Chapter 3

Atomistic Study of Disclinations in Nanostructured Metals

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3.1 Introduction

3.1.1 Various Deformation Modes in Nanostructured Metals

Nanostructured materials generally have unique mechanical properties that cannot be easily expressed by extrapolating the mechanical properties of coarse-grained materials (Gleiter 2000; Valiev et al. 2000; Meyers et al. 2006; Yinmin et al. 2002; Lu et al. 2009; Wang et al. 2011). A possible reason for these unique mechanical properties is that the activated plastic deformation modes in nanostructured materials are different from those in coarse-grained materials. Intrinsically, each crystalline material has various plastic deformation modes: *plaston* (Tsuji et al. 2020), as discussed in detail in the previous chapters of this book. Among the several candidates of plastic deformation modes, one is strongly activated in relation to factors such as constituent elements, structure size, and environment. For example, the number of dislocations in each structure decreases with the decrease in the structure size below the sub-micron level when the dislocation density does not depend on the structure size. For example, if the dislocation density is 10^{14} $1/\text{m}^2$, there would be 10,000 dislocations in a 10 μm grain but only 1 dislocation in a 100 nm grain. Therefore, in nanostructured metals, the generation of a new plastic deformation mode from the interface between neighboring structures is more important than the plastic phenomena that start from the intragranular region. Then, unique lattice defects can develop in nanostructured materials.

An example of the structure dependence of activated deformation modes is shown in Fig. 3.1, which also shows the grain size dependence of the (a) (b) strength and (c) (d) deformation mechanism in nanopolycrystalline Al, which was obtained using

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Fig. 3.1 Grain size dependence of the strength and deformation mechanism in nanostructured Al. **a** Temperature dependence of strength (Shimokawa 2012). **b** Grain boundary structure dependence of strength (Shimokawa 2012). **c** Collective dislocation motion constrained by the grain boundary ($d = 80$ nm) (Shimokawa et al. 2005). **d** Grain rotation of grains A and B and grain boundary sliding between grains C and D ($d = 5$ nm) (Shimokawa et al. 2005). Reprinted with permission from Springer and American Physical Society

molecular dynamic simulations (Shimokawa et al. 2005; Shimokawa 2012). The transition from the grain size strengthening (Hall-Petch relation) to grain size softening (inverse Hall-Petch relation) (Chokshi et al. 1989; Fougere et al. 1992; Schiøtz and Jacobsen 2003) occurred as shown in Fig. 3.1a, b. In the Hall-Petch region, dislocation pile-ups against the grain boundary can be observed in Fig. 3.1c. Hence, the dominant deformation mechanism was caused by intragranular deformation modes. However, in the inverse Hall-Petch region, the geometrical misfit caused by the grain boundary sliding of grains C and D can be accommodated by the grain rotation of grains A and B, as shown in Fig. 3.1d. Thus, the dominant deformation mechanism was caused by intragranular deformation modes. Figure 3.1a shows the temperature dependence of the strength and grain size relation and the maximum grain size changes with the following temperatures: 20 nm at 100 K, 30 nm at 300 K, and 40 nm at 500 K (Shimokawa 2012). The black lines represent the fitting results of the Hall-Petch relation: $\sigma = \sigma_0 + kd^{-1/2}$. Also, k does not show the temperature dependence but σ_0 shows it. This is because the grain boundary-mediated plastic deformation

Fig. 3.2 Relationship between the critical shear stress and the characteristic length of the dislocation source of Al estimated by molecular dynamics simulations. Reproduced from Shimokawa and Kitada (2014) with permission from The Japan Institute of Metals and Materials

contains more thermal-activated processes than intragranular deformation. On the other hand, Fig. 3.1b shows the grain boundary structure dependence of the strength and grain size relation (Shimokawa 2012). Case-1 and case-2 have the same texture but different grain boundary structures by changing the grain positions. In the strengthening region, case-1 is stronger than case-2, but in the softening region, case-2 is stronger than case-1. These results show that the role of the grain boundary in strength is influenced by the structure. Consequently, the active deformation modes were changed by the grain size and temperature, and this phenomenon influences the mechanical properties of nanostructured metals.

Figure 3.2 shows the relationship between the critical shear stress to nucleate the dislocation and the characteristic length (Shimokawa and Kitada 2014). The solid circles, triangles, and squares represent the dislocation multiplication results from a Frank-Read source, the dislocation emission from the (112) tilt grain boundaries, and the homogeneous nucleation from a perfect crystal, respectively (Shimokawa and Kitada 2014). The characteristic length of the grain boundary is the distance between the structural units that can act as a dislocation source (Shimokawa 2010), and the homogeneous nucleation length is the Burgers vector. This result clearly shows that the active deformation mode changes with the decrease in the characteristic length.

