Thermodynamics of orientation discontinuity surface: small misorientation approach

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THE THERMODYNAMICS of a crystal lattice reorientation process proceeding on low angle grain boundary is presented. In material science, the influence of lattice misorientation on the grain boundary energy is well established. On the other hand, in thermodynamics of discontinuity surface the influence of misorientation vector on the surface energy is usually ignored as yet. Therefore, in the present paper, attention is focused on this influence. To obtain the driving forces conjugate to relative grain reorientation, the continuum theory of dislocations has been applied. Starting from the energy balance law and assuming that the free energy of discontinuity surface depends strongly on the jump in crystal orientation field, the mathematical relations for the misorientation vector and the conjugated thermodynamic force are derived. The mentioned force contributes to the total driving force governing the grain boundary migration process. The problem of constitutive modelling of the surface motion is considered. The main result of this analysis is the incorporation of grain orientation jump into the thermodynamic description of driving forces of the grain reorientation process.

Key Words: Continuum theory of dislocations, misorientation, discontinuity of crystal surface.

1. Introduction

GRAIN REORIENTATION process plays an important role in mechanical behaviour of metals. Unfortunately, there are many factors, which may influence reorientation. To obtain a complete thermodynamic description of the reorientation process, the mechanical properties and geometry of individual grains (orientation, existing defects etc.) and boundary (its structure, defects existing on the boundary, possibility to move and glide, jump in respective thermodynamics parameters), interaction between defects in grains with the boundary should be incorporated. To avoid an extremely complex description in mathematical models of the polycrystal deformation, it is often assumed that the reorientation of grains depends only on the jump in the plastic deformation tensor. The influence of misorientation vector on the grain reorientation phenomenon is usually ignored, see Fig. 1.
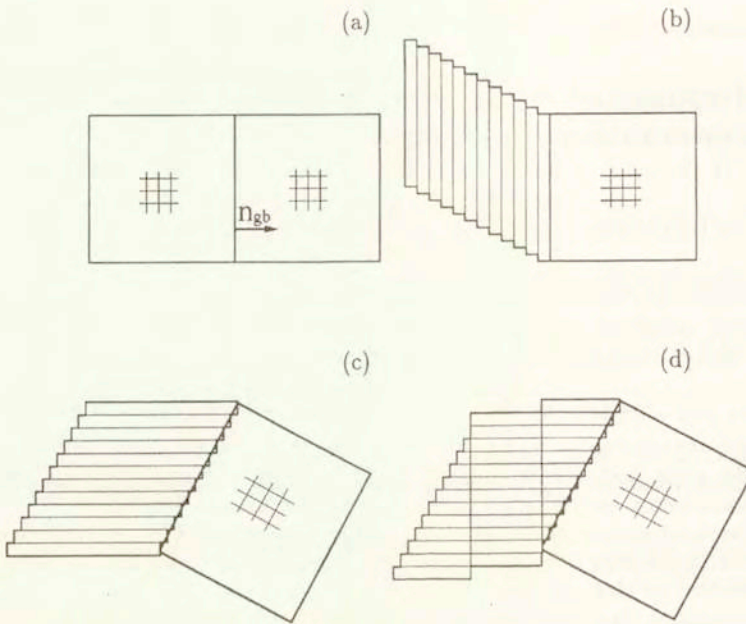
FIG. 1. Influence of slip orientation on grain reorientation: a) initial state; b) – d) state of deformed crystal.

The thermodynamic description of grain boundary motion considered in terms of the discontinuity surface has been considered in many papers [1, 3, 8, 13, 15]. However, in most of the papers a major premise is that driving traction originates from the balance of energy stored outside the boundary, cf. [1, 8, 13]. Additionally, the comparison of different thermodynamic approaches is difficult due to a variety of the used measures of crystal lattice defects, coordinate systems, tangent vector basis in which the position of measures are described, postulated deformation types (only elastic, elastoplastic etc.), cf. [2, 5, 6, 9, 18, 21, 24]. This is beyond our abilities to present most of them. In author's opinion, many of above approaches are not suitable for the considered type of discontinuity surface. For instance, the disclination theory can be a useful framework description of some of epitaxial layer interfaces [27] or defects in liquid crystals [16], while micropolar continuum description are much more complicated than the present framework. Therefore, we limit our references to the papers most representative for the approach developed here. Configurational forces play an important role in our analysis. Those forces are pivotal for the direction of the process evolution. For this reason, we distinguish the driving forces of the reorientation process originated from different grounds. Similar analysis based on a quite different axiomatic basis was presented by Cermelli and Sellers [2, 3]. They described the Bravais crystal with existence of the defects of lattice in the

form of dislocations, vacancies, interstitials and, contrary to our analysis, they did not use elastic-plastic decomposition. Additionally they discussed the widely used Born rule, see also [30]. Many other approaches have been formulated, e.g. [10, 11, 31], or more recently [15]. A common practice in the field of continuum mechanics is incorporation of internal variables to describe meso- or micro- proceses, which influence the macroscopic behaviour of the material. For the case of dislocation influence, the dislocation vector, dislocation tensor or lattice directors are incorporated into the constitutive equation, cf. [2, 12].

On the other hand, in the material science, the effect of lattice misorientation on the energy of low angle grain boundaries is well established, cf. [14, 28]. Moreover, the surface density of the free energy has been catalogued with respect to lattice misorientation vectors for given crystal lattices.

