 2 in the considered model, a combined action of both mechanisms was observed: joint sliding of pair grain-boundary dislocations and their splitting with the change of dislocations-partners. In connection with this, the displacements of atoms in Fig. 4 at migration of ⟨1 1 1⟩ 30°/20°/10° and ⟨1 1 1⟩ 15°/15°/30° junctions had the form of a hexagonal grid.

The following characteristics of the triple junctions migration were considered: υ – velocity of the migration; H_{tj} – activation energy of the triple junctions migration; A_{0tj} – pre-exponential factor in the Arrhenius equation. According to [3,6], the specific mobility of the triple junction is determined by the formula

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

Here a is the distance between boundaries 1 and 2 in the model; σ is the surface tension of boundaries 1 and 2 (in the model from [3,6]

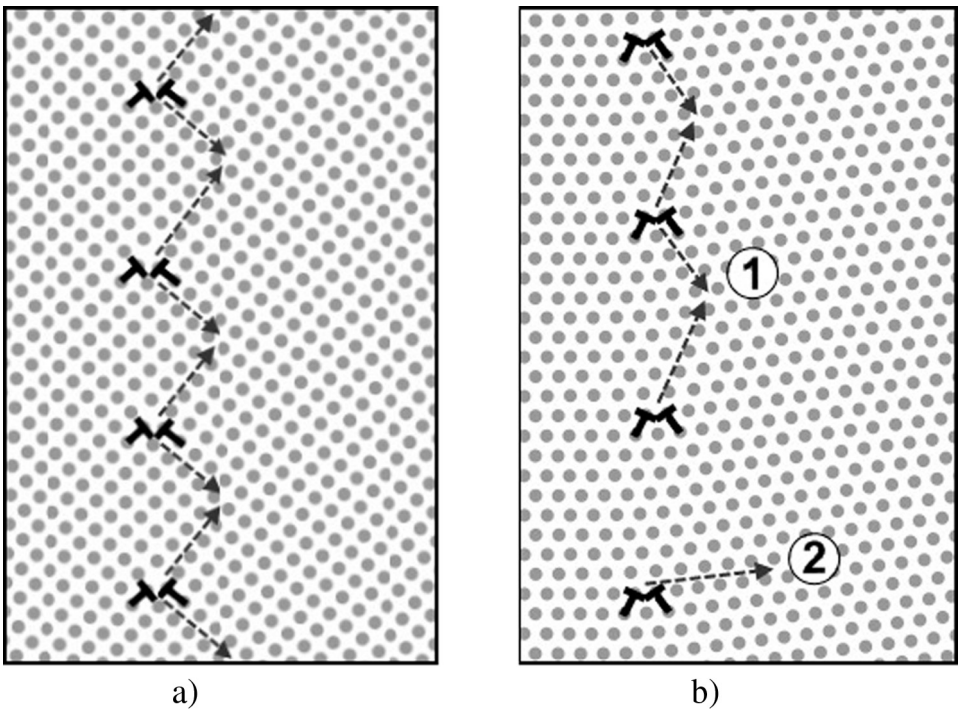

Fig. 5. Scheme of the migration mechanism of low-angle ⟨1 0 0⟩ and ⟨1 1 1⟩ tilt boundaries in a monoatomic plane: (a) ⟨1 0 0⟩ 10° boundary: change of the dislocations-partners; (b) ⟨1 1 1⟩ 7° boundary: 1 – change of the dislocations-partners, 2 – joint sliding of the pair dislocations.

it is assumed that the boundaries 1 and 2 have equal tensions); σ_3 is the surface tension of boundary 3; k is the Boltzmann constant and T is the temperature.

Before carrying out measurements of the triple junction migration velocity, an additional study of the dependence of the migration velocity on time from the beginning of the computer experiment was made. It was found that the migration velocity is not constant during all simulation: at the first stage, the "contraction" of boundaries 1 and 2 occurs (Fig. 1). The junction itself practically does not move at this time. When boundaries 1 and 2 are stretched, they begin to "pull" the triple junction and the boundary 3 down. At the end of the movement, the velocity gradually falls due to a change in the direction of the tension vectors of boundaries 1 and 2. In this connection the velocity of migration of the triple junction was measured only in the middle region, when the driving force and the angles between grain boundaries at the junction are constant.

The method of determining the ratio of the boundaries tensions in the triple junction σ_3/σ consisted in finding the ratio of grain boundaries energies. It was assumed that the tension of 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.

In addition, the tensions ratio was verified by carrying out long-term computer experiments by searching for an equilibrium correlation of the angles between boundaries at the junction and determining the ratio through the Yang relation [22].