As a result, the deformation mode *plaston* can be selected by designing structures, elements, and environments. Afterward, materials with excellent mechanical properties can be obtained. Recent attempts have been made to design materials with excellent mechanical properties by making heterogeneous microstructures, such as gradient nanotwinned metals (Cheng et al. 2018; Sun et al. 2018) and harmonic materials (Zhang et al. 2014; Sawangrat et al. 2014). Such excellent properties might

be closely related to a mix of various structure-specific deformation modes in such heterogeneous structure materials.

3.1.2 Disclinations

In this chapter, we considered disclination as an example of plaston. Disclination is a line defect in which rotational symmetry is violated (Romanov and Vladimirov 1992). Although it is generally difficult for crystalline materials to contain disclinations in a stable form in intragranular regions, disclinations have recently been recognized as typical defects that can influence the mechanical properties of nanostructured metals (Valiev et al. 2000; Gutkin and Ovid'ko 2004), as seen in nanostructure materials (Murayama et al. 2002). Moreover, the stability of disclinations at the grain boundaries of bicrystalline nanowires has been studied using computer simulations (Zhou et al. 2006, 2007). Here, we introduced three examples of disclinations that can be observed in nanostructured materials under deformation through atomic simulations.

The first example is disclinations in a grain, as shown in Fig. 3.3a. Since a perfect disclination is hard to exist in grains due to the huge elastic strain energy, generally partial disclinations with plane defects exist in grains. Plane defects have a misorientation angle; hence, partial disclinations can divide a grain into several regions with misorientation angles. In Sect. 3.2, we discussed the grain refinement mechanism by severe plastic deformation focusing on the formation and movement of partial disclinations (Shimokawa et al. 2016). The next example shows disclinations at the junctions of grain boundaries, as shown in Fig. 3.3b. The formation of these disclinations brings grain rotation (Shimokawa et al. 2005, 2006), as already shown in Fig. 3.1d. The possible mechanism of the grain rotation with disclinations was proposed by Gutkin et al. (2003). The last example shows disclinations at the grain boundaries, as shown in Fig. 3.3c. The disclination dipole at a grain boundary changes the misorientation angle at the grain boundary region, and its stress field is formed in the grain. These stress fields can improve the fracture toughness of nanostructured

Fig. 3.3 Disclinations **a** in a grain, **b** at the grain boundary junctions, and **c** at the grain boundary. Each disclination state brings grain subdivision (Shimokawa et al. 2016), grain rotation (Shimokawa et al. 2005), and improved fracture toughness (Shimokawa et al. 2011; Shimokawa and Tsuboi 2015), respectively. The thick and thin solid lines represent the grain boundary and a common lattice of grains, respectively

metals (Shimokawa et al. 2011; Shimokawa and Tsuboi 2015). A detailed discussion can be found in Sect. 3.3.

3.2 Grain Subdivision: Disclinations in Grains

3.2.1 Strain Gradients in Severe Plastic Deformation Processes

The severe plastic deformation (SPD) process is a method of producing nanostructured metals in bulk. As shown in Fig. 3.4, the main types of SPD are equal-channel angular pressing (ECAP) (Iwahashi et al. 1996; Valiev and Langdon 2006), accumulative roll-bonding (Saito et al. 1999), and high-pressure torsion (HPT) (Valiev et al. 1996). Bulk ultra-fine-grained (UFG) metals, which could not be obtained before, could be produced by repeatedly introducing large strains into specimens. Hence, the research on the mechanical properties of UFG metals has dramatically developed. The common feature of these SPD processes is the introduced strain gradient into specimens. In the cases of ECAP and ARB, the strain gradient appeared at the border between the deformed and undeformed regions, and in the case of HPT, the strain gradient appeared along the radius direction. In the strain gradient regions, there were dislocations that could accommodate the plastic deformation gaps. These dislocations are called geometrically necessary dislocations (GNDs) (Ashby 1970). As a result, a large number of GNDs are introduced during SPD processes, and this phenomenon causes grain refinement. The concept of *grain subdivision* was proposed by Hansen et al. (2001) to explain grain refinement through SPD, where an original grain domain is finely divided by rearranging several GNDs, which are introduced by SPD into energetically stable structures.

However, it is still not clear why introducing GNDs into specimens results in grain subdivisions due to the difficulty of directly observing the structural changes in bulky metallic specimens during SPD processes. Hence, molecular dynamic simulations of the SPD process were performed using the analysis model shown in Fig. 3.5 (Shimokawa et al. 2016). To simplify the SPD process, a quasi-two-dimensional model was employed. The crystal structure is a hexagonal close-packed structure, where two $\{0001\}$ planes are arranged along the y -direction. Adopting the periodic boundary condition in the y -direction realized three equivalent prismatic slip systems. The outer region of the analysis model was set to the displacement controlled layer, and the shear strain $\gamma = \lambda/A$ was introduced by changing the shape of the layer along the z -direction at a velocity v . The strain gradient appeared at the border of the shear and non-shear zones. Our SPD process is similar to the multi-pass ECAP (Nakashima et al. 2000) and ECAP in parallel channels (Raab 2005). Two types of crystal orientations, as shown in Fig. 3.5c, were adopted in the analysis models to investigate the crystal orientation influence on the activated slip systems in the vicinity of the strain gradient regions. The embedded atom method for copper (Mishin

Fig. 3.4 Relationship among the severe plastic deformation processes, strain gradient, and grain refinement

Fig. 3.5 **a, b** Analysis model for investigating the relationship through molecular dynamic simulations. **c** Two types of crystal orientation were used in the analysis models. Reproduced from Shimokawa et al. (2016) with permission from The Japan Institute of Metals and Materials

et al. 2001) was used for the atomic interactions. Although the most stable phase of the EAM potential is the face-centered cubic phase, the transformation from the hexagonal close-packed phase to the face-centered cubic phase did not occur during the SPD simulations because of the boundary conditions.