In this paper starting from the energy balance law and assuming that the free energy of discontinuity surface depends on the jump in orientation field, the relations for the misorientation vector and conjugate thermodynamical force are derived. This force contributes to the total driving force of the grain boundary migration process. The problem of constitutive modelling of the surface movement is considered. Due to the assumption of dislocation model of the grain boundary, the current analysis concerns only the low angle grain boundary. State of the dislocated crystal lattice near the boundary depends strongly on the exerted strain, cf. [28]. Thus in the first step, we have limited consideration to small deformation approach.

In the present analysis, incorporation of dislocation density tensor enables the description of the existence of dislocation in the bulk and on the grain boundary. The classical balance laws with symmetric stress tensor are used and no additional balance laws for couple stress are needed. To describe the orientation jump on the surface, the jump in the elastic and plastic deformation tensors are considered.

In the following section the kinematics of small deformation with continuous distribution of dislocations is presented. The notion of curvature tensor is introduced and its connection with the dislocation density tensor, which is a defect measure of the body, is considered. Particular attention is focused on the curvature measure of the dislocated continuum. The relation between the elastic, plastic and total curvature measure are also investigated. Section 3 concerns the compatibility conditions for deformation field on the grain boundary. The relations of the dislocation density to the grains misorientation are formulated. The importance of analysis in Sec. 4 consists in describing thermodynamics of the continuum theory of dislocations applied to the grain boundary reorientation process. Balance laws and the forms of driving forces are described explicitly. Proposition of a general form of the constitutive equation for grain boundary migration is proposed in Subsec. 4.3. Finally, in Sec. 5, summary of the analysis is presented.

2. Crystal lattice versus kinematics of the oriented continuum

In the case of small deformations, we assume an additive decomposition of the displacement gradient

$$(2.1) \qquad \nabla \mathbf{u} = \mathbf{w} + \varepsilon_e + \varepsilon_p,$$

where $\mathbf{w}$, ε_e and ε_p denote the antisymmetric tensor of lattice rotation, symmetric tensor of elastic deformation, and generally unsymmetrical tensor of plastic deformation, respectively. Let us consider the conservative movement of dislocations (slips). Then, the plastic deformation tensor can be expressed as

$$\varepsilon_p = \sum_{i=1}^{n} \gamma_i \, \mathbf{s}_i \otimes \mathbf{m}_i,$$

where $\gamma_i, \mathbf{s}_i, \mathbf{m}_i$ denote the plastic slip value on the i-th slip system, vector parallel to the i-th slip system and vector perpendicular to the i-th slip system, respectively. The displacement integrability condition takes the following form:

$$(2.2) \qquad \mathrm{curl}(\nabla \mathbf{u}) = \mathbf{0}.$$

Substituting (2.1), we obtain

$$(2.3) \qquad -\alpha + \alpha_e + \alpha_p = 0,$$

where

$$(2.4) \qquad \alpha \overset{df}{=} -\mathrm{curl}\mathbf{w},$$

$$(2.5) \qquad \alpha_e \overset{df}{=} \mathrm{curl}\varepsilon_e,$$

$$(2.6) \qquad \alpha_p \overset{df}{=} \mathrm{curl}\varepsilon_p.$$

In the above equations α, α_e, α_p denote measures of the continuum curvature, which originates from the total, elastic and plastic deformations, respectively. The close relation between elastic and plastic curvature in (2.3) is explained by the general deformation rule, i.e. elastic and plastic strains separately do not satisfy the compatibility relation (2.2), cf. [19]. There exists another group of curvature measures κ, κ_e, κ_p. Tensors kappa are related with tensors alpha by the linear, mutually reversible relationships, noted by NYE, cf. [25],

$$(2.7) \qquad \begin{aligned} \alpha_{...} &= -\kappa_{...}^{T} + \mathbf{1}\,\mathrm{tr}\,\kappa_{...}^{T}, \\ \kappa_{...} &= -\alpha_{...}^{T} + \frac{1}{2}\,\mathrm{tr}\,\alpha_{...}^{T}. \end{aligned}$$

This relation is a consequence of geometrical nature of current consideration. The choice of measure depends on convenience in its application to particular cases. Burgers vector can be determined as an integral over a Burgers circuit c around a given dislocation

$$\mathbf{b_d} = \oint_c \varepsilon_p d\mathbf{r}.$$

Using the Stokes theorem, we obtain

$$\mathbf{b_d} = \int_s \text{curl} \varepsilon_p d\mathbf{s}.$$

This means that from the mathematical point of view, we can define using Eqs. (2.1), (2.4), (2.5), (2.6), the following vectors:

$$\mathbf{b} \overset{df}{=} \int_s \alpha d\mathbf{s},$$

$$\mathbf{b_e} \overset{df}{=} \int_s \alpha_e d\mathbf{s},$$

$$\mathbf{b_p} \overset{df}{=} \int_s \alpha_p d\mathbf{s},$$

where $\mathbf{b_p} = \mathbf{b_d}$. By analogy to the classical Burgers vector, the above vectors can be called the total, elastic and plastic Burgers vectors. From Eq. (2.3) we find

$$\mathbf{b} = \mathbf{b_e} + \mathbf{b_p}.$$

Relationship between the dislocation density tensor and the curvature tensors were first introduced by NYE, cf. [25]. However, he didn't specify which of curvature tensor corresponded to the dislocation density tensor. According to the above consideration it is easy to note that the dislocation density tensor corresponds to a measure of plastic curvature similar to κ_p, cf. [7, 8].

