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Disorientations in dislocation boundaries: formation and spatial correlation

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Abstract

During plastic deformation dislocation boundaries appear separating regions of different orientation. The occurrence of disorientations across these boundaries is discussed with emphasis on several types of boundaries. For incidental dislocation boundaries a statistical origin of disorientations is considered, additional deterministic contributions arising from geometrical reasons are taken into account for geometrically necessary boundaries. The resulting diversity in the modelled boundary behaviour explains the experimentally observed differences in the dependence of the average disorientation angle on plastic strain. Spatial correlations between disorientation angles of neighbouring boundaries are investigated.

Keywords: Disorientation; Disorientation angle; Dislocation boundary; Model; Plastic deformation; Correlation

1. Introduction

With increasing plastic strain dislocation loops are emitted from dislocation sources. After carrying the plastic deformation along their free path, mobile dislocations are stored within the material. Dislocations of opposite sign of the Burgers vector are present in equal number, but their spatial distribution is inhomogeneous. A local surplus of dislocations of a preferred sign leads to a disorientation between adjacent regions.

The excess dislocations causing disorientations tend to gather into dislocation rotation boundaries and two types of boundaries can be distinguished [1]: incidental dislocation boundaries (IDBs) as a result of a statistical mutual trapping of dislocations and geometrically necessary boundaries (GNBs) with a different activity of slip systems on each side of the boundary.

The formation of disorientations is modelled for both kinds of boundaries emphasizing the process of separation of dislocations of opposite sign. For IDBs excess dislocations and, consequently, disorientations accumulate statistically from fluctuations in the density of mobile dislocations [2,3].

For GNBs an additional contribution arises (by definition) from a different activity of the slip systems on either side of the boundary leading to creation of disorientations even if no statistical fluctuations occur and no disorientations are present initially. Depending on the actual geometry there might be a further contribution to the accumulation of disorientations arising from misfit dislocations deposited at the boundary as soon as small disorientation angles appear. The same processes responsible for the formation of disorientations across individual boundaries cause correlations between the disorientations of neighbouring boundaries also.

2. Disorientations and excess dislocations

Mobile dislocations carrying the plastic deformation are partially trapped in dislocation boundaries (or dislocation walls) during their passage as illustrated in Fig. 1. The mean free path $\bar{\lambda}$ of mobile dislocations moving with velocity $v = j/\rho^{\mathrm{m}} = \dot{\gamma}/b\rho^{\mathrm{m}}$ determines their life time $\tau = \bar{\lambda}/v$. The dislocation fluxes $j^{\rightarrow} = v\rho_{\perp}^{\mathrm{m}}$ and $j^{\leftarrow} = v\rho_{\top}^{\mathrm{m}}$ in both directions are depleted by trapping of mobile dislocations and dislocations of both signs of the Burgers vector ($\perp$ and $\top$) are stored in the boundary. The accumulation of dislocations of positive sign

$$\frac{\mathrm{d}\rho_{\perp}}{\mathrm{d}t} = \frac{j^{\rightarrow}}{\bar{\lambda}} = \frac{P}{d} j^{\rightarrow} \tag{1}$$

is governed by the dislocation flux $j^{\rightarrow}$ through the boundary to the right-hand side. In an analogous manner, dislocations of opposite sign are trapped. The capturing probability $P = d/\bar{\lambda}$ is determined by the mutual distance d between boundaries and the mean free path $\bar{\lambda}$ of mobile dislocations

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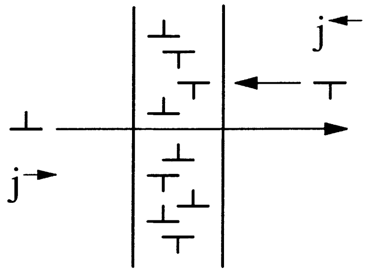

Fig. 1. Dislocation boundary with penetrating dislocation fluxes of a single slip system.

which can be obtained from slip line length ($2\bar{\lambda}$) measurements. In case of tensile deformation along the [0 0 1] axis of copper single crystals, in average three boundaries are passed before a mobile dislocation is immobilized in a dislocation boundary leading to $P = \frac{1}{3}$ [4].