Figure 3.6 shows the crystal orientation influence on the activated slip systems around the strain gradient regions. The crystal orientation of case-1 has the slip system iii parallel to the x -direction of the shear deformation direction, and the crystal orientation of case-2 has the slip system III orthogonal to the slip system iii. The analysis conditions are $\gamma = 0.2$, $v = 500$ m/s, and $T = 300$ K. Figure 3.6a, b

Fig. 3.6 Influence of the crystal orientation on the activated slip systems at the vicinity of the strain gradient regions with $\gamma = 0.2$. **a, c** Crystal slip histories colored by the atomic strain. **b, d** Crystal rotation angle from the initial state

shows the atomic strain during shear deformation, where the black lines represent the crystal slip histories. In case-1, the slip system III was mainly activated. However, in case-2, the primarily slip system was III. As mentioned before, these slip systems are orthogonal to each other, so the same shear stress magnitude was applied to all of them. Figure 3.6c, d shows the change in the crystal orientation for each crystal orientation. The atomic color represents the crystal rotation angle from the initial state. The average rotation angle θ_{AVE} in the shear zone in case-2 was larger than that in case-1. Hence, the accommodation mechanism of the strain gradient changed due to the activated slip systems, as shown in Fig. 3.6e, f. In this chapter, SPD simulations were performed using case-2.

3.2.2 Grain Subdivision by Severe Plastic Deformation

Figure 3.7 shows the taken snapshots during the SPD simulations with $\gamma = 0.7$ and $v = 500$ m/s. The atomic color represents the crystal rotation angle from the initial state, and the black atoms are those in a defect structure. A clear difference in the crystal orientation appeared around the strain gradient regions, and the boundaries with a misorientation angle propagated along with the specimen. Finally, distinct regions with different crystal orientations were formed in the specimen after the SPD process, as shown in Fig. 3.7g, where grain subdivisions occurred in the simple atomic simulations.

Figure 3.8 shows the influence of the local shear strain γ on the microstructure after the SDP process. In the cases of small γ , as shown in Fig. 3.8a, b, no microstructures appeared after the SPD process. However, in the cases of larger γ , as shown in

Fig. 3.7 Grain subdivision caused by the SPD process with the propagation of the local shear strain $\gamma = 0.7$. The atomic colors other than black represent the rotation angle from the initial state, and the black atoms represent the defect structures defined using the common neighbor analysis. Reproduced from Shimokawa et al. (2016) with permission from The Japan Institute of Metals and Materials

Fig. 3.8 Dependence of the local shear strain γ on the observed microstructures after the SPD process. Crystal orientation maps after the SPD processes of **a** $\gamma = 0.2$, **b** $\gamma = 0.5$, **c** $\gamma = 0.7$, and **d** $\gamma = 1.0$. **e** Atomic configurations around the grain boundary indicated by a white broken box in (c). Reproduced from Shimokawa et al. (2016) with permission from The Japan Institute of Metals and Materials

Fig. 3.11c, d, new grains were formed by the SPD process. Figure 3.8e shows the detailed atomic configurations in the broken box in Fig. 3.8c. Two types of defects can be observed: one is the line defects that do not bring crystal misorientations, and the other is the grain boundaries with a misorientation angle. To quantify the influence of γ on the microstructure formation, Fig. 3.9 shows the proportion of the defect atoms

Fig. 3.9 Proportions of the defect atoms: line defect and grain boundary. The proportion of the defect atoms was calculated in the central region of the specimens, as shown in the inset of (a). **a** Local shear strain dependence ($v = 500$ m/s). **b** Propagation speed dependence ($\gamma = 0.7$ and 1.0). Reproduced from Shimokawa et al. (2016) with permission from The Japan Institute of Metals and Materials

f_{def} with respect to (a) γ and (b) v after the SPD process. Here, f_{def} was measured for each defect type, and the analysis region for f_{def} is the central region surrounded by the broken line shown in the insert figure in Fig. 3.9a. It was confirmed that f_{def} of the line defects increases with γ . Since most line defects are vacancy arrays formed by interactions between dislocations with the same slip system but opposite Burgers vectors, the f_{def} of the line defects reflected the number of dislocations activated during the SPD process. The results show that many dislocations were nucleated with the increase in γ . However, f_{def} of the grain boundaries showed almost zero for $\gamma \leq 0.6$ but showed a constant value for $\gamma \geq 0.7$. This indicates that a critical value of γ existed to realize the grain subdivision in the atomic simulations. Figure 3.8b shows the influence of the propagation speed of the local shear zone v on f_{def} for $\gamma = 0.7$ and 1.0 . f_{def} of the grain boundaries was also influenced by v , as a smaller v could not form new microstructures in the specimen that was even larger than γ . These results imply that the necessary conditions for grain subdivision in SPD simulations not only contain geometrical aspects but also kinematic aspects.