In the case when in the continuum there exists a discontinuity surface of displacement gradient, on the basis of (2.4) we can assume the following relation for the total measure of continuum curvature

(2.8)
$$\int_v \alpha dv = \int_{v^+} \alpha dv + \int_{\partial v^\pm} \alpha_s ds - \int_{v^-} \alpha dv,$$

where $\int_{\partial v^\pm} \alpha_s ds$ denotes the measure of continuum curvature due to existence of the discontinuity surface. The last equation may be expressed as

(2.9)
$$-\int_v \text{curl} \mathbf{w} dv = -\int_{v^+} \text{curl} \mathbf{w} dv + \int_{\partial v^\pm} \alpha_s ds + \int_{v^-} \text{curl} \mathbf{w} dv$$

and

$$-\int_{\partial v} \mathbf{w} \times d\mathbf{s} = -\int_{\partial v^+} \mathbf{w} \times d\mathbf{s} + \int_{\partial v^\pm} \alpha_s ds + \int_{\partial v^-} \mathbf{w} \times d\mathbf{s},$$

what leads to the following integral form:

$$\int_{\partial v^\pm} \alpha_s ds = -\int_{\partial v^\pm} \lceil \mathbf{w} \rceil \times d\mathbf{s}$$

and the local form, namely

(2.10) $$\alpha_s = -\lceil \mathbf{w} \rceil \times \mathbf{n}.$$

Here $\lceil \cdot \rceil$ and $\mathbf{n}$ denote the jump in the respective quantity across the grain boundary, e.g. $\lceil \varepsilon_p \rceil = \varepsilon_p^+ - \varepsilon_p^-$, and the unit normal to the surface. Relation (2.10) defines a curvature measure on the discontinuity surface of the displacement gradient. Now, we can define the curvature measure on the grain boundary corresponding to the jump in: the displacement gradient, the elastic deformation tensor and the plastic deformation tensor, namely

(2.11) $$\alpha_{\mathrm{gb}} \stackrel{df}{=} -\lceil \mathbf{w} \rceil \times \mathbf{n}_{\mathrm{gb}},$$

(2.12) $$\alpha_{\mathrm{gbe}} \stackrel{df}{=} \lceil \varepsilon_e \rceil \times \mathbf{n}_{\mathrm{gb}},$$

(2.13) $$\alpha_{\mathrm{gbp}} \stackrel{df}{=} \lceil \varepsilon_p \rceil \times \mathbf{n}_{\mathrm{gb}},$$

and

(2.14) $$\kappa_{\mathrm{gb}} \stackrel{df}{=} -\alpha_{\mathrm{gb}}^T + \frac{1}{2}\mathrm{tr}, \quad \alpha_{\mathrm{gb}}^T = \lceil \varphi \rceil \otimes \mathbf{n}_{\mathrm{gb}},$$

(2.15) $$\kappa_{\mathrm{gbe}} \stackrel{df}{=} -\alpha_{\mathrm{gbe}}^T + \frac{1}{2}\mathrm{tr}\, \alpha_{\mathrm{gbe}}^T,$$

(2.16) $$\kappa_{\mathrm{gbp}} \stackrel{df}{=} -\alpha_{\mathrm{gbp}}^T + \frac{1}{2}\mathrm{tr}\, \alpha_{\mathrm{gbp}}^T,$$

where $\varphi = -\mathbf{w} : \mathbf{e}$. The quantities φ, $\mathbf{e}$, $\mathbf{n}_{\mathrm{gb}}$ denote the vector of lattice orientation, alternating symbol and the unit vector normal to the grain boundary, respectively. It is worth emphasizing that equation (2.14) connects continuous curvature of the grain boundary with jump in the lattice orientation, cf. critical notes in [30]. Equations (2.11) to (2.16) visualize the correspondence between the classical measures of structure discontinuity and oriented continuum curvature measures. By analogy to the additive curvature decomposition (2.3), let us define the jump in the orientation caused by elastic and plastic deformation, respectively.

$$\lceil \varphi_e \rceil \stackrel{df}{=} \kappa_{\mathrm{gbe}} \cdot \mathbf{n}_{\mathrm{gb}},$$

$$\lceil \varphi_p \rceil \stackrel{df}{=} \kappa_{\mathrm{gbp}} \cdot \mathbf{n}_{\mathrm{gb}}.$$

From the above definitions, we get additional curvature measure relations on the grain boundary, namely

$$\alpha_{...}(x) = -\alpha_{...}^-(x)\frac{H(x^3_{gb} - x^3)}{\sqrt{g^{33}}} + \alpha_{gb\,...}\frac{\delta(x^3_{\,gb})}{\sqrt{g^{33}}} + \alpha_{...}^+(x)\frac{H(x^3 - x^3_{gb})}{\sqrt{g^{33}}},$$

$$\kappa_{...}(x) = -\kappa_{...}^-(x)\frac{H(x^3_{gb} - x^3)}{\sqrt{g^{33}}} + \kappa_{gb\,...}\frac{\delta(x^3_{\,gb})}{\sqrt{g^{33}}} + \kappa_{...}^+(x)\frac{H(x^3 - x^3_{gb})}{\sqrt{g^{33}}},$$

where by $H(\cdot)$, x^3, x^3_{gb}, $\sqrt{g^{33}}$, $\delta(\cdot)$ we denote the Heaviside function, any curvilinear coordinate perpendicular to the surface, its value at the intersection point on the surface, the respective component of the metric tensor and the Dirac function, respectively.