If dislocations of one sign ($\perp$) of the Burgers vector exceed the number of dislocations of opposite sign ($\top$), an excess dislocation density $\Delta\rho = \rho_\perp - \rho_\top$ arises and the boundary is associated with a disorientation angle

$$\alpha = bd\Delta\rho \tag{2}$$

between both adjacent regions according to the Read–Shockley relation [5]. Assuming that the boundary spacing d does not change significantly during the passage time of an individual mobile dislocation through the boundary, a change in the disorientation angle

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = Pb(j^{\rightarrow} - j^{\leftarrow}) = Pb\Delta j \tag{3}$$

is obtained from any bias $\Delta j = j^{\rightarrow} - j^{\leftarrow}$ of the dislocation fluxes passing the boundary from both sides. A possible annihilation of dislocations of opposite sign will affect the total dislocation density, but has no effect on the accumulation of excess dislocations.

3. Stochastic formation of disorientations [2]

In homogeneously deforming single crystals, a bias Δj_{fluc} is caused solely by statistical fluctuations. Fluctuations are considered stemming only from the number of mobile dislocations of each sign simultaneously present in an equiaxed region (dislocation cells) of size d [7]. If the fluctuations in the number of mobile dislocations on both sides of a boundary are independent of each other, a fluctuation amplitude

$$(\Delta j_0)^2 = \frac{v^2}{d^2}\rho_{\mathrm{m}} \tag{4}$$

results (deviating by a factor of 2 from earlier results [2,3] where a strong anti-correlation was assumed). Fluctuations in the mobile dislocation density are restricted to the life time of mobile dislocations $\tau = \bar{\lambda}/v$ and correlations between fluctuations can be expected only for shorter times. The correlation function is then given by an instantaneous correlation

$$\langle \Delta j(t')\Delta j(t'')\rangle = (\Delta j_0)^2\tau\delta(t' - t'') \tag{5}$$

with Dirac's δ-function. For any random noise, the ensemble average over the system disappears ($\langle\Delta j(t)\rangle = 0$).

For continuous deformations on time scales large compared to τ (like unidirectional deformation without spontaneous strain rate changes), a normal distribution

$$f(\alpha) = \frac{1}{\sqrt{2\pi\sigma_\alpha^2}}\exp\left(-\frac{\alpha^2}{2\sigma_\alpha^2}\right) \tag{6}$$

for the disorientation angles results with a vanishing mean value $\langle\alpha\rangle = 0$ and a standard deviation

$$\sigma_\alpha^2 = \langle\alpha^2\rangle = \int_0^\gamma \frac{bP}{d}\,\mathrm{d}\gamma' \tag{7}$$

After normalization of the disorientation angles by the average modulus $\langle|\alpha|\rangle = \sigma_\alpha\sqrt{2/\pi}$, the resulting distribution does not depend on the standard deviation σ_α or on strain γ any longer, i.e. scaling behaviour.

Similar expressions can be obtained by slightly different arguments [8]: during plastic deformation, dislocation loops are emitted from randomly and uniformly distributed dislocation sources. Each dislocation (of the two dislocations of opposite sign forming a loop) travels along a path λ before it is stopped in a boundary. The mean free path $\bar{\lambda}$ determines the separation of the dislocations of opposite sign and leads in consequence to a correlation between the disorientation angles over distances comparable to $\bar{\lambda}$.

4. Deterministic formation of disorientations

4.1. Activation imbalance

For GNBs, by definition, a certain difference in the activation of slip systems on both sides exists due to either an activation of a different set of slip systems [1] or a different activation of the same set of slip systems [9].