3.2.3 Partial Disclinations Induced by the Strain Gradient

Figure 3.10a, b shows the atomic configurations at the vicinity of the grain gradient regions for $\gamma = 0.2$ and 0.7 . The atomic color represents the rotation angle from the initial state. As shown in the figure, defect boundaries with misorientation angles appeared around the strain gradient regions. Figure 3.10d, e shows the defect distributions of the same areas of Fig. 3.10a, b. A defect analysis was performed by drawing the Burgers circuits for each defect atom, as shown in Fig. 3.10f. In both cases of $\gamma = 0.2$ and 0.7 , geometrically necessary boundaries (GNBs) were formed

Fig. 3.10 Distributions of the lattice defects around the strain gradient regions during SPD processes. **a, c** $\gamma = 0.2$. **b, d** $\gamma = 0.7$. **c** A higher resolution image of the region marked out by a box in **(b)**. **f** Burgers circuits for determining the defect structure types. Partial disclinations accompanied by finite dislocation arrays and a plane defect. The structures of the partial disclination boundaries change according to the local shear strain γ . The filled and unfilled triangles denote the positive and negative partial disclinations, respectively. Reproduced from Shimokawa et al. (2016) with permission from The Japan Institute of Metals and Materials

by the finite edge dislocation arrays with the same sign of the slip system for the left side of the strain gradient regions. The GNBs could accommodate the strain gradient fields. The distance between the dislocations in the GNBs became shorter with the increase in γ , as the misorientation angle at the GNBs became larger. With the increase in the misorientation angle, it is difficult to express GNBs as dislocation arrays. Hence, the GNB was expressed as a plane defect as shown on the right side of the strain gradient region in Fig. 3.10e. This plane defect did not cross the specimen, so a rotational type of defect field appeared in the specimen. As a result, this defect can be regarded as a partial disclination (Romanov and Vladimirov 1992) with a plane defect. Notice that the finite dislocation arrays on the left side also can be regarded as partial disclinations. That is, the plane defect structure transitions with the magnitude of the Frank vector ω , which represents the disclination strength, as shown in Fig. 3.11.

Partial disclination mobility is important for grain subdivisions, as strain gradient regions travel through specimens during the SPD process. If the partial disclination mobility was small, the GNBs would not have been able to follow the moving strain gradient regions in the specimen. Consequently, they would have remained in the specimen and formed a microstructure. Since partial disclinations are accompanied by grain boundaries, the mobility of grain boundaries is closely related to the grain subdivision process. Furthermore, the interactions between dislocations and partial disclinations are also important since many dislocations are generated in SPD processes. Also, the mobility of the partial disclinations interacting with lattice dislocations strongly depends on their grain boundary structure. When a structure is represented as a lattice dislocation array in the case of a small ω , as shown on the left

Fig. 3.11 Grain subdivision mechanism obtained by a severe plastic deformation process through molecular dynamic simulations

side of Fig. 3.11, it is hardly affected by external dislocations. However, when it is represented as a structural unit in the case of a large ω , as shown on the right side of Fig. 3.11, it is strongly affected by external dislocations, resulting in the formation of new microstructures by grain subdivision with GNBs remaining in the specimen (Shimokawa et al. 2016). The critical misorientation angle of the grain boundary transition in the partial disclination from the dislocation array to the structural units corresponded to the critical γ required for the grain subdivision in this simulation (Shimokawa et al. 2016). These are the geometrical and kinematic reasons for the existence of the critical local shear strain γ in the grain subdivision of the present simulation.

3.3 Fracture Toughness: Disclinations at the Grain Boundary

3.3.1 High Strength and High Toughness

In general, it is difficult to achieve both high strength and high fracture toughness with single-crystal materials from the viewpoint of dislocation mobility, but it has been reported that UFG materials with enhanced strength can achieve both high strength and high fracture toughness by reducing the grain size to the sub-micron order (Hodge et al. 1949; Tsuji et al. 2004; Tanaka et al. 2008). Since UFG materials have more grain boundaries than coarse-grained materials, it is important to understand the role of grain boundaries in crack-initiated fracture phenomena. In this section, a new shielding process was presented via grain boundaries (Shimokawa et al. 2011; Shimokawa and Tsuboi 2015) based on the lattice defects evolution, as shown in Figs. 3.12 and 3.13, and it may be one of the mechanisms for improving the fracture

toughness of UFG materials based on the dislocation shielding theory (Rice and Thomson 1974; Majumdar and Burns 1981) and molecular dynamic simulations.