3. Misorientation vector on the grain boundary

From the point of view of the oriented continuum mechanics, a grain boundary can be considered as a surface of jump in the orientation field. Non-zero misorientation vector $\Delta\varphi$ ($\Delta\varphi = \lceil\varphi\rceil/\sqrt{g_{33}}$ for $x^3 = x^3_{gb}$) can be attributed to all points on this surface. In such a case, the curvature tensor on grain boundary κ (Eq. (2.14)) can be restated in the form

$$\kappa = \delta(x^3 - x^3_{gb})\sqrt{g_{33}}\,\Delta\varphi \otimes \mathbf{n}_{gb},$$

and, by the NYE relation (2.7), the tensor alpha is determined

$$\alpha = \delta(x^3 - x^3_{gb})\sqrt{g_{33}}\left(-\mathbf{n}_{gb} \otimes \Delta\varphi + (\mathbf{n}_{gb} \cdot \Delta\varphi)\mathbf{1}\right).$$

By making use of (2.3), we define the following misorientation vectors:

(3.1)
$$\Delta\varphi = \left(+\lceil\mathbf{w}\rceil \times \mathbf{n}_{gb} - \frac{1}{2}\mathrm{tr}(\lceil\mathbf{w}\rceil \times \mathbf{n}_{gb})\right)\mathbf{n}_{gb},$$

$$\Delta_e\varphi = \left(-\lceil\varepsilon_e\rceil \times \mathbf{n}_{gb} + \frac{1}{2}\mathrm{tr}(\lceil\varepsilon_e\rceil \times \mathbf{n}_{gb})\right)\mathbf{n}_{gb},$$

$$\Delta_p\varphi = \left(-\lceil\varepsilon_p\rceil \times \mathbf{n}_{gb} + \frac{1}{2}\mathrm{tr}(\lceil\varepsilon_p\rceil \times \mathbf{n}_{gb})\right)\mathbf{n}_{gb}.$$

The above relation shows that in the case of elastic-plastic crystal deformation, we can define elastic and plastic vectors of lattice misorientation. This implies that

representation of the dislocation density tensor in orthogonal base $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}$ takes the form

$$[\alpha_{\text{gb}}] = \rho_{\text{gb}} \begin{bmatrix} -b_3 & 0 & 0 \\ 0 & -b_3 & 0 \\ b_1 & b_2 & 0 \end{bmatrix},$$

where

$$\mathbf{n}_3 = \mathbf{n}_{\text{gb}},$$
$$b_i = -a\,(\Delta_{\text{p}}\varphi \cdot \mathbf{n}_i),$$
$$\rho_{\text{gb}} = \frac{\delta(x^3 - x_{\text{gb}}^3)\sqrt{g_{33}}}{a}.$$

Parameter a plays the role of the length scale, e.g. it corresponds to the length of crystal cell. It is easy to notice that the grain boundary dislocation tensor corresponds to a superposition of two families of dislocation lines lying on the considered surface. As an alternative, dislocation density vector can be included, cf. [12].

4. Thermodynamics

In order to obtain the form of driving forces of the process, we should complete the thermodynamical description. In Subsec. 4.1 we derive the constitutive relations for the body without discontinuity surface and next, in Subsec. 4.2, the discontinuity surface in continuum is described. From the viewpoint of balance equations, our approach differs from the classical elastic-plastic continuum thermodynamics only by the dislocation energy flux term included in the energy balance.

4.1. Continuum theory of dislocations

For a dislocated crystal, we postulate the balance equations in the form

$$\frac{d}{dt}\int_v \rho\,dv = 0,$$

$$\frac{d}{dt}\int_v \rho\mathbf{v}\,dv = \int_s \boldsymbol{\sigma}\,ds + \int_v \rho\mathbf{j}\,dv,$$

$$\frac{d}{dt}\int_v \mathbf{x}\times\rho\mathbf{v}\,dv = \int_s \mathbf{x}\times\boldsymbol{\sigma}\,ds + \int_v \mathbf{x}\times\rho\mathbf{j}\,dv,$$

$$\frac{d}{dt} \int\limits_{v} \left(\rho u + \frac{1}{2} \rho \mathbf{v} \mathbf{v} \right) dv = \int\limits_{s} (\mathbf{v} \boldsymbol{\sigma} - \mathbf{q}_T - \mathbf{q}) ds + \int\limits_{v} (\rho \mathbf{j} \mathbf{v} + \rho h) dv,$$

$$\frac{d}{dt} \int\limits_{v} \rho \eta \, dv \geq - \int\limits_{s} \frac{\mathbf{q}_T}{T} ds + \int\limits_{v} \frac{\rho h}{T} dv,$$

where ρ, $\boldsymbol{\sigma}$, $\mathbf{j}$, $\mathbf{v}$, u, $\mathbf{q}_T$, h, η denote the mass density, Cauchy stress tensor, body force density, velocity, internal energy density, heat flux and heat source density, respectively, while $\mathbf{q}$ denotes the vector of the energy flux due to the relation between free energy and the dislocation density tensor. The above integral relations imply the following local form of balance equations:

(4.1)
$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0,$$
$$\operatorname{div} \boldsymbol{\sigma} + \rho \mathbf{j} - \rho \dot{\mathbf{v}} = \mathbf{0},$$
$$\boldsymbol{\sigma} - \boldsymbol{\sigma}^T = \mathbf{0},$$
$$-\rho \dot{u} + \boldsymbol{\sigma} : \nabla \mathbf{v} - \operatorname{div} \mathbf{q} - \operatorname{div} \mathbf{q}_T + \rho h = 0,$$

(4.2)
$$\rho \dot{\eta} + \operatorname{div}\left(\frac{\mathbf{q}_T}{T}\right) - \frac{\rho h}{T} \geq 0.$$

Using the free energy function ($\psi = u - \eta T$), the last inequality can be expressed as

(4.3)
$$-\rho \dot{\psi} - \rho \eta \dot{T} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_e + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p - \operatorname{div} \mathbf{q} - \frac{\mathbf{q}_T}{T} \nabla T \geq 0.$$

To find the driving forces on the dislocation field, let us assume that the specific free energy of the dislocated crystal depends not only on the elastic strain and temperature, but also on the dislocation density tensor corresponding to the plastic curvature (induced by permanent rebuilding of the lattice by plastic deformation). Thus, let the free energy take the form

(4.4)
$$\psi = \psi(\boldsymbol{\varepsilon}_e, \boldsymbol{\alpha}_p, T).$$

The similar dependency were assumed by many other authors, e.g. [29]. Substituting this equation into (4.3) and making use of (2,6), we obtain

(4.5)
$$(\boldsymbol{\sigma} - \boldsymbol{\sigma}_p) : \dot{\boldsymbol{\varepsilon}}_p - \frac{\mathbf{q}_T}{T} \nabla T \geq \mathbf{0}.$$

To hold this inequality for all processes, the Cauchy stress tensor resulting from elastic strain, the stress resulting from existence of dislocations (tending to minimize the free energy due to dislocation distribution), and the energy flux as

an effect of dislocation distribution and finally, the entropy have to satisfy the following equations:

$$\sigma = \rho \frac{\partial \psi}{\partial \varepsilon_e},$$

(4.6)

$$\sigma_p = -\mathrm{curl}\left(\rho \frac{\partial \psi}{\partial \alpha_p}\right),$$

$$\mathbf{q} = -\left(\rho \frac{\partial \psi}{\partial \alpha_p}\right) \dot{\times} \dot{\varepsilon}_p,$$

$$\eta = -\frac{\partial \psi}{\partial T}.$$

In (4.6) symbol $\dot{\times}$ denotes the double product: the scalar one over the first indices and the vector one over the second indices, i.e. $\dfrac{\partial \psi}{\partial \alpha_{pij}} \dot{\varepsilon}_p^{ik} e^j{}_{kl}$. Fundamental equation describing the plastic flow in the continuum theory of dislocations takes the form

(4.7) $$\dot{\varepsilon}_p = \alpha_p \times \mathbf{v}_p,$$

where $\mathbf{v}_p$ denotes the dislocation velocity vector, cf. [19, 23].

4.2. Driving forces on the dislocation field

The driving force is a sum of Peach-Koehler forces and the configuration force. Peach-Koehler force describes the influence of stress field on dislocation, cf. [26] and more general [10], while configuration force describes the influence of spatial configuration of all dislocation on each dislocation. The configuration force is responsible for minimization of the stored energy due to dislocations configuration. The favorable dislocations configurations are often called the low energy dislocation structures [20]. This force gives direct information on the direction of the reorientation process. Using (4.7), relations (4.5) and (4.6) can be rewritten in the form

$$(\mathbf{f} - \mathbf{f}_p)\mathbf{v}_p + \frac{q_T}{T}\nabla T \geq 0,$$

$$\mathbf{q} = k_p \mathbf{v}_p,$$

where

(4.8)

$$\mathbf{f} = \sigma \dot{\times} \alpha_p,$$

$$\mathbf{f}_p = \sigma_p \dot{\times} \alpha_p,$$

$$k_p = \frac{\partial \psi}{\partial \alpha_p} : \alpha_p.$$

In the above equations $\mathbf{f}$ denotes the elastic force acting on the dislocation field – the Peach-Koehler force, while $\mathbf{f}_p$ denotes the configuration force. According to the obtained thermodynamic restrictions, the dislocation velocity constitutive equation (plastic flow equation) can be assumed in the following form:

$$(4.9) \qquad\qquad \mathbf{v}_p = \mathbf{v}_p(\mathbf{f} - \mathbf{f}_p, \alpha_p, T).$$

The configuration force $\mathbf{f}_p$ is responsible mainly for the self-reorganization of dislocation field towards formation of the grain boundaries. This force is parallel to the gradient of dislocation density field, but takes usually the opposite sign to the above gradient. Therefore, a continuous field of unbalanced (monomial) dislocation tends to concentrations in narrow regions, what in terms of the continuum theory of dislocations corresponds to the process of subgrain boundary formation. Similar role on discrete dislocations plays the Peach-Koehler force. The energy of local stress field around dislocations must be taken into account in the energy equation assumed on the continuum dislocation field level, see (4.4). The role of configuration force can be also considered in terms of the Baushinger force (by analogy to the Baushinger stress) induced e.g. by the pile-up of discrete dislocations on the existing grain boundaries.

