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Tangential continuity of elastic/plastic curvature and strain at interfaces

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The continuity vs discontinuity of the elastic/plastic curvature & curvature rate, and strain & strain rate tensors is examined at non-moving surfaces of discontinuity, in the context of a field theory of crystal defects (dislocations and disclinations). Tangential continuity of these tensors derives from the conservation of the Burgers and Frank vectors over patches bridging the interface, in the limit where such patches contract onto the interface. However, normal discontinuity of these tensors remains allowed, and Kirchhoff-like compatibility conditions on their normal discontinuities across the concurring interfaces are derived at multiple junctions. In a simple plane case and in the absence of surface-disclinations, the compatibility of the normal discontinuities in the elastic curvatures assumes the form of a Young's law between the grain-to-grain disorientations and the sines of the dihedral angles. Complete continuity of the plastic strain rate tensor at triple junctions also derives from the compatibility of the normal discontinuities in the plastic strain rates in such conditions.

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1. Introduction

In crystalline media, grain boundaries are rotational defects resulting in certain discontinuities of the elastic/plastic strain and/or curvature fields. Modeling efforts at describing grain boundaries include dislocation-based and disclination-based approaches (see respectively (Frank, 1950; Bilby, 1955) and (Li, 1972; Shih and Li, 1975; Gertsman et al., 1989)) and atomistic simulations (Sutton et al., 1983). In dislocation-based models, surface-dislocation densities are considered as the source of disorientation between grains, *i.e.* an arbitrary disorientation is accommodated by an appropriate distribution of surface-dislocations. Such approaches may be successful in predicting geometrical properties of grain boundaries, such as the coupling factor relating the normal tilt boundary motion to an imposed shear displacement (Cahn et al., 2006). However, surface-dislocations-based models are limited to small misorientation angles. Indeed, as implied by Frank's equation, the distance between surface-dislocations decreases when the misorientation angle increases, to the point where dislocation core overlapping occurs (Li, 1972). In addition, surface-dislocations are singularly supported by an infinitely thin interface, a premise at odds with the atomistic rendering of grain boundaries, which features elementary structures spreading over a finite-width layer, perhaps as thin as a nanometer, but definitely not vanishingly thin (Sutton et al., 1983).

Being themselves rotational defects, disclinations may seem to be more appropriate than dislocations for grain boundary modeling (Li, 1972). Discrete disclination dipole walls were indeed introduced to represent grain boundaries (Li, 1972; Shih and Li, 1975; Gertsman et al., 1989). These models are built on linear arrays of discrete disclination dipoles, for which closed-form expressions of the elastic energy, strain and curvature fields were first derived by Huang and Mura (1970) and de Wit (1973). However, this approach suffers from several limitations. In the first place, it only describes relative misorientation with respect to reference boundaries – corresponding to cusps in the variation of the grain boundary energy with misorientation. Second, it also confines the disclination distribution to the plane of the interface where it exhibits discontinuities. It may again seem paradoxical to attempt modeling of a thin, but non vanishingly small, material layer where the crystal lattice encounters a finite rotation, by using a crystal defect distribution supported by an infinitely thin interface.

The aim of the present work is to contribute to a non-singular description of grain boundaries, by dismissing surface-defects pertaining to an infinitely thin interface, and using a volumetric field representation of dislocations and disclinations by their aerial density (Nye, 1953; de Wit, 1970). A continuous elasto-plastic theory of crystal defect (dislocation and disclination) fields was recently proposed, in which disclination dipoles are indeed seen as objects extended in space and used to model high-angle tilt boundary segments with a finite thickness (Fressengeas et al., 2011). In this theory, the material displacements as well as the density and motion of dislocations/disclinations can be derived uniquely from initial

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and boundary conditions, provided constitutive information for elasticity and the dislocation/disclination velocities is supplied. In the present paper, our specific intent is to clarify the issue of continuity vs discontinuity of the elastic/plastic strain and curvature tensor fields across a surface of discontinuity, in the framework of this theory. Although discontinuities in these fields are allowed, necessary tangential continuity conditions on the elastic strain and curvature tensors will be derived at smooth interfaces, and some of their implications investigated. In doing so, we clearly benefit from earlier investigation of the continuity conditions on the plastic distortion rate in the field theory of dislocations (Acharya, 2007). Interfaces with kinks or ledges, as occurs in phase transformation, are beyond the scope of the present investigation, although they can be treated using discrete disclination dipoles (see for example the review (Romanov and Kolesnikova, 2009)), because characterization of such features in a continuous framework requires defining crystal defects of higher order than dislocations and disclinations (Acharya and Fressengeas, 2012).