3.3.1.1 Dislocation Shielding

In general, there is a trade-off relationship between the yield stress and fracture toughness of crystalline materials with a high Peierls stress, and it is known that the fracture toughness decreases with the increase in the yield stress. Since the yield stress is negatively correlated with temperature, a brittle-ductile transition behavior can be observed for such materials at a certain temperature. Previous experiments have shown that the activation energy of the brittle-ductile transition is well correlated with the activation energy of dislocation mobility (Giannattasio et al. 2007), and it has been reported that the elemental mechanism controlling the behavior of brittle-ductile transition is the mobility of dislocations. In other words, as the dislocation motion is suppressed at lower temperatures, the material becomes more brittle, and the fracture toughness value decreases. This phenomenon can be explained by considering the dislocations shielding effect on the crack tip mechanical field, as shown in Fig. 3.12a (Rice and Thomson 1974). For a coarse-grained material in which the distance between the crack and grain boundary is sufficiently large, the mechanical field at the crack tip is shielded by the mechanical field of the dislocations emitted from the crack. This effect is called *dislocation shielding*. If the dislocation stays near the crack tip, it is difficult to emit subsequent dislocations from the crack tip, which then reaches a cleavage failure environment with a small stress intensity factor. Hence, to obtain a large fracture toughness value, the emitted dislocations from a crack tip have to move far enough away to shield it by a large number of dislocations. In other words, the mechanical field at a crack tip, which governs the fracture toughness, is determined by the competition between “the expansion speed of the stress concentrated field (K-field) with the increase in the external force” and “the expansion speed of the plastic region (dislocation mobility)”.

3.3.1.2 Grain Boundary Shielding

As known in the Hall-Petch relation, grain refinement is one of the methods for strengthening materials. The researches on the fracture toughness of UFG materials have shown that at low temperatures, the brittle-ductile transition temperature is shifted to lower temperatures and that the fracture toughness is improved (Tsuji et al. 2004; Tanaka et al. 2008). In short, grain size refinement is expected to be an excellent method for achieving both high strength and high toughness. However, since the activation energies of the brittle-ductile transition between coarse- and fine-grained materials are almost the same (Tanaka et al. 2009), it can be deduced that the dislocation mobility is not affected by the grain size. Therefore, it is clear that to understand the grain size dependence of fracture toughness, it is necessary to extend the conventional shielding theory to consider another dominant factor that shows the

Fig. 3.12 Schematics of **a** the dislocation shielding and **b** grain boundary shielding. **c, d** Stress fields around the crack tip with/without a dislocation at the grain boundary under the same applied loading. A grain boundary shielding can be clearly confirmed in (c). Reprinted with permission from Shimokawa et al. (2011). Copyright 2011 by American Physical Society

grain size dependence in addition to the dominant factor of the dislocation mobility that controls the brittle-ductile transition behavior. The major difference between coarse and fine-grained materials is the volume fraction of grain boundaries. As shown in Fig. 3.12b, in the conventional shielding theory, if the grain boundaries role is considered as an obstacle to dislocations, a dislocation emitted from a crack can only move up to the grain boundaries. In this case, the shielding effect at the crack tip by the dislocations entering the grain boundary is termed as *grain boundary shielding*, which is clearly observed in Fig. 3.12c, d. The stress field ahead of the crack tip decreased with the existence of a dislocation at the grain boundary. With the decrease in the grain size, dislocations piled up against the grain boundary in the vicinity of the crack, and the back stress suppressed the release of dislocations from the crack tip. As a result, it is not possible to easily increase the number of dislocations emitted from a crack tip, and the fracture toughness is reduced (Noronha and Farkas 2004; Zeng and Hartmaier 2010). This result cannot explain the actual experimental results, so it was necessary to extend the role of grain boundaries to resolve this discrepancy.

3.3.1.3 Disclination Shielding

The atomic simulations of the interactions among dislocations, crack tip, and grain boundary showed that this contradiction can be resolved by considering the role of the grain boundary as a dislocation generation site (Shimokawa et al. 2011). If dislocations are continuously emitted from a grain boundary, disclination dipoles can be formed, as shown in Fig. 3.13. The stress field in this disclination dipole can reduce the stress field at the crack tip, meaning that the mechanical field at the crack tip can be shielded without losing the plastic deformation ability near the crack by the dislocations emission from the grain boundary. This is called *disclination shielding*. The details of the disclination shielding mechanism are described below.