4.3. Thermodynamics of the orientation discontinuity surface

Let us consider translational motion of the orientation discontinuity surface. Due to dislocation models of the grain boundary, we consider only a small angle discontinuity surface (e.g. up to $15°$ for germanium). For such a case we assume the following conditions:

1. The surface possesses densities of mass, energy and entropy, but the fluxes of the above quantities vanish on the surface.

2. The surface density of mass on the discontinuity surface is constant.

3. The displacement field is continuous with the piecewise continuous first and second-order derivatives, i.e. the grain boundary sliding is excluded.

4. The temperature field is continuous on the orientation discontinuity surface.

The attributes of such a surface allow to call it stationary discontinuity. Let us denote the discontinuity surface velocity by $\mathbf{w}_{gb}$. Then the local velocity vector of the surface motion (grain boundary velocity) is $\mathbf{v}_{gb} = \mathbf{w}_{gb} - \mathbf{v}$. Additionally, we assume convection parameterization of the surface. The velocity of a material point lying on the discontinuity surface at a given time denoted by $\mathbf{v}$ can be decomposed into normal and tangential parts

$$\mathbf{v} = v_n \mathbf{n}_{gb} + v^\alpha \mathbf{i}_\alpha,$$

where $\mathbf{i}_\alpha$ denotes the local base vectors tangent to the coordinates on the surface. This allows us to define the time derivative of arbitrarily chosen scalar density ω for points lying outside the surface and ω_{gb} for points inside the surface, see [17].

$$\dot{\omega} \equiv \frac{\partial \omega}{\partial t}|_{X=\text{const}} + \operatorname{grad} \omega \cdot \mathbf{v},$$

$$\overset{\circ}{\omega}_{gb} \equiv \frac{\partial \omega_{gb}}{\partial t}|_{i_\alpha=\text{const}} + \omega_{gb,\alpha}\mathbf{v}^\alpha.$$

Due to the mass balance and the assumed zero surface flux of mass, the mass flux across the discontinuity surface satisfies the condition

(4.10) $$\pi_{gb} = \rho^+\mathbf{v}_{gb}^+ \cdot \mathbf{n}_{gb} = \rho^-\mathbf{v}_{gb}^- \cdot \mathbf{n}_{gb}.$$

With respect to the kinematical constraints, total velocity of the surface must assume the same value on both sides of this surface, i.e.

$$(\mathbf{v}_{gb}^+ + \mathbf{v}^+)\mathbf{n}_{gb} = (\mathbf{v}_{gb}^- + \mathbf{v}^-)\mathbf{n}_{gb},$$

which implies the relation of jump in local velocity of the grain boundary to the jump in the continuum velocity, namely

(4.11) $$\lceil\mathbf{v}_{gb}\rceil\mathbf{n}_{gb} = -\lceil\mathbf{v}\rceil\mathbf{n}_{gb}.$$

Such restriction implies the following set of equations on the discontinuity surface, cf. (4.1) – (4.2),

(4.12)
$$\lceil\rho\mathbf{v}_{gb}\rceil\mathbf{n}_{gb} = 0,$$
$$\lceil\sigma + \rho\mathbf{v} \otimes \mathbf{v}_{gb}\rceil\mathbf{n}_{gb} = \mathbf{0},$$

(4.13) $$\lceil\rho u\mathbf{v}_{gb} + \frac{1}{2}\rho(\mathbf{v} \cdot \mathbf{v})\mathbf{v}_{gb} + \mathbf{v}\sigma - \mathbf{q}_T - k_p(\mathbf{v}_p - \mathbf{v}_{gb})\rceil\mathbf{n}_{gb} = \rho_{gb}\overset{\circ}{u}_{gb},$$

(4.14) $$\lceil-\rho\eta\mathbf{v}_{gb} + \frac{\mathbf{q}_T}{T}\rceil\mathbf{n}_{gb} + \rho_{gb}\overset{\circ}{\eta}_{gb} \geq 0,$$

where ρ_{gb} denotes the surface mass density. Substituting (4.10) and (4.11) into (4.13), inequality (4.14) takes the form

(4.15) $$\pi_{gb}\lceil\psi\rceil + \mathbf{n}_{gb}\sigma\lceil\mathbf{v}\rceil - \lceil k_p(\mathbf{v}_p - \mathbf{v}_{gb})\rceil\mathbf{n}_{gb} - \rho_{gb}\overset{\circ}{\psi}_{gb} - \rho_{gb}\eta_{gb}\overset{\circ}{T} \geq 0,$$

where $\sigma = \frac{1}{2}(\sigma^+ + \sigma^-)$. To determine the thermodynamical driving forces on the surface we must postulate the state variables on surface. Our approach is based

on the assumption that misorientation should be incorporated into constitutive modelling of the reorientation process. To do this let us assume, that the constitutive equation for the surface free energy density depends on misorientation and temperature, i.e.