This is illustrated for a single crystal in plane strain compression, where only the two slip systems of Fig. 2 are

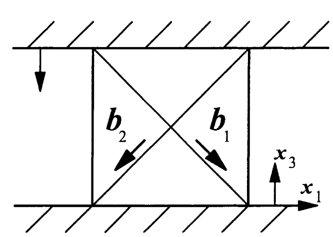

Fig. 2. Plane strain compression of a single crystal on two slip systems (coordinate system is indicated).

assumed to be active. [1] The distortion rate tensors corresponding to the two slip systems

$$\mathbf{L}_{\mathrm{pl},1} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & -1 \end{pmatrix} \frac{\dot{\gamma}_1}{2},$$

$$\mathbf{L}_{\mathrm{pl},2} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} \frac{\dot{\gamma}_2}{2} \quad (8)$$

lead to the same deformation rate tensor $\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^{\mathrm{T}})$, but differ in their antisymmetric part. A different activation of both slip systems $\dot{\gamma}_1 = \dot{\gamma}(1 + \Gamma)$ and $\dot{\gamma}_2 = \dot{\gamma}(1 - \Gamma)$ is characterized by an activation parameter $-1 < \Gamma < 1$ describing how the slip systems share the prescribed deformation (rate) leading to a plastic distortion rate tensor

$$\mathbf{L}_{\mathrm{pl}} = \begin{pmatrix} 1 & 0 & \Gamma \\ 0 & 0 & 0 \\ -\Gamma & 0 & -1 \end{pmatrix} \dot{\gamma} \quad (9)$$

During compression the compression tool remains planar, requiring a vanishing component of the total distortion rate tensor: $L_{31} = 0$. This boundary condition forces an orientation change of the single crystal with a rate $\omega = \Gamma\dot{\gamma}$ depending on the activation parameter Γ [10].

For GNBs a certain imbalance between both sides in sharing the plastic strain (rate) between the activated slip systems is expected. The difference $\Delta\Gamma$ between the activation parameters Γ_i on both sides of the boundary gives rise to a geometrical bias in the dislocation fluxes $\Delta j_{\mathrm{gn}} = \Delta\Gamma j$ and a change in the disorientation angle across the GNB

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \Delta\omega = \Delta\Gamma\dot{\gamma} \quad (10)$$

4.2. Misfit dislocations

A further possibility for deterministic formation of disorientations arises from the mutual disorientation between the two regions adjacent to the boundary depending on the geometry of the boundary (and may be differently activated slip systems) [6,13]. If both sides of a boundary are slightly disoriented, mobile dislocations from both adjacent sides cannot annihilate completely. The misfit dislocations lead to elastic stresses and strains on both sides ensuring compatibility of the deformation. By forming ledges, the boundary remains free of long range stresses (obeying Frank's formula [11]) and "rotates" [12]. Thus, instead of producing elastic stresses, the misfit dislocations contribute to the disorientation angle (compare [6]):

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = r\alpha bj \quad (11)$$

The geometrical factor $-1 < r < 1$ reflects that misfit dislocations affect the disorientation angle in either an enforcing or a lessening way.

5. Evolution of disorientation angles

All three mechanisms (based on statistical fluctuations, activation imbalance and misfit dislocations) are summarized in an evolution equation for the disorientation angle [6]

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = bP\Delta j_{\mathrm{fluc}} + b\Delta\Gamma j + r\alpha bj \quad (12)$$

Taking into account a Gaussian process for statistical fluctuations in the bias of dislocation fluxes (Δj_{fluc}) as in Section 3, Eq. (12) is solved by a Gaussian distribution

$$f(\alpha) = \frac{1}{\sqrt{2\pi\sigma_\alpha^2(\gamma)}} \exp\left(-\frac{1}{2\sigma_\alpha^2(\gamma)}(\alpha - \bar{\alpha}(\gamma))^2\right) \quad (13)$$

for constant boundary spacing d and constant imbalance $\Delta\Gamma$. With initial values $\bar{\alpha}(0) = 0$ and $\sigma_\alpha(0) = 0$ for an undeformed material the mean disorientation angle and the standard deviation become

$$\bar{\alpha}(\gamma) = \langle\alpha\rangle = \frac{\Delta\Gamma}{r}(\exp(r\gamma) - 1) \quad (14)$$

$$\sigma_\alpha^2(\gamma) = \frac{bP}{2rd}(\exp(2r\gamma) - 1) \quad (15)$$

Depending on the relative contribution of the three mechanisms, several types of behaviour of the disorientation angles with strain displayed in Fig. 3 can be distinguished:

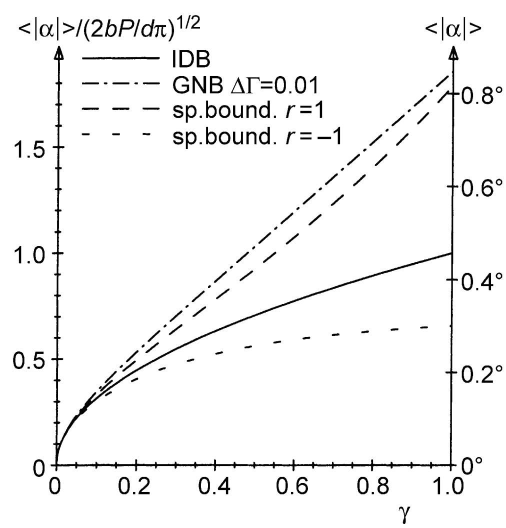

Fig. 3. Modelled evolution of the average modulus $\langle|\alpha|\rangle$ of the disorientation angle for different conditions. Type 1: pure statistical accumulation (IDBs), type 2: imbalance in slip activity $\Delta\Gamma = 0.01$ (GNBs), and type 3: creation of misfit dislocations (special boundaries with $r = 1$ or -1). For the numerical values, $b = 3 \times 10^{-10}$ m, $P = \frac{1}{3}$, and $d = 10^{-6}$ m was used.

[1] Similar conditions are met, for instance, in plane strain compression of f.c.c. crystals in cube orientation. The four active slip systems are forming two pairs with an equal activity of the two slip systems in each pair due to plane strain conditions [12].

1. A pure stochastic process leads to a square root behaviour of the average modulus of the disorientation angle

$$\langle|\alpha|\rangle = \sqrt{\frac{2}{\pi}}\sigma_\alpha = \sqrt{\frac{2bP}{\pi d}}\sqrt{\gamma} \tag{16}$$

(non-constant boundary spacings d modify the behaviour slightly, compare Eq. (7) and [2]).

2. An imbalance $\Delta\Gamma$ in the activation of slip systems on both sides of a boundary causes a linear increase of the mean angle

$$\langle\alpha\rangle = \bar{\alpha} = \Delta\Gamma\gamma \tag{17}$$

The entity measured experimentally, the average modulus of the disorientation angles $\langle|\alpha|\rangle$, will depend on the presence of fluctuations. Taking fluctuations into account (and $r = 0$), an increasing deviation from an initial square root behaviour can be detected in Fig. 3 and the slope $\partial\langle|\alpha|\rangle/\partial\gamma$ approaches $\Delta\Gamma$ with increasing strain.

3. An accumulation of disorientations from misfit dislocations without an imbalance ($\Delta\Gamma = 0$) leads to

$$\langle|\alpha|\rangle = \sqrt{\frac{2}{\pi}}\sigma_\alpha = \sqrt{\frac{2bP}{\pi d}}\sqrt{\frac{\exp(2r\gamma) - 1}{2r}} \tag{18}$$

showing a stronger increase for a positive r or a levelling off at large strains to $\langle|\alpha|\rangle_\infty = \sqrt{bP/\pi|r|d}$ for negative r.

The first type of behaviour with pure statistical accumulation corresponds clearly to IDBs, whereas the second type with an imbalance in the activities of the slip systems matches the definition of GNBs. The proposed mechanism of an accumulation of disorientation angles from misfit dislocations of the third type is quite obvious for a different selection of slip systems on both sides of a boundary, but also applicable to special boundaries remaining free of long range stresses.

The predicted enhanced accumulation of disorientation angles resulting from deterministic contributions compared to a pure statistical accumulation (as obvious from Fig. 3) is supported by experimental investigations of the different types of boundaries (IDBs and GNBs). In cold rolled aluminium polycrystals, Hughes et al. [14] found a square root dependence of the disorientation angle on plastic strain for IDBs, but larger disorientation angles for GNBs as well as a stronger increase with strain of disorientations across GNBs.

