

Misorientation and crystal lattice distortions as the source of driving force for grain boundary movement

P. Dłużewski

Institute of Fundamental Technological Research, Swietokrzyska 21, 00-049 Warsaw, Poland
E-Mail: pdluzew@ippt.gov.pl

Abstract

A thermodynamic theory of the movement of misorientation surface is considered. This theory is based on the tensorial measures of elastic-plastic distortions and curvatures (contortions). The crystal plasticity is described by vector constitutive equations stated for dislocation movement and for grain boundary migration. The compatibility equations across the discontinuity surface together with the well-known balance laws have been used to find the driving forces acting on the surface. Using the derived relations the constitutive modelling of the movement of defects is considered. The constitutive equations presented take into account the elastic strain, dislocation density and temperature. Special attention is given to the dependency of free energy on the misorientation vector on the grain boundary.

1 Introduction

In this paper the continuum theory of dislocations is developed in terms of an oriented continuum. Usually, an oriented continuum is unjustly identified with the idea of the couple stress introduced by Cosserat, cf. e.g. Truesdell & Toupin [1], Eringen & Kafadar [2], Dłużewski [3]. In the current approach the couple stresses are not used and the main attention is focused on kinematical relations for evolution of the microstructure orientation, cf. Mandel [4], Dłużewski [5].

In Section 2 the mathematical foundations for the relations between of the dislocation theory and the oriented continuum are presented. Section 3
deals with the thermodynamics of dislocation field movement. Making some assumptions on the properties of a discontinuity surface, the driving force on a grain boundary is found as a thermodynamic force needed to balance the energy on the moving grain boundary. The thermodynamical considerations complete the discussion on the constitutive modelling of the grain boundary migration.

2 An oriented continuum

Usually, for elastic-plastic deformation of crystalline solids the following decomposition of the deformation gradient is assumed

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$$  \hspace{1cm} (1)

where $\mathbf{F}_e$ denotes the elastic deformation tensor, while $\mathbf{F}_p$ is the corotational measure of the plastic deformation — corotational with the crystal lattice rotation. If the elastic displacements of dislocations are negligibly small then it is easy to show that the lattice rotation is described by the orthogonal tensor $\mathbf{R}_e$ obtained in the polar decomposition of $\mathbf{F}_e^*$. In such a case the elastic stretch of the crystal lattice is described by the symmetric tensor $\mathbf{U}_e$. So, from the viewpoint of the oriented continuum, cf. Dlużewski [5,6], we can distinguish the microstructure rotation by using the following multiplicative decomposition

$$\mathbf{F} = \mathbf{Q} \mathbf{F}_e \mathbf{F}_p$$  \hspace{1cm} (2)

where $\mathbf{Q} \equiv \mathbf{R}_e$ and $\mathbf{U}_e \equiv \mathbf{F}_e$.

In this paper our consideration has been limited to the linear theory. In such a case the above decomposition can be replaced by the additive decomposition of the displacement gradient

$$\nabla \mathbf{u} = \mathbf{w} + \mathbf{\epsilon}_e + \mathbf{\epsilon}_p$$  \hspace{1cm} (3)

where $\mathbf{w}$ denotes the asymmetric tensor of crystal lattice rotation, $\mathbf{\epsilon}_e$ is the elastic strain tensor, while $\mathbf{\epsilon}_p$ is the generally nonsymmetric tensor of plastic strain (distortion). Considering the conservative movement of dislocations this tensor can be determined as a sum of simple shear deformations $\gamma_i$ induced in $n$ slip systems, i.e.

$$\mathbf{\epsilon}_p = \sum_{i=1}^{n} \gamma_i \mathbf{s}_i \otimes \mathbf{m}_i$$  \hspace{1cm} (4)

where $\mathbf{s}_i$ and $\mathbf{m}_i$ denote the respective unit vectors.