$$(4.16) \qquad \boxed{\psi_{gb} = \psi_{gb}(\Delta_p \varphi, T).}$$

If we take into account that in our formalism the Born rule holds, then the same restriction for the surface free energy density is obtained as those assumed by CERMELLI and SELLERS in [3]. This postulate is crucial for the analysis and it has strong consequences on the shape of driving forces. Substituting (4.16) to (4.15) we get

$$(4.17) \qquad \pi_{gb}\lceil\psi\rceil + \mathbf{n}_{gb}\sigma\lceil\mathbf{v}\rceil - \lceil k_p(\mathbf{v}_p - \mathbf{v}_{gb})\rceil\mathbf{n}_{gb} - \mathbf{m}_p \overset{\circ}{\Delta_p\varphi}$$

$$- \rho_{gb}\overset{\circ}{T}\left(\frac{\partial \psi_{gb}}{\partial T} + \eta_{gb}\right) \geq 0,$$

where

$$(4.18) \qquad \mathbf{m}_p = \rho_{gb}\frac{\partial \psi_{gb}}{\partial \Delta_p\varphi}.$$

To satisfy (4.17) for all possible process, we find

$$(4.19) \qquad \eta_{gb} = -\frac{\partial \psi_{gb}}{\partial T}.$$

It is easy to realize that $\mathbf{m}_p$ has the meaning of the misorientation vector driving force. Traditionally η_{gb} in (4.19) denotes entropy density of the grain boundary. Additionally, using (4.11) and (4.12), the jump in continuum velocity can be expressed as

$$(4.20) \qquad \lceil\mathbf{v}\rceil = -\lceil\frac{1}{\rho}\rceil\mathbf{n}_{gb}\pi_{gb}.$$

Let us define the right and left dislocation flux vectors to the boundary, namely

$$\pi_p^\pm = \mp\mathbf{n}_{gb} \cdot (\mathbf{v}_p^\pm - \mathbf{v}_{gb}^\pm).$$

It can be established, that[1]

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[1]Using (3.1) we find $\overset{\circ}{\Delta_p\varphi} = -\mathbf{n}_{gb} \cdot \lceil\overset{\circ}{\varepsilon_p}\rceil \times \mathbf{n}_{gb} + \frac{1}{2}\mathbf{n}_{gb}\text{tr}\left(\lceil\overset{\circ}{\varepsilon_p}\rceil \times \mathbf{n}_{gb}\right)$

$= -\mathbf{n}_{gb} \cdot \lceil\dot{\varepsilon}_p + \nabla\varepsilon_p \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb} + \frac{1}{2}\mathbf{n}_{gb}\text{tr}(\lceil\dot{\varepsilon}_p + \nabla\varepsilon_p \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb})$

$= -\mathbf{n}_{gb} \cdot \lceil\dot{\varepsilon}_p + \nabla_{<\varepsilon_p>} \mathbf{v}_{gb} + \nabla_{(\varepsilon_p)} \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb}$
$\quad + \frac{1}{2}\mathbf{n}_{gb}\text{tr}(\lceil\dot{\varepsilon}_p + \nabla_{<\varepsilon_p>} \mathbf{v}_{gb} + \nabla_{(\varepsilon_p)} \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb})$

$= -\mathbf{n}_{gb} \cdot \lceil\alpha_p \times \mathbf{v}_p + \nabla_{<\varepsilon_p>} \mathbf{v}_{gb} + \nabla_{(\varepsilon_p)} \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb}$
$\quad + \frac{1}{2}\mathbf{n}_{gb}\text{tr}(\lceil\alpha_p \times \mathbf{v}_p + \nabla_{<\varepsilon_p>} \mathbf{v}_{gb} + \nabla_{(\varepsilon_p)} \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb})$

$= -\mathbf{n}_{gb} \cdot \lceil\alpha_p \times (\mathbf{v}_p - \mathbf{v}_{gb}) + \nabla_{(\varepsilon_p)} \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb} + \frac{1}{2}\mathbf{n}_{gb}\text{tr}(\lceil\alpha_p \times (\mathbf{v}_p - \mathbf{v}_{gb}) + \nabla_{(\varepsilon_p)} \mathbf{v}_{gb}\rceil \times \mathbf{n}_{gb}).$

(4.21) $\Delta_p \overset{\circ}{\varphi} = \pi_p^+ \, \mathrm{angl}(\alpha_p^+ \times \mathbf{n}_{gb}) + \pi_p^- \, \mathrm{angl}(\alpha_p^- \times \mathbf{n}_{gb})$

$$+ \pi_{gb} \, \mathrm{angl}\lceil \frac{\nabla_{(\varepsilon_p)} \cdot \mathbf{n}_{gb}}{\rho} \rceil,$$

where, for each tensor $\mathbf{t}$, operator $\mathrm{angl}\, \mathbf{t}$ is defined as

$$\mathrm{angl}\, \mathbf{t} \overset{df}{=} \mathbf{n}_{gb} \cdot \mathbf{t} \times \mathbf{n}_{gb} + \frac{1}{2}\mathbf{n}_{gb}\mathrm{tr}\mathbf{t}.$$

By the use of (4.21), the entropy inequality (4.17) in the isothermal conditions can be rewritten in the form

(4.22) $t_{gb}\pi_{gb} + t_p^+ \pi_p^+ + t_p^- \pi_p^- \geq 0,$

where

(4.23) $t_{gb} = \lceil \psi \rceil - \mathbf{n}_{gb} \cdot \sigma \cdot \mathbf{n}_{gb}\lceil \frac{1}{\rho} \rceil - \mathbf{m}_p \cdot \mathrm{angl}\lceil \frac{\nabla_{(\varepsilon_p)} \cdot \mathbf{n}_{gb}}{\rho} \rceil,$

(4.24) $t_p^{\pm} = k_p^{\pm} - \mathbf{m}_p \cdot \mathrm{angl}(\alpha_p^{\pm} \times \mathbf{n}_{gb}).$

In above equations t_{gb} and t_p denote driving forces conjugate to: the jump in the respective quantities on the boundary and the existing dislocation around the boundary. In order to complete the thermodynamical formulation of the theory, the manner in which the grain boundary migrates, should be given.