Fig. 3.13 Schematics of the disclination shielding with a dislocation emission from the grain boundary observed in atomic simulations to realize the improving fracture toughness. **a** Intragranular crack and **b**, **c** intergranular cracks. Reprinted with permission from Shimokawa et al. (2011). Copyright 2011 by American Physical Society

3.3.2 Dislocation Emission from the Grain Boundary

The grain boundary that achieved disclination shielding changed the grain boundary misorientation in the dislocation-emitted region. In other words, the grain boundary structure must transition to another grain boundary structure with the release of a dislocation. One grain boundary that satisfies this is the $\langle 112 \rangle$ symmetrical tilt grain boundary in the face-centered cubic system. Figure 3.14a shows the relationship between the grain boundary misorientation angle and the grain boundary energy of the Al $\langle 112 \rangle$ symmetrical tilt grain boundaries (Shimokawa 2010). The numbers near the plot represent the Σ value of each grain boundary. There is a $\Sigma 11$ grain boundary with minimum energy at $\theta = 62.96^\circ$. Figure 3.14b, c shows the grain boundary structure of the $\Sigma 11$ grain boundary and the $\Sigma 15$ grain boundary, which has a larger misorientation angle than the $\Sigma 11$ grain boundary. The structure of the $\Sigma 11$ grain boundary can only be represented by the B -structural unit, while the structure of the $\Sigma 15$ grain boundary can be represented by the periodic arrangement of the B and C structural units. To investigate the relationship between the two structures, the displacement shift complete (DSC) lattice (Bollmann 1970) and coincidence site lattice (CSL) of the $\Sigma 11$ grain boundary were demonstrated as thin and thick solid lines, respectively, as shown in Fig. 3.14d. Figure 3.14e shows the DSC lattice of the $\Sigma 11$ grain boundary applied to the $\Sigma 15$ grain boundary. This indicates that there was a grain boundary dislocation in the C -structural unit of the $\Sigma 15$ grain boundary that formed a change in the misorientation angle from the $\Sigma 11$ grain boundary structure. The Burgers vector of the grain boundary dislocation is $\mathbf{b}^{\text{gb}+} = \frac{2}{11}[\bar{1}\bar{3}\bar{1}]_{\text{II}}$. Here, the Burgers vector of the slip system, which was activated by applying a tensile load perpendicular to the interface of the $\Sigma 15$ grain boundary, was $\mathbf{b}^{\text{t}} = \frac{1}{2}[1\bar{1}0]_{\text{II}}$, and the response of the Burgers vectors when a lattice dislocation was emitted using a grain boundary dislocation is as follows:

Fig. 3.14 a Grain boundary energy and misorientation angle relationship of the aluminum $\langle 112 \rangle$ tilt grain boundaries. The Σ values are shown near the symbols. b, c The grain boundary structures of $\Sigma 11$ and $\Sigma 15$ are represented by the B and C structural units. d, e The DSC lattices of $\Sigma 11$ and $\Sigma 15$. The atomic colors represent the different depths of the stacking atomic layers along the $[1\bar{1}2]$ direction. The thick and thin lines represent the CSL and DSC lattices of $\Sigma 11$, respectively. Reprinted with permission from Shimokawa (2010). Copyright 2010 by American Physical Society

$$\begin{aligned}
 b^{\text{gb}+} - b^{\text{lt}} &= 2b_2^{\text{dsc}} - b^{\text{lt}} \\
 &= \frac{2}{11}[1\bar{3}\bar{1}]_{\text{II}} - \frac{1}{2}[1\bar{1}0]_{\text{II}} \\
 &= \frac{1}{22}[\bar{7}\bar{1}\bar{4}]_{\text{II}} = -b_1^{\text{dsc}}.
 \end{aligned} \tag{3.1}$$

This means that the residual Burgers vector at the grain boundary is the same as in the transverse DSC lattice and that there are no grain boundary dislocations that form grain boundary misorientation angles. In other words, the $\Sigma 15$ grain boundary can transition to the $\Sigma 11$ grain boundary by emitting lattice dislocations under tensile deformation. Such a dislocation emission accompanied by a grain boundary transition has also been observed in the case of a symmetrical tilt grain boundary of $\langle 110 \rangle$ (Spearot 2008). Notice that, in the case of compressive deformation at the $\Sigma 15$ grain boundary, the Burgers vectors of the lattice dislocations were in the opposite direction to b^{lt} , so a dislocation cannot be emitted from the grain boundary dislocation, as the magnitude of the residual Burgers vector becomes larger than that of the grain boundary dislocation. The grain boundary structure transition by compressive deformation occurred at the grain boundaries with a smaller misorientation angle

than that of the $\Sigma 11$ grain boundary, which is the case with the $\Sigma 21$ grain boundary, where the Burgers vector of the grain boundary dislocation was $-\mathbf{b}^{\text{gb}+}$ when the $\Sigma 11$ was the reference structure. Consequently, if the Burgers vectors of the grain boundary dislocations and lattice dislocations, which can be activated under an applied loading, are close to each other, lattice dislocations can easily be generated from the grain boundary accompanied by a grain boundary structure transition into the stable boundary, which forms a disclination dipole at the grain boundary.

3.3.3 Intragranular Crack

To investigate the disclination shielding effect on the fracture toughness, the interactions among the crack tip, dislocations, and grain boundary were simulated using molecular dynamics (Shimokawa et al. 2011). Here, we used the $\Sigma 15$ grain boundary ($|BBC|$ period), which has a high dislocation source ability in the tensile deformation described in the previous section.