6. Correlation of disorientations of neighbouring boundaries

The disorientations of neighbouring dislocation boundaries of the same type are coupled by the formation processes for disorientations across individual boundaries (IDBs or GNBs). If disorientations of individual boundaries are totally independent of each other [8], the disorientation angle across n boundaries increases proportional to the square root of the number n of boundaries ($\langle|\alpha_{(n)}|\rangle = \langle|\alpha|\rangle\sqrt{n}$).

6.1. IDBs

Disorientation angles in neighbouring IDBs are not independent, because dislocations of opposite Burgers vector corresponding to the same dislocation loop are not separated to infinity, but only to a finite distance $2\bar{\lambda}$. Therefore, in the absence of any bending or gradients in the plastic strain (rate), disorientations cannot be cumulative over several boundaries and the disorientation across n boundaries will level-off after an initial increase. A detailed treatment of this idea [8] shows that the average modulus of the disorientation angle across n boundaries is

$$\langle|\alpha_{(n)}|\rangle = \langle|\alpha_{(\infty)}|\rangle\sqrt{1 - \exp(-nP/2)} \tag{19}$$

increases with the number of boundaries n towards a saturation value

$$\langle|\alpha_{(\infty)}|\rangle = \sqrt{\frac{4b\gamma}{\pi d}} \tag{20}$$

The correlation coefficient

$$r(n) = \frac{\langle\alpha_i\alpha_{i+n}\rangle}{\sqrt{\langle\alpha_i^2\rangle\langle\alpha_{i+n}^2\rangle}} \tag{21}$$

$$r(n) = \exp\left(-\frac{nP}{2}\right)\frac{1 - \cosh(P/2)}{1 - \exp(-P/2)} < 0 \quad \forall n > 0 \tag{22}$$

is always negative and indicates a (weak) tendency for neighbouring boundaries having disorientations of opposite sign compared to the boundary under consideration.

6.2. GNBs

Correlations between the disorientation angles of adjacent GNBs appear from a different reason. In the lamellar arrangement of GNBs separating cell blocks shown in Fig. 4, each cell block j is characterized by an individual activation parameter Γ_j. Per definitionem, the Γ_j are different in adjacent cell blocks leading to a change in the

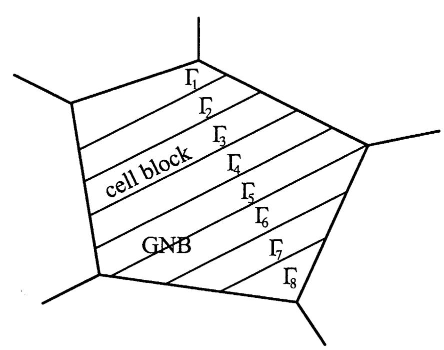

Fig. 4. Scheme of a grain subdivided into several cell blocks by a single set of planar and parallel GNBs. Each individual cell block j is characterized by a certain activation parameter Γ_j.

disorientation angle of boundary i

$$\frac{d\alpha_i}{dt} = \Delta\Gamma_i\dot{\gamma} = (\Gamma_{i+1} - \Gamma_i)\dot{\gamma} \tag{23}$$

owing to the activation imbalance $\Delta\Gamma_i$.

If the activation parameter Γ_j, i.e. the degree of freedom in the activation of the slip systems, is selected randomly in every cell block j, $\langle\Gamma_i\Gamma_j\rangle = \langle\Gamma^2\rangle\delta_{ij}$ results (with Kronecker's symbol δ_{ij}). Then, the average modulus of the disorientation angle across several boundaries $\langle|\alpha_{(n)}|\rangle = \langle|\alpha|\rangle$ is equal to the average modulus of the disorientation angle across a single boundary and does not depend on the number of boundaries. Beside the auto-correlation coefficient $r(0) = 1$, the correlation coefficient has only one non-vanishing value $r(1) = -\frac{1}{2}$ indicating that disorientations of adjacent boundaries are more likely to be opposite than of the same sign. For more distant boundaries, any correlation vanishes ($r(n) = 0\,\forall n > 1$) and a correlation exists only between closest neighbours. This is in contrast to IDBs where the mean free path of the dislocations causes a correlation over several boundaries.