Constitutive equation for a grain boundary migration. According to known experimental data i.e. [4], the mobility of grain boundary depends mainly on misorientation, temperature, concentration of precipitations and driving forces described by (4.23) and (4.24). According to the thermodynamic restrictions obtained in the previous subsection we can assume a constitutive equation for fluxes across the boundary. Taking into account the driving forces, misorientation and temperature, the constitutive equations for the mass and dislocation flux through the grain boundary can be stated in the form

(4.25) $\pi_{gb} = \pi_{gb}(t_{gb}, \Delta_p\varphi, T),$

(4.26) $\pi_p^{\pm} = \pi_p^{\pm}(t_p^{\pm}, \Delta_p\varphi, T).$

Equation (4.26) does not mean that a single dislocations have to overcome a grain boundary, but it means that the proportion between the annihilation of dislocations on one side and production of them on the second side subject to a limitation imposed on this process by energy of the grain boundary, according to (4.26) and (4.24). According to the thermodynamic balance we have determined

a thermodynamic force t_p yielding from the change of grain misorientation energy inherently related to the production and annihilation of dislocations on the grain boundary. For example, it is known that some orientations of grains in polycrystals are observed more often than others. Our paper is devoted to thermodynamic reasons of this effect obtained from thermodynamics of the grain reorientation process. It is worth emphasizing that in terms of the classical theory of crystal plasticity, this effect cannot be described as far as the grain misorientation energy will be incorporated into thermodynamic considerations on elastic-plastic deformations.

The constitutive equation (4.25) describes the mass flux over the grain boundary, what means that this equation describes nothing more than the migration of grain boundary. This is induced by the jump in the specific free energy on the opposite sides of boundary, cf. (4.25) and (4.23). In real crystals another component of the driving force often exists when the strongly dislocated structure on one side of the grain is recovered on the second side in the form of the nucleation and growth of new (undislocated) grain. So, the force t_{gb} can be treated here only as a part of the resulting driving force governing the migration of grain boundaries in real crystals. The main part of this force results from the difference of the free energy of dislocated and recovered grains on opposite sides of the grain boundary. Equation (4.23) describes a component induced by unbalanced dislocations, which bend crystal lattice within grains.

5. Final remarks

In this paper, a thermodynamical solution for the grain reorientation process and the conjugated driving forces has been derived. In the presented approach it has been assumed that the surface density of the free energy depends on the misorientation vector. It is worth emphasizing that in material science the influence of lattice misorientation on the energy of low angle grain boundaries is well established, cf. [14], while from the viewpoint of continuum thermodynamics of plastic deformation such a dependence is usually ignored.

According to the symmetry of crystal lattice, to a given boundary several vectors of jump in orientation can be attributed. Even in the case of asymmetric unit there exist two misorientation vectors with the lengths: $\Delta\varphi$ and $\Delta\varphi' = (2\pi - \Delta\varphi)$. In real crystal lattices e.g. for fcc crystal, we can assign 48 mutually different orientation vectors for a single boundary. The choice of real vector of jump in orientation corresponds to the choice of a certain inner grain boundary structure. This suggests that in oreder to describe properly the single-valued grain reorientation process, initial orientations of grains around boundary should be included.

The effect of grain reorientation has been described here in the spirit of the macroscopic dislocation theory. We have shown, how the influence of the grains misorientation on the reorientation process can be described in terms of continuum theory of dislocations. As a result of the dependence of surface energy on the misorientation vector, additional terms have been obtained in the equation of driving force of grain boundary motion.

On the other hand, from the viewpoint of the general continuum theory of defects our approach concerns only a thermodynamic solution obtained in terms of the dislocation theory. For example, in terms of the disclination theory we should assume that a constitutive dependence for surface energy takes into account not only the dependence on the misorientation vector, but also on its gradient along the boundary. This gradient corresponds to continuous distribution of disclinations along grain the boundary. For a discrete wedge disclination, understood as a line bounding the grain boundary within a crystal, the gradient will reduce to the delta distribution at the edge of the grain boundary identified with disclination line. Therefore the disclination model needs the determination of the discontinuity conditions of higher order than those considered in the present paper. It is most probable that to balance the energy, which is dependent on the misorientation gradient along the grain boundary, the polar elasticity could appear to be indispensable. Then the polar elasticity could play a similar role as the symmetric elasticity employed here to the dislocation theory. Thus, our approach concerns thermodynamics of crystal lattice misorientation considered in terms of a discontinuity surface analyzed in the framework of the dislocation theory and the symmetric elasticity. It is worth emphasizing that in real crystals the grain boundaries usually show a constant misorientation vector along the boundary; moreover, boundaries do not end within a crystal by disclinations – therefore, from the viewpoint of the authors, the dislocational model of the grain boundary seems to be much closer to thermodynamics of low-angle grain boundaries than the considerably more advanced disclination/dislocation model.

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