The paper is organized as follows. In Section 2, notation conventions are settled. For completeness, a brief review of the incompatible elastic defect theory (de Wit, 1970) is provided in Section 3. In Section 4, the existence in this framework of tangential continuity conditions on the elastic/plastic strain and curvature at material surfaces of discontinuity is shown. Kirchhoff-type compatibility conditions on the normal discontinuities at multiple junctions are derived in Section 5. Illustration of these concepts is proposed in Section 6 with the two-dimensional case of triple junctions built from tilt boundaries. Concluding remarks follow.

2. Notations

A bold symbol denotes a tensor. When there may be ambiguity, an arrow is superposed to represent a vector: $\vec{\mathbf{V}}$. The symmetric part of tensor $\mathbf{A}$ is denoted $\{\mathbf{A}\}$. Its skew-symmetric part is $\}\mathbf{A}\{$. The tensor $\mathbf{A}\cdot\mathbf{B}$, with rectangular Cartesian components $A_{ik}B_{kj}$, results from the dot product of tensors $\mathbf{A}$ and $\mathbf{B}$, and $\mathbf{A}\otimes\mathbf{B}$ is their tensorial product, with components $A_{ij}B_{kl}$. A : represents the trace inner product of the two second order tensors $\mathbf{A}:\mathbf{B} = A_{ij}B_{ij}$, in rectangular Cartesian components, or the product of a higher order tensor with a second order tensor, e.g., $\mathbf{A}:\mathbf{B} = A_{ijkl}B_{kl}$. The cross product of a second-order tensor $\mathbf{A}$ and a vector $\mathbf{V}$, the **div** and **curl** operations for second-order tensors are defined row by row, in analogy with the vectorial case. For any base vector $\mathbf{e}_i$ of the reference frame:

$$(\mathbf{A}\times\mathbf{V})^t\cdot\mathbf{e}_i = (\mathbf{A}^t\cdot\mathbf{e}_i)\times\mathbf{V} \tag{1}$$

$$(\mathbf{div}\,\mathbf{A})^t\cdot\mathbf{e}_i = \mathbf{div}(\mathbf{A}^t\cdot\mathbf{e}_i) \tag{2}$$

$$(\mathbf{curl}\,\mathbf{A})^t\cdot\mathbf{e}_i = \mathbf{curl}(\mathbf{A}^t\cdot\mathbf{e}_i) \tag{3}$$

In rectangular Cartesian components:

$$(\mathbf{A}\times\mathbf{V})_{ij} = e_{jkl}A_{ik}V_l \tag{4}$$

$$(\mathbf{div}\,\mathbf{A})_i = A_{ij,j} \tag{5}$$

$$(\mathbf{curl}\,\mathbf{A})_{ij} = e_{jkl}A_{il,k} \tag{6}$$

where e_{jkl} is a component of the third-order alternating Levi–Civita tensor $\mathbf{X}$. A vector $\vec{\mathbf{A}}$ is associated with tensor $\mathbf{A}$ by using its trace inner product with tensor $\mathbf{X}$:

$$(\vec{\mathbf{A}})_k = -\frac{1}{2}(\mathbf{A}:\mathbf{X})_k = -\frac{1}{2}e_{ijk}A_{ij} \tag{7}$$

A superposed dot represents a material time derivative. In the component representation, the spatial derivative with respect to a Cartesian coordinate is indicated by a comma followed by the component index.