The dependences $\ln A_{tj}$ on T^{-1} were obtained for the considered triple junctions with the help of which the corresponding activation energies of the migration and the pre-exponential factors were calculated. Modeling of migration was carried out at temperatures from 1200 K to 1700 K. The duration of computer experiments was ranged from 500 ps to 2000 ps depending on the migration velocity of the junction. The obtained values σ_3/σ, υ, H_{tj} and A_{0tj} for the considered triple junctions are given in Table 1.

It is seen that the velocity values correlates with the values of the ratio of the boundaries tensions: the smaller the ratio σ_3/σ, the higher the velocity υ. But, as mentioned earlier, besides the influence of the ratio σ_3/σ, the mobility of the boundaries itself affects to the junction mobility. In particular, the angle of misorientation affects: high-angle boundaries migrate faster than low-angle boundaries.

The activation energy of migration of the triple junctions of ⟨1 0 0⟩ boundaries, as can be seen from the table, turned out to be almost three times higher than the activation energy of migration of the junctions of ⟨1 1 1⟩ boundaries. The reason for this, as mentioned above, is connected with the presence of the additional mechanism, in contrast to ⟨1 0 0⟩ boundaries, which consists in the joint slipping of grain-boundary pair dislocations and has a relatively low activation energy.

Another interesting result, which follows from Table 1, is the approximate equality of the activation energies of migration of the boundaries with the same misorientation axis regardless of the misorientation angle. The activation energy was 0.26–0.31 eV for all considered junctions of ⟨1 1 1⟩ tilt boundaries. For junctions of ⟨1 0 0⟩ boundaries, the activation energy was 1.04–1.10 eV. This result indicates that the migration of tilt boundaries with the same misorientation axis occurs by the same mechanism. The activation energy is determined by the work that must be spent on the implementation of an elementary act of migration. The frequency of elementary acts of migration (which in our case is proportional to the density of grain-boundary dislocations) is theoretically proportional to the pre-exponential factor. However, due to the relatively high error, the dependence A_{0tj} on the misorientation angle is implicit (Table 1).

4. Conclusions

In the present work, the study of the atomic mechanisms of migration of triple junctions of tilt boundaries with misorientation axes ⟨1 1 1⟩ and ⟨1 0 0⟩ on the example of nickel was performed by

Table 1
Characteristics of migration of triple junctions in Ni for the temperature range 1200–1700 K.

Triple junction	$\frac{\sigma_3}{\sigma}$	υ (m/s) (at 1700 K)	H_{tj} (eV)	A_{0tj} (10^{-5} m^2/s)
⟨1 1 1⟩ 30°/25°/5°	0.4	16.4	0.28	0.11
⟨1 1 1⟩ 30°/20°/10°	0.7	12.8	0.31	0.13
⟨1 1 1⟩ 15°/15°/30°	1.3	2.9	0.26	0.09
⟨1 0 0⟩ 30°/25°/5°	0.4	4.6	1.04	4.96
⟨1 0 0⟩ 30°/20°/10°	0.6	3.6	1.10	6.52
⟨1 0 0⟩ 15°/15°/30°	1.3	1.2	1.08	4.45

the method of molecular dynamics. It was found that migration and elongation of low-angle ⟨1 0 0⟩ boundaries is realized through slipping of pair grain-boundary dislocations with the subsequent change of dislocations-partners. During the changing of dislocation-partners, the decomposed dislocations slipped, the climb of the dislocations was not observed. The migration of ⟨1 1 1⟩ tilt boundary occurred as a result of the combined action of two mechanisms: the mechanism described above and the mechanism consisting in the joint slipping of pair grain-boundary dislocations, which, in contrast to grain-boundary dislocations in ⟨1 0 0⟩ boundaries, have common slip planes. The second mechanism has relatively low activation energy, as a result of which ⟨1 1 1⟩ boundaries are much more mobile than ⟨1 0 0⟩ boundaries.

During the triple junction migration, at least one of the boundaries is lengthened. A new, geometrically necessary, dislocation appeared, as a rule, from the migrating triple junction, after which the dislocation-partners are redistributed in the elongating boundary near the junction as a result of their split and subsequent merging with the formation of zigzag atomic displacements.

The values of the migration activation energy were calculated by the molecular dynamics simulation for the triple junctions under consideration. It is shown that the activation energies have similar values for junctions of boundaries with the same misorientation axis, which indicates the similarity of the migration mechanism for such boundaries. The migration energy of triple junctions of ⟨1 1 1⟩ boundaries turned out to be almost three times lower than the activation energy of migration of the junctions of ⟨1 0 0⟩ boundaries.

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