3.3.3.1 Transition of the Dislocation Sources from the Crack Tip to the Grain Boundary

Figure 3.15a–c shows the evolution of the lattice defects in a model with intergranular cracks under tensile loading with a strain rate of 2×10^7 1/s at 100 K. The color of the atoms represents the rotation angle extent from the initial state. The embedded atom method proposed by Mishin et al. was adopted to simulate the atomic interactions. Mishin et al. (1999). First, since the crack tip became a strong source of stress concentration, dislocations were generated from the crack tip, as shown in Fig. 3.15a, and these dislocations penetrated into the grain boundary. These dislocations also shielded the crack tip and reduced the stress concentration capability: *dislocation shielding and grain boundary shielding*. However, as shown in Fig. 3.15b, c, a large number of dislocations were generated from the $\Sigma 15$ grain boundary due to the stress concentration caused by the lattice dislocations near the grain boundary. As shown in Fig. 3.15d, the lattice dislocations were emitted from the C structural units, which contained the grain boundary dislocations, and the grain boundary structure transitioned to the more stable $\Sigma 11$ grain boundary (B only). Also, a disclination dipole was formed at its boundary. This can be confirmed by the rotation of the region in which the dislocations were emitted, as shown in Fig. 3.15c.

3.3.3.2 Improving the Fracture Toughness by Disclination Shielding

Figure 3.16 shows the effect of the mechanical field of the disclination dipole formed at the grain boundary on the crack tip. Figure 3.16a shows the stress field of the grain boundary shielding by a lattice dislocation emitted from the crack tip, and

Fig. 3.15 **a, b, c** Translation of the dislocation source from the crack tip to the grain boundary in model A. The atomic color represents the rotation angle from the initial state of each atom with an FCC structure, $\Delta\theta$. The black atoms represent the defect structures. **d** Change in the grain boundary structures from $\Sigma 15$ to $\Sigma 11$ after the dislocation emissions from the C structural units. This atomic structure corresponds to a higher resolution image of the white box shown in (c). The dark and light gray atoms indicate that the nearest-neighboring atomic configurations correspond to stacking fault structures and other defects, respectively. The atoms shown in other colors form an FCC structure. Reprinted with permission from Shimokawa et al. (2011). Copyright 2011 by American Physical Society

Fig. 3.16b, c shows the stress field of the disclination dipole with the same Frank vector but with a different length a_{discli} by introducing the $\Sigma 11$ grain boundary region into the $\Sigma 15$ grain boundary. These are all unloaded conditions. With the increase in a_{discli} , a negative stress field was generated at the crack tip, indicating that the disclination dipole shielded the crack tip. To more quantitatively evaluate this effect, Fig. 3.16d shows the value of the local stress intensity factor due to the disclination dipole k_{discli} , which was normalized by the local stress intensity factor k_{gb,l_i} due to the grain boundary shielding shown in Fig. 3.16a. It was confirmed that the shielding effect of the crack tip increased with the increase in a_{discli} . Thus, the fracture toughness of the crack tip could be increased by the disclination dipole. The positional relationship between the crack tip and dislocations emitted from the grain boundary changed as a result of the dislocation motion, but the positional relationship between the disclination dipole and crack tip remained unchanged. Therefore, the dislocation emission from the grain boundary allowed the disclination dipole to grow while maintaining the plastic deformation capacity around the crack tip. It could also

Fig. 3.16 Disclination shielding and its dependence on the distance between the disclination dipoles, a_{discli} . Distributions of σ_z by the **a** grain boundary shielding, $k_{\text{gb,lt}}$, **b** disclination shielding, k_{discli} with $a_{\text{discli}} = 3$ nm, and **c** k_{discli} with $a_{\text{discli}} = 6$ nm when the applied stress σ_a was zero. **d** The normalized disclination shielding effect $k_{\text{discli}}/k_{\text{gb,lt}}$ as a function of a_{discli} . The inset figure represents the grain boundary structure through the combination of the structural units *B* and *C*, two semi-infinite walls of the grain boundary dislocations, and a disclination dipole. Reprinted with permission from Shimokawa et al. (2011). Copyright 2011 by American Physical Society

better shield the mechanical field at the crack tip and improve the fracture toughness with the progress in the plastic deformation. As a result, it can be concluded that one of the mechanisms for improving the fracture toughness of UFG materials is that grain boundaries act as a source of dislocations and create a shielding field by the disclination dipole in the grain boundary region against the mechanical field at the crack tip, which can be realized by the grain boundary transformation through dislocation emissions.

