Computational Materials Science 148 (2018) 184–189

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

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

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ARTICLE INFO

Article history:
Received 21 November 2017
Received in revised form 20 February 2018
Accepted 20 February 2018

Keywords:
Triple junction
Grain boundary
Migration
Tilt boundary
Molecular dynamics
Grain boundary dislocation

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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https://doi.org/10.1016/j.commatsci.2018.02.047
0927-0256/

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.

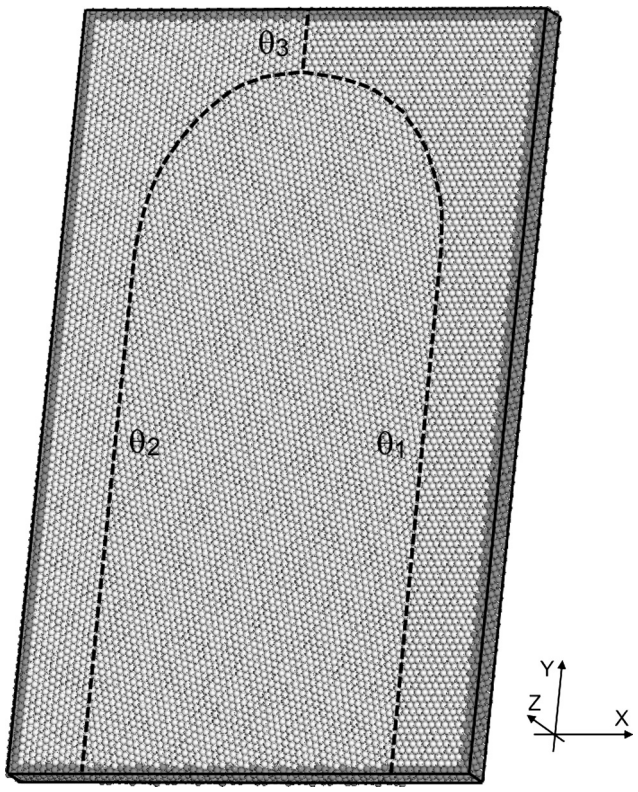

Fig. 1. Calculation block for modeling the migration of ⟨1 1 1⟩ 15°/15°/30° triple junction. Dark-gray atoms at the edge of the calculation block remained motionless during the computer experiment (rigid boundary conditions). θ_1, θ_2, θ_3 are misorientation angles of grains.

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