Migration of tilt boundaries in nickel and Ni$_3$Al intermetallide: a molecular dynamics study

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Abstract. The study of migration of <100> and <111> tilt boundaries in Ni and the Ni$_3$Al intermetallide is performed by the molecular dynamics method. It is shown that in Ni and Ni$_3$Al, the low-angle <100> boundaries migrate much slower than the <111> boundaries (approximately twice at a temperature of 1700 K) due to the difference in the mechanisms of migration of the low-angle <100> and <111> boundaries. According to the obtained results, the migration rate of similar boundaries in the Ni$_3$Al intermetallide is much lower than in Ni (approximately three times at 1700 K). The reason for this is mainly the additional energy expenditure for the formation of a disordered area in Ni$_3$Al behind the migrating boundary. Due to the relatively low mobility of the boundaries in Ni$_3$Al, the contribution of diffusion displacements of atoms in the process of boundary migration is higher than in Ni.

1. Introduction

Grain boundary migration plays a crucial role in the process of recrystallization and in many cases of phase transformations. Despite the long-standing interest in the problem of migration of grain boundaries, there are still disagreements and unresolved issues related to the migration mechanism. It is believed that low-angle tilt boundaries migrate through the combined action of two mechanisms: slip and climb of grain boundary dislocations [1]. In [2, 3], for example, the authors come to the conclusion that the main mechanism of migration of the tilt boundaries is the climbing of grain boundary dislocations. But, on the other hand, it is known that in fcc metals the low-angle <111> tilt boundaries have the highest mobility, while the <100> tilt boundaries, for example, migrate much more slowly [1, 3], although the density of jogs on grain boundary dislocations within the <100> boundaries is higher, i.e. the climb intensity should be greater than within <111> boundaries. The reason for this difference in the mobility of the <111> and <100> boundaries, as well as the migration mechanism, is not completely clear.

The migration of grain boundaries in ordered alloys and intermetallides is scantily known. One of the interesting and promising intermetallic compounds is Ni$_3$Al, which has a fcc lattice and ordering of the L1$_2$ type. The intermetallic compound Ni$_3$Al is distinguished from a number of similar ordered alloys by
unique physical and mechanical properties, which include, first of all, a positive temperature dependence of the yield stress and high thermal stability (the order-disorder phase transition temperature for Ni₃Al is above the melting point) [4]. Therefore, this intermetallic compound is of practical significance as a heat-resistant structural material.

The present work is devoted to the study of the features of the migration of <100> and <111> tilt boundaries in Ni and the Ni₃Al intermetallide by the molecular dynamics method.

2. Model description

A clearly defined boundary was created in the form of a loop or arch, as in figure 1 (black dotted line). The tension of the boundary, which, like a surface tension, arises from the tendency of the boundary to minimize its energy, is the reason for the directed movement of the boundary, which decreases its area. The force that provokes the migration and the boundary migration velocity remained constant throughout almost the entire movement of the boundary, smoothly decreasing by the end of the computer experiment.

The three-dimensional computational block in the molecular dynamics model was created in the form of a plate with a thickness of 12 atomic layers (figure 1). This thickness is sufficient for the appearance of effects associated with the jogs of grain boundary dislocations. In the case of the <111> tilt boundaries, the nickel computational block had a height of 18.0 nm, a width of 12.0 nm and a thickness of 2.4 nm. For the <100> boundaries, the dimensions were 18.2 nm, 12.1 nm and 2.2 nm, respectively. The computational blocks of Ni₃Al were slightly larger due to the difference in the lattice parameters of Ni and Ni₃Al. The blocks contained approximately 50,000 atoms. Along the Z-axis (figure 1), an infinite repetition of the structure was simulated, i.e. periodic boundary conditions were imposed. At the edge of the computational block, the grain boundaries must be fixed, which implies preserving the orientation of the crystal lattice of two different grains at the border of the block. In this connection, along the X and Y axes, the block borders (highlighted in dark gray in figure 1) were rigidly fixed to preserve the given misorientation of the grains.

Figure 1. Computational block for modeling the migration of <111> 30° tilt boundary. The dark-gray atoms on the edge of the block remained motionless during the computer experiment (rigid boundary conditions).

To describe the interatomic interactions in Ni and in the Ni₃Al intermetallide, the Cleri–Rosato tight-binding EAM potentials were used [5]. Potentials of this type have been repeatedly used in models of
molecular dynamics and have been tested for a large number of characteristics [6–10]. The experience of their application shows that their use allows describing various properties of metals and alloys. The time step in the molecular dynamics method was equal to 2 fs. The temperature in the model was set through the initial velocities of the atoms according to the Maxwell-Boltzmann distribution, wherein the thermal expansion of the calculation blocks was taken into account. To maintain a constant temperature during the simulation, the Nose-Hoover thermostat was used.