Experimental evidence for a preferred opposite sign of the disorientations rather than cumulative disorientations is gained from the often observed alternating signs of disorientation angles across neighbouring GNBs, e.g. [15].

The original idea that the selection of active slip systems is different on both sides of a GNB [1] (instead of a slightly different sharing the strain between the same active slip systems [9]) leads to a much stronger correlation. If each cell block of the lamellar structure in Fig. 4 deforms only on one of the two possible slip systems, the activation parameter Γ becomes either 1 or -1. With only two possibilities, every second cell block has the same activation parameter and directly adjoined cell blocks have the opposite one ($\Delta\Gamma = \pm 2$). All disorientation angles become exactly $\alpha = \pm 2\gamma$ with alternating signs showing a perfect anti-correlation between the disorientation angles of neighbouring GNBs.

7. Conclusions

Disorientations across dislocation boundaries developing during plastic deformation are discussed. Statistical fluctuations as well as deterministic contributions from imbalances in the slip activity or misfit dislocations are incorporated in a model for the evolution of disorientation angles. The distribution function of the disorientation angles and the dependence of their average modulus on strain are obtained analytically. Already established boundary types are identified based on the relative importance of the different contributions. This distinction rationalizes the experimentally observed differences in the evolution of disorientations between IDBs and GNBs.

The existence of correlations between the disorientation angles in neighbouring boundaries is predicted from the same considerations. For both types of boundaries, a negative correlation occurs differing qualitatively between IDBs and GNBs. In case of IDBs, the correlation length is given by the mean free path of mobile dislocations. For GNBs, a correlation is expected only for the next neighbours if the activation of the same slip systems differs slightly, whereas a highly ordered structure with alternating disorientation angles arise for a different selection of slip systems.

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References

[1] D. Kuhlmann-Wilsdorf, N. Hansen, Scripta Metall. Mater. 25 (1991) 1557.
[2] W. Pantleon, Acta Mater. 46 (1998) 451.
[3] W. Pantleon, Mater. Sci. Eng. A 234–236 (1997) 567.
[4] Y. Kawasaki, T. Takeuchi, Scripta Metall. 14 (1980) 183.
[5] W.T. Read, W. Shockley, Phys. Rev. 78 (1950) 275.
[6] W. Pantleon, in: J.B. Bilde-Sørensen, et al. (Eds.), Proceedings of the 20th International Risø Symposium on Deformation-induced Microstructures: Analysis and Relation to Properties, Risø National Laboratory, Roskilde, Denmark, 1999, pp. 123–146.
[7] F.R.N. Nabarro, Scripta Metall. Mater. 30 (1994) 1085.
[8] W. Pantleon, D. Stoyan, Acta Mater. 48 (2000) 3005 and 4179 (Erratum).
[9] J.A. Wert, Q. Liu, N. Hansen, Acta Mater. 43 (1995) 4153.
[10] U.F. Kocks, H. Chandra, Acta Metall. 30 (1982) 695.
[11] F.C. Frank, Report on a Symposium on Plastic Deformation of Crystalline Solids, Carnegie Institute of Technology and Office of Naval Research, US Government Printing Office, Washington, DC, 1950, pp. 150–151.
[12] W. Pantleon, N. Hansen, in: J.V. Carstensen, et al. (Eds.), Proceedings of the 19th International Risø Symposium on Modelling of Structure and Mechanics of Materials from Microscale to Product, Risø National Laboratory, Roskilde, Denmark, 1998, pp. 405–410.
[13] W. Pantleon, Mater. Sci. Eng. A (2001), in press.
[14] D.A. Hughes, Q. Liu, D.C. Chrzan, N. Hansen, Acta Mater. 45 (1997) 105.
[15] Q. Liu, D. Juul Jensen, N. Hansen, Acta Mater. 46 (1998) 5819.