Let us consider the compatibility condition for displacements

$$\text{curl} ( \nabla \mathbf{u} ) = 0$$  \hspace{1cm} (5)
Substituting (3) we find the following conditions for the curvature tensors
\[ -\mathbf{\alpha} + \mathbf{\alpha}_e + \mathbf{\alpha}_p = 0 \] (6)
where
\[ \mathbf{\alpha} \triangleq \text{curl } \mathbf{w} \] (7)
\[ \mathbf{\alpha}_e \triangleq \text{curl } \mathbf{\varepsilon}_e \] (8)
\[ \mathbf{\alpha}_p \triangleq \text{curl } \mathbf{\varepsilon}_p \] (9)

It is worth recalling that a second group of the curvature measures exists: \( \kappa, \kappa_e, \kappa_p \), cf. Dłużewski [5,6]. The kappa tensors relate to the respective alpha tensors by the linear, mutually reversible relations, see Nye [7],
\[ \mathbf{\alpha}_{...} = -\kappa^T_{...} + 1 \text{ tr } \kappa^T_{...} \] (10)
\[ \kappa_{...} = -\mathbf{\alpha}^T_{...} + \frac{1}{2} \text{ tr } \mathbf{\alpha}^T_{...} \] (11)
The subscript \( ... \) can be replaced e.g. by \( p, e \) or by a space, respectively. On the other hand, it can be shown that the plastic curvature tensor \( \mathbf{\alpha}_p \) is nothing more as the well known dislocation density tensor. According to the definition of the Burgers vector the vector can be determined by means of the following integral over the Burgers circuit \( c \) around the dislocations piercing the surface region \( s \),
\[ \mathbf{b}_d = \oint_c \mathbf{\varepsilon}_p d\mathbf{r} \] (12)
Using the Stokes theorem it can be rewritten in the form
\[ \mathbf{b}_d = \int_s \text{curl } \mathbf{\varepsilon}_p ds \] (13)
So, from the mathematical point of view, we can define the following vectors
\[ \mathbf{b} \triangleq \int_s \mathbf{\alpha} ds \] (14)
\[ \mathbf{b}_e \triangleq \int_s \mathbf{\alpha}_e ds \]
\[ \mathbf{b}_p \triangleq \int_s \mathbf{\alpha}_p ds \]
where \( \mathbf{b}_p \equiv \mathbf{b}_d \). By analogy to the Burgers vector, we can call the above vectors the total, elastic and plastic Burgers vectors, respectively. Due to (6) we find
\[ \mathbf{b} = \mathbf{b}_e + \mathbf{b}_p \] (15)
The relation between the dislocation density and curvature tensors has been noted first by Nye [7]. It is worth emphasizing that J.F.Nye did not precise which of the curvature tensors relates to the dislocation density tensor. On the basis of the present considerations we can state precisely that the dislocation density tensor \( \mathbf{\alpha}_d \) relates to the plastic curvature tensor \( \kappa_p \).
Crystal misorientation on grain boundary  

From the viewpoint of the oriented continuum a grain boundary can be defined as a surface which separates two differently oriented regions of the continuum. To each point of the discontinuity surface the misorientation vector $\Delta \varphi$ can be assigned. In such a case for the discontinuity surface the curvature tensor $\kappa$ is obtained as

$$\kappa = \delta(x^3 - x^3_{gb}) \sqrt{g_{33}} \Delta \varphi \otimes n_{gb}$$  \hspace{1cm} (16)

where $\delta(\cdot)$ is the Dirac function, $x^3$ is any curvilinear coordinate perpendicular to the surface, $x^3_{gb}$ is its value at the intersection point of the surface and $g_{33}$ is the respective component of the metric tensor, $\otimes$ denotes the diadic product, while $n_{gb}$ is the unit normal to the grain boundary. Using the Nye relation, (10), we can determine the respective alpha tensor

$$\alpha = \delta(x^3 - x^3_{gb}) \sqrt{g_{33}} (-n_{gb} \otimes \Delta \varphi + (n_{gb} \cdot \Delta \varphi) 1)$$  \hspace{1cm} (17)

On the other hand, using the integral form of (9) the following misorientation vectors can be determined

$$\Delta \varphi = +n_{gb} \cdot [w] \times n_{gb} - \frac{1}{2} \text{tr} ([w] \times n_{gb}) n_{gb}$$  \hspace{1cm} (18)

$$\Delta_e \varphi = -n_{gb} \cdot [\varepsilon_e] \times n_{gb} + \frac{1}{2} \text{tr} ([\varepsilon_e] \times n_{gb}) n_{gb}$$  \hspace{1cm} (19)

$$\Delta_p \varphi = -n_{gb} \cdot [\varepsilon_p] \times n_{gb} + \frac{1}{2} \text{tr} ([\varepsilon_p] \times n_{gb}) n_{gb}$$  \hspace{1cm} (20)