3. Results and discussion

Figure 2a shows the dependences of the migration rate of <100> and <111> tilt grain boundaries in nickel at a temperature of 1700 K on the misorientation angle. Special and symmetrical boundaries were not considered in the paper. The tension of the grain boundaries is proportional to their energy: as the misorientation angle increases, both energy and tension increase as well [11].

The boundary migration rate of during the computer experiment remained practically constant and high enough at the considered temperature of 1700 K, and at misorientation angles above 10°, which made it possible to make the required measurements in the molecular dynamics model. The angle of the grain misorientation θ varied from 10° to 45° for the <100> boundaries and to 40° for the <111> boundaries. In the case of <100> boundaries, 45° is the maximum misorientation angle. In the case of the <111> boundaries, it was taken into account that the <111> tilt boundaries with the misorientation angle of 38° have the highest mobility, according to, for example, [1, 12]. As the misorientation angle increases, the migration rate of the boundaries increases similarly to the well-known regularity [1, 11].

![Figure 2](image)

**Figure 2.** The rate of migration of <100> (white triangles) and <111> (black dots) tilt boundaries at 1700 K (b), depending on the misorientation angle θ in Ni (a) and the Ni₃Al intermetallic.

It should be noted that at the angles of misorientation above 25° the high-angle <100> and <111> boundaries migrate with approximately the same velocity (30–37 m/s at 1700 K), while the migration rates of the low-angle <100> and <111> tilt boundaries differ significantly – the low-angle <100> boundaries migrate about twice as slow as the <111> boundaries. Earlier in [10], we found that the migration of the <100> boundary is carried out by splitting of the paired grain boundary dislocations with a subsequent change of the dislocations partners. The dislocations partners are replaced through the slip of split dislocations. The migration of the <111> tilt boundary is accomplished by the combined action of two mechanisms: the mechanism described above and the mechanism consisting in joint sliding of the paired grain boundary dislocations, which, in contrast to the grain boundary dislocations within <100> boundaries, have common slip planes. The joint sliding of the
paired dislocations has a relatively low activation energy. As a result, the low-angle $<111>$ tilt boundaries are more mobile than the $<100>$ boundaries.

Figure 2b shows the dependences of the migration rate of the boundaries in Ni$_3$Al on the misorientation angle. Despite the relatively higher energy of the boundaries and, hence their tension, the migration rate of the boundaries in the Ni$_3$Al intermetallide proved to be significantly lower compared to Ni, approximately three times at the same temperature of 1700 K. This is apparently due to the additional expenditure of energy for disordering and the rupture of Ni-Al bonds during the motion of the boundaries in Ni$_3$Al. Figure 3 shows an example of the formation of a disordered area behind the migrating $<111>$ 20° boundary. The order does not have enough time to recover. The ordering process in this case is much slower than the boundary migration.

![Figure 3. Formation of a disordered area behind the moving boundary (1 – initial position of the boundary, 2 – current position) during the migration of $<111>$ 30° tilt boundary at a temperature of 1700 K in the course of 800 ps.](image)

As in the case of boundaries in Ni, the low-angle $<100>$ boundaries in Ni$_3$Al were approximately two times lower in mobility than the $<111>$ boundaries (figure 2b). The mechanism of migration of low-angle boundaries, in general, in Ni$_3$Al was the same as in Ni. Due to the relatively low rate of migration of boundaries in Ni$_3$Al, one of the significant differences was a greater contribution of the diffusion displacements of atoms in the migration process.

4. Conclusions
In the present work, the study of the features and mechanism of migration of $<100>$ and $<111>$ tilt boundaries in Ni and the Ni$_3$Al intermetallide was performed the molecular dynamics method. The dependences of the migration rate of the considered boundaries at a temperature of 1700 K on the misorientation angle are obtained. It is shown that the high-angle $<100>$ and $<111>$ boundaries migrate at approximately the same rate at a given temperature, while the low-angle $<100>$ boundaries migrate about twice as slower as the $<111>$ boundaries. According to our previous work [10], this is due to the difference in the mechanisms of migration of low-angle $<100>$ and $<111>$ boundaries. As the molecular dynamics studies demonstrated, the migration rate of similar boundaries in Ni$_3$Al intermetallide is much lower than in Ni (approximately three times at 1700 K). In particular, the reason for this is the formation of a disordered area behind the migrating boundary in Ni$_3$Al. In general, the mechanism of the migration
of low-angle boundaries in Ni₃Al was the same as in Ni. Due to the relatively low rate of boundary migration in Ni₃Al, one of the significant differences was a greater contribution of the diffusion displacements of atoms in the migration process.

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