3.3.4 Intergranular Crack

The same kind of disclination shielding was also observed in the intergranular cracks, as shown in Fig. 3.13b, c (Shimokawa and Tsuboi 2015). Based on the energy equilibrium, the following equations should be satisfied for the propagation of intergranular cracks (Sutton and Balluffi 1995):

$$\mathcal{G}_c = \mathcal{G} > (2\gamma_s - \gamma_{gb}) + \gamma_p. \quad (3.2)$$

Here, $\mathcal{G}$, γ_s , γ_{gb} , and γ_p represent the strain energy release rate, surface energy, grain boundary energy, and work done by the plastic strain near the crack tip, respectively. $\mathcal{G}$ is the crack extension force, and $(2\gamma_s - \gamma_{gb}) + \gamma_p$ is the crack extension resistance. Generally, since γ_p is much larger than $(2\gamma_s - \gamma_{gb})$, it can be predicted that the grain boundary fracture is not affected by the grain boundary structure. However, it has been reported that the fracture toughness is significantly affected by the segregation amount at grain boundaries (Guttmann and McLean 1979), which is contrary to the prediction of Eq. (3.2). It has been proposed that this contradiction can be resolved by considering γ_p to be a function of $(2\gamma_s - \gamma_{gb})$ (Jokl et al. 1980). In other words, the plasticity capacity near the intergranular cracks may be affected by the grain boundary characteristics. In this section, a tensile deformation analysis was conducted for the intergranular cracks of $\Sigma 15$ and $\Sigma 73$, which tend to emit dislocations under tensile loading as in the previous section, using molecular dynamic simulations to investigate the relationship between the grain boundary characteristics and fracture toughness while focusing on disclination shielding (Shimokawa and Tsuboi 2015). The analysis material was aluminum, the strain rate was 1×10^8 1/s, and the temperature was maintained at 100 K.

3.3.4.1 Propagation of the Stress Concentration Field

The results of the uniaxial tensile simulation of the analytical model with a crack on the right side of the $\Sigma 15$ grain boundary are shown in Fig. 3.17. The colors of the atoms represent the normal stress components in the loading direction. The grain boundary dislocations in front of the intergranular crack were continuously emitted from the C structural unit. When dislocations were emitted from the grain boundary, the $\Sigma 15$ grain boundary structure became $\Sigma 11$, and the grain boundary misorientation angle changed. This implies that a disclination dipole was formed at the grain boundary, as shown in Fig. 3.17c, d. As a result, the stress concentration field at the crack tip shifted to the left along the grain boundary, as if an intergranular crack was growing. In other words, the mechanical field due to the crack tip was shielded by the disclination dipole, which increased the fracture toughness. In addition, the energy of the grain boundary decreased after the dislocation emissions, meaning that the grain boundary was transitioned to one that is less likely to be the cleavage fracture.

3.3.4.2 Nanograin Formation

A crack was introduced at the left side of the $\Sigma 73$ grain boundary ($|BBBBBBC|$ period), and the results of the uniaxial tensile analysis perpendicular to the crack plane are shown in Fig. 3.18. As dislocations were emitted from the crack tip, grain boundary dislocations in front of the crack tip were also emitted. The grain boundary

Fig. 3.17 Shift of the stress concentration ahead of the intergranular crack tip of the $\Sigma 15$ boundary by the disclination shielding shown in Fig. 3.13b, which was caused by the continuous dislocation emissions from the grain boundary. Reprinted with permission from Shimokawa and Tsuboi (2015) from Elsevier

Fig. 3.18 Nanograin formation near the crack tip caused by the dislocation emission from the crack tip and the $\Sigma 73$ grain boundary. **d** Schematic of the disclination dipoles ahead of the crack tip. The nanograin with a wedge disclination with ω_3 at the triple junction among the original $\Sigma 73$ boundary, $\Sigma 11$, and low angle grain boundary. Reprinted with permission from Shimokawa and Tsuboi (2015) from Elsevier

structure at the crack tip was branched into the $\Sigma 11$ grain boundary and a small-angle grain boundary, and a new nanocrystal grain was formed in front of the crack. If the sum of the misorientation angle θ_{73} of the original grain boundary, θ_{11} of the $\Sigma 11$ boundary, and θ_L of the small-angle grain boundary, 11, is not equal, there is a disclination with the Frank vector ω_3 at the triple junction, as shown in Fig. 3.18d. In the grain boundaries with $\theta > \theta_{11}$, the greater the θ of the original grain boundary, the greater the θ_L of the small-angle grain boundary formed near the crack, resulting in a larger negative Frank vector ω_3 in front of the crack that can shield the intergranular crack. Therefore, by controlling the character and strength of disclinations near the crack tip caused by the lattice defect evolution, which is closely related to the role of GBs as dislocation sources, materials with excellent strength and ductility can be obtained.

3.4 Conclusion

In this chapter, two different studies involving the disclination-mediated plastic phenomena observed in atomic simulations were reviewed to show the potential of

disclination, which exposes the attractive properties of nanostructured metals. The first reviewed study discussed a grain subdivision mechanism related to the mobility of partial disclination under severe plastic deformation processes. The second one thoroughly discussed an improving fracture toughness mechanism in which the disclination shielding effect appears at the grain boundary after dislocation emission. These atomic simulations with the geometrical restrictions of boundary conditions showed the possibility of selecting a plastic deformation mode by designing structures, elements, and environments to obtain materials with excellent mechanical properties.

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