where $\times$ and $[\cdot]$ denote the vector product and the jump in the respective quantity across the grain boundary, e.g. $[\varepsilon_p] = \varepsilon_p^+ - \varepsilon_p^-$. The above equations show that in the case of the elastic-plastic deformation of dislocated crystals we can determine the elastic and plastic misorientation vectors, respectively. They compose together the vector of total misorientation. In such a case the representation of the dislocation density tensor in the orthonormal basis $\{n_1, n_2, n_3\}$ takes the form, cf. (11),

$$[\alpha_{gb}] = \rho_{gb} \begin{bmatrix} -b_3 & 0 & 0 \\ 0 & -b_3 & 0 \\ b_1 & b_2 & 0 \end{bmatrix}$$  \hspace{1cm} (19)

where

$$n_3 = n_{gb}$$  \hspace{1cm} (20)

$$b_i = -a (\Delta_p \varphi \cdot n_i)$$  \hspace{1cm} (21)

$$\rho_{gb} = \frac{\delta(x^3 - x^3_{gb}) \sqrt{g_{33}}}{a}$$  \hspace{1cm} (22)

$a$ takes the role of a scale parameter, e.g. the fundamental dimension of the crystal cell. It means that the tensor of grain boundary dislocations corresponds to a superposition of two families of dislocations lying on the surface.
3 Thermodynamics and balance laws

For dislocated crystals the conservation laws for the mass, momentum, moment of momentum, energy as well as the entropy production inequality can be assumed in the following form, respectively,

\[ \frac{d}{dt} \int_{V} \rho d\mathbf{v} = 0 \]  
\[ \frac{d}{dt} \int_{V} \rho \mathbf{v} d\mathbf{v} = \int_{S} \mathbf{\sigma} dS + \int_{V} \rho j d\mathbf{v} \]  
\[ \frac{d}{dt} \int_{V} \mathbf{x} \times \rho \mathbf{v} d\mathbf{v} = \int_{S} \mathbf{x} \times \mathbf{\sigma} dS + \int_{V} \mathbf{x} \times \rho j d\mathbf{v} \]  
\[ \frac{d}{dt} \int_{V} (\rho \mathbf{u} + \frac{1}{2} \rho \mathbf{v} \mathbf{v}) d\mathbf{v} = \int_{S} (\mathbf{v} \mathbf{\sigma} - \mathbf{q} \mathbf{T} - \mathbf{q}) dS + \int_{V} (\rho j \mathbf{v} + \rho h) d\mathbf{v} \]  
\[ \frac{d}{dt} \int_{V} \rho \mathbf{\eta} d\mathbf{v} \geq - \int_{S} \frac{\mathbf{q} \mathbf{r}}{T} dS + \int_{V} \frac{\rho h}{T} d\mathbf{v} \]

where \( \rho, \mathbf{\sigma}, \mathbf{j}, \mathbf{v}, \mathbf{u}, \mathbf{q}, \mathbf{T}, \mathbf{h}, \mathbf{\eta} \) denote the mass density, Cauchy stress tensor, body force density, velocity, internal energy density, heat flux, heat source density, entropy density, respectively; while \( \mathbf{q} \) denotes the vector of the energy flux due to the dependency of free energy on dislocation density tensor. It is worth emphasizing that no dependency of free energy on the elastic curvature will be assumed below. It gives the possibility to avoid the couple stress in balance equations. Under the above assumptions the integral equations lead to the following field equations

\[ \dot{\mathbf{\rho}} + \rho \text{ div } \mathbf{v} = 0 \]  
\[ \text{div} \mathbf{\sigma} + \rho \mathbf{j} - \rho \dot{\mathbf{v}} = 0 \]  
\[ \mathbf{\sigma} - \mathbf{\sigma}^T = 0 \]  
\[ - \rho \ddot{\mathbf{u}} + \mathbf{\sigma} : \dot{\mathbf{v}} - \text{div} \mathbf{q} - \text{div} \mathbf{q} \mathbf{T} + \rho h = 0 \]  
\[ \rho \dot{\mathbf{\eta}} + \text{div} \left( \frac{\mathbf{q} \mathbf{r}}{T} \right) - \frac{\rho h}{T} \geq 0 \]

Using the Helmholtz free energy function the inequality can be rewritten in the form

\[ - \rho \dot{\psi} - \rho \eta \dot{T} + \mathbf{\sigma} : \dot{\mathbf{\epsilon}} + \mathbf{\sigma} : \dot{\mathbf{\epsilon}}_p - \text{div} \mathbf{q} - \frac{\mathbf{q} \mathbf{r}}{T} \nabla T \geq 0 \]

where \( \psi = u - \eta T \).

Let us assume that the free energy density depends on the elastic strain, plastic curvature (dislocations), and on temperature,

\[ \psi = \psi(\mathbf{\epsilon}_e, \mathbf{\alpha}_p, T) \]
Substituting the above function into (31) and using (9) we find

\[(\sigma - \sigma_p) : \dot{\varepsilon}_p - \frac{q^T}{T} \nabla T \geq 0\]  

(33)

where by assumption

\[\sigma = \rho \frac{\partial \psi}{\partial \varepsilon_e}\]  

(34)

\[\sigma_p = - \text{curl} \left( \rho \frac{\partial \psi}{\partial \alpha_p} \right)\]  

(35)

\[q = - (\rho \frac{\partial \psi}{\partial \alpha_p}) \times \dot{\varepsilon}_p\]  

(36)

\[\eta = - \frac{\partial \psi}{\partial T}\]  

(37)

\[\times\] denotes the double product over two sequential indices: the scalar one over the first indices and the vector one over the second indices \[\left( \frac{\partial \psi}{\partial \alpha_{pij}} \varepsilon^i_p e^j_{kl} \right)\].

### 3.1 Driving force on dislocation field

Considering the plastic deformation as a result of dislocation motion the material derivative of the plastic strain is governed by the well known relation

\[\dot{\varepsilon}_p = \alpha_p \times v_p\]  

(38)

where \(v_p\) denotes the dislocation velocity, cf. Mura [9], Kröner [10,11,12]. Using (38) the inequality (33) and equation (36) can be rewritten in the form

\[(f - f_p)v_p + \frac{q^T}{T} \nabla T \geq 0\]  

(39)

\[q = k_p v_p\]  

(40)

where

\[f = \sigma \times \alpha_p\]  

(41)

\[f_p = \sigma_p \times \alpha_p\]  

(42)

\[k_p = \frac{\partial \psi}{\partial \alpha_p} : \alpha_p\]  

(43)

\(f\) denotes the elastic force acting on dislocation field. Equation (41) is nothing else than a continuum counterpart of the well-known Peach-Koehler formula, [8]. \(f_p\) denotes the configurational force on dislocation field — the force is responsible for the formation of low energy dislocation structures.

To satisfy the inequality of the entropy production a general constitutive equation governing the dislocation field movement can be stated in the following form

\[v_p = v_p(f - f_p, \alpha_p, T)\]  

(44)
3.2 Thermodynamic forces on grain boundary

In a general case the description of the grain boundary migration needs the use of a very complex thermodynamic system with many internal freedom degrees, e.g. to determine the surface tension or the movement of impurities along the boundaries the surface densities of the free energy, mass, impurity atoms, etc. should be considered. This leads to enlarged thermodynamic balance equations, see e.g. Kosiński [13]. With respect to the limited space of this paper we consider a simplified system under the following assumptions:

1. The displacement field is continuous with piecewise continuous first and second derivatives. Due to the kinematical constraints the total velocity of the grain boundary must reach the same value on the opposite sides of the boundary, i.e.

\[ (v_{gb}^+ + v^-) n_{gb} = (v_{gb}^- + v^-) n_{gb} \]  \hspace{1cm} (45)

where \( v_{gb} \) is perpendicular to the grain boundary surface, i.e. \( v_{gb}^\perp = v_{gb} \cdot n_{gb} \). The condition (45) means that the jump in the local velocity of the grain boundary must be equal to the continuum velocity jump, i.e.

\[ [v_{gb}] n_{gb} = -[v] n_{gb} \]  \hspace{1cm} (46)

2. The change of the surface mass is negligibly small. In such a case the mass flux through the grain boundary can be defined as

\[ \pi_{gb} = \rho^+ v_{gb}^+ \cdot n_{gb} = \rho^- v_{gb}^- \cdot n_{gb} \]  \hspace{1cm} (47)

This leads to the following dependence on jump in velocity of material

\[ [v] = -\left[ \frac{1}{\rho} \right] n_{gb} \pi_{gb} \]  \hspace{1cm} (48)

3. The temperature is continuous at the grain boundary, i.e.

\[ [T] = 0 \]  \hspace{1cm} (49)

4. The internal energy and entropy of the surface are taken into account. The corresponding flux vectors on the surface are neglected.

From the viewpoint of thermodynamics the above assumptions lead to the following equations for jumps

\[ [\rho u v_{gb} + \frac{1}{2} \rho (v \cdot v) v_{gb} + v \sigma - q_T - k_p (v_p - v_{gb})] n_{gb} = \rho_{gb} \dot{u}_{gb} \]  \hspace{1cm} (50)

\[ [-\rho \eta v_{gb} + \frac{q_{gb}}{T}] n_{gb} + \rho_{gb} \dot{h}_{gb} \geq 0 \]  \hspace{1cm} (51)
where $\rho_{\text{gb}}$ is the surface density of the mass while $\dot{\psi}_{\text{gb}}, \eta_{\text{gb}}$ denote the time derivatives of the respective densities. By making the use of (46) and (49) the inequality (51) can be rewritten in the form

$$\pi_{\text{gb}}[\psi] + n_{\text{gb}}\sigma[v] - \left[k_p(v_p - v_{gb})\right]n_{\text{gb}} - \rho_{\text{gb}}\dot{\psi}_{\text{gb}} - \rho_{\text{gb}}\eta_{\text{gb}}\dot{T} \geq 0$$

where the stress at the boundary (without ceil brackets) is found as $\sigma = \frac{1}{2}(\sigma^+ + \sigma^-)$.

To determine the driving tractions on grain boundary let us assume the following constitutive equation for the surface density of free energy

$$\psi_{\text{gb}} = \psi_{\text{gb}}(\Delta_p \varphi, T)$$

Substituting (53) into (52) we find

$$\pi_{\text{gb}}[\psi] + n_{\text{gb}}\sigma[v] - \left[k_p(v_p - v_{gb})\right]n_{\text{gb}} - m_p \Delta_p \varphi \geq 0$$

where by assumption

$$m_p = \rho_{\text{gb}} \frac{\partial \psi_s}{\partial \Delta_p \varphi}$$
$$\eta_{\text{gb}} = - \frac{\partial \psi_{\text{gb}}}{\partial T}$$

Let us define the left and right dislocation flux to the grain boundary as

$$\pi_p^\pm = (v_p^\pm - v_{gb}^\pm) \cdot (\mp n_{\text{gb}})$$

Using (18c) and (38) it can be shown that the inequality (54) can be rewritten as

$$t_{gb} \pi_{gb} + t_p^+ \pi_p^+ + t_p^- \pi_p^- \geq 0$$

where, cf. (43),

$$t_{gb} = \left[\psi\right] - n_{\text{gb}}\sigma n_{\text{gb}} \left[\frac{1}{\rho}\right]$$
$$t_p^\pm = k_p^\pm - m_p(\alpha_p^\pm T - \frac{1}{2} \text{tr} \alpha_p^\pm 1)n_{\text{gb}}$$

**Constitutive equations**

According to many experimental data the mobility of grain boundaries depends mainly on the driving forces, misorientation, concentration of impurity atoms and on temperature, [14,15]. Taking into account the driving force, misorientation and temperature the constitutive equations for grain boundary migration and for dislocation flux can be stated in the following form

$$\pi_{gb} = \pi_{gb}(t_{gb}, \Delta_p \varphi, T)$$
$$\pi_p^\pm = \pi_p^\pm(t_p^\pm, \Delta_p \varphi, T)$$
4 Final remarks

It is worth emphasizing that in the most models of polycrystals it is assumed that the reorientation of grains depends only on the jump in the plastic deformation, while here it has been shown, cf. (18), that the reorientation depends strongly on the orientation of the grain boundary. Moreover, if the plastic misorientation vector and the jump in plastic deformation are given then the grain boundary can take only a certain orientation, cf. (18c). Usually, in the mathematical models of polycrystals this restriction is ignored.

Due to the crystal lattice symmetry, we find many misorientation vectors for a real grain boundary. Even for a discontinuity surface in the continuum composed of the unsymmetric unit, two rotations $\Delta \varphi$ and $\Delta \varphi' = (2\pi - \Delta \varphi)$ can be traced in the orientation space. Obviously, for real crystal structures we can determine a considerably larger number of misorientation vectors, e.g. in f.c.c. bicrystals we find as many as 48 possible misorientation vectors for a single grain boundary, cf. Dłużewski [16]. The change of the misorientation vector can correspond to the reorganization of the grain boundary internal structure.

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