3. Review of the incompatible elasto-static defect theory

In the framework of the field models (de Wit, 1970; Fressengeas et al., 2011), the displacement vector $\mathbf{u}$ is defined continuously at any point of a simply-connected body undergoing elasto-plastic deformation. Hence, it is required that the displacement field represent a consistent shape change, possibly defined between atoms, below interatomic distance. Therefore, the total distortion tensor $\mathbf{U}$ is defined as the gradient of the displacement:

$$\mathbf{U} = \mathbf{grad}\,\mathbf{u} \tag{8}$$

As such, it is curl-free:

$$\mathbf{curl}\,\mathbf{U} = 0 \tag{9}$$

This equation is a necessary condition for the integrability of the distortion $\mathbf{U}$, referred to as the compatibility condition for $\mathbf{U}$. Conversely, Eq. (9) is sufficient to assure the existence of a single-valued continuous solution $\mathbf{u}$ to Eq. (8), up to a constant translation. Generally, in the presence of dislocations, the plastic, $\mathbf{U}_p$, and elastic, $\mathbf{U}_e$, components of the total distortion are not curl-free. Indeed, the plastic distortion tensor has an incompatible part, $\mathbf{U}_p^{\perp}$, associated with the presence of Nye's dislocation density tensor $\boldsymbol{\alpha}$ (Nye, 1953). An opposite incompatible elastic distortion of the lattice, $\mathbf{U}_e^{\perp}$, also arises to maintain lattice continuity. Curl-free compatible components, $\mathbf{U}_e^{\parallel}$ and $\mathbf{U}_p^{\parallel}$, may additionally exist to satisfy the balance of momentum and boundary conditions, and the following relations are therefore satisfied:

$$\mathbf{U} = \mathbf{U_e} + \mathbf{U_p} \tag{10}$$

$$\mathbf{U_e} = \mathbf{U_e^{\perp}} + \mathbf{U_e^{\parallel}} \tag{11}$$

$$\mathbf{U_p} = \mathbf{U_p^{\perp}} + \mathbf{U_p^{\parallel}} \tag{12}$$

$$0 = \mathbf{U_e^{\perp}} + \mathbf{U_p^{\perp}} \tag{13}$$

$$\mathbf{curl}\,\mathbf{U_e^{\perp}} = -\mathbf{curl}\,\mathbf{U_p^{\perp}} = \boldsymbol{\alpha} \tag{14}$$

Composing Eqs. (10)–(12) allows showing that Eq. (13) is needed to ensure satisfaction of the compatibility condition (9). The right-hand-side incompatibility Eq. (14) defines the incompatible plastic distortion $\mathbf{U}_p^{\perp}$ associated with the presence of $\boldsymbol{\alpha}$, while the left-hand-side equation provides the incompatible elastic distortion $\mathbf{U}_e^{\perp}$ offsetting the latter to ensure the continuity of matter.[1] Since $\mathbf{U}_e^{\parallel}$ and $\mathbf{U}_p^{\parallel}$ are curl-free, Eq. (14) is still true when $\mathbf{U}_e^{\perp}$ and $\mathbf{U}_p^{\perp}$ are respectively replaced with $\mathbf{U}_e$ and $\mathbf{U}_p$:

$$\mathbf{curl}\,\mathbf{U_e} = -\mathbf{curl}\,\mathbf{U_p} = \boldsymbol{\alpha} \tag{15}$$

Therefore, to ensure that the incompatible part $\mathbf{U_p^{\perp}}$ vanishes identically throughout the body when $\boldsymbol{\alpha} = 0$, Eq. (14) must be augmented with the side conditions $\mathbf{div}\,\mathbf{U_p^{\perp}} = \mathbf{0}$ and $\mathbf{U_p^{\perp}}\cdot\mathbf{n} = \mathbf{0}$ on the boundary with unit normal $\mathbf{n}$ (see for example Acharya and Roy, 2006). Defining the strain tensor $\boldsymbol{\epsilon}$ as the symmetric part of the distortion $\mathbf{U}$, the rotation tensor $\boldsymbol{\omega}$ as its skew-symmetric part and the associated rotation vector $\vec{\boldsymbol{\omega}}$ as:

[1] By virtue of Stokes' theorem: $\int_C \mathbf{U}\cdot\mathbf{dl} = \int_S \mathbf{curl}\,\mathbf{U}\cdot\mathbf{n}\,dS$ on a closed curve C surrounding surface S of normal $\mathbf{n}$. In compatible theory, the distortion tensor $\mathbf{U}$ is a gradient and its line integral along curve C is zero on the left hand side. Thus, from the right hand side, the compatibility condition (9) is satisfied with sufficient continuity. In the presence of a net content of dislocations threading S, a discontinuity in the elastic displacement arises, and the closure defect of circuit C : $\mathbf{b} = \int_C \mathbf{U_e}\cdot\mathbf{dl}$ is non zero. $\mathbf{b}$ is referred to as the Burgers vector of the dislocations threading S. It characterizes the incompatibility in the elastic displacement along circuit C. The left Eqs. (14), (15) are now satisfied, and the net dislocation content is also characterized in a continuous manner by Nye's tensor $\boldsymbol{\alpha}$.

$$\vec{\omega} = -\frac{1}{2}\boldsymbol{\omega} : \mathbf{X} \tag{16}$$

Eq. (9) becomes:

$$\mathbf{curl}\,\epsilon + div(\vec{\omega})\mathbf{I} - \mathbf{grad}^{\mathbf{t}}\vec{\omega} = 0 \tag{17}$$

where $\mathbf{I}$ is the identity tensor. Transposing, then taking the **curl** of Eq. (17) leads to:

$$\mathbf{curl}\,\mathbf{curl}^{\mathbf{t}}\epsilon = 0 \tag{18}$$

This relation is the classical Saint–Venant compatibility condition for the strain ϵ. It is a necessary condition for the integrability of the displacement $\mathbf{u}$. The trace of Eq. (17) similarly yields the necessary condition:

$$div(\vec{\omega}) = 0 \tag{19}$$

which is a compatibility condition for the rotation $\vec{\omega}$. Applying the same curl-trace procedure to the elastic restriction of Eq. (15), we obtain from the curl operation, with self-evident notations, an equation parallel to Eq. (17):

$$\mathbf{curl}\,\epsilon_e + div(\vec{\omega}_e)\mathbf{I} - \mathbf{grad}^{\mathbf{t}}\vec{\omega}_e = \boldsymbol{\alpha} \tag{20}$$

and a similar equation for the plastic part of Eq. (15):

$$\mathbf{curl}\,\epsilon_p + div(\vec{\omega}_p)\mathbf{I} - \mathbf{grad}^{\mathbf{t}}\vec{\omega}_p = -\boldsymbol{\alpha} \tag{21}$$

From the trace operation, we find an equation parallel to Eq. (19):

$$div(\vec{\omega}_e) = -div(\vec{\omega}_p) = \frac{1}{2}tr(\boldsymbol{\alpha}) \tag{22}$$

Motivated by the Saint–Venant compatibility condition (18), we transpose Eqs. (20), (21) and further rearrange with the help of Eq. (22), to obtain:

$$\mathbf{grad}\,\vec{\omega}_e = \mathbf{curl}^{\mathbf{t}}\,\epsilon_e + \mathbf{K} \tag{23}$$

$$\mathbf{grad}\,\vec{\omega}_p = \mathbf{curl}^{\mathbf{t}}\,\epsilon_p - \mathbf{K} \tag{24}$$

$$\mathbf{K} = \frac{1}{2}tr(\boldsymbol{\alpha})\mathbf{I} - \boldsymbol{\alpha}^t \tag{25}$$

At this point, we can define the elastic, $\boldsymbol{\kappa}_e$, and plastic, $\boldsymbol{\kappa}_p$, curvature tensors as:

$$\boldsymbol{\kappa}_e = \mathbf{grad}\,\vec{\omega}_e \tag{26}$$
$$\boldsymbol{\kappa}_p = \mathbf{grad}\,\vec{\omega}_p \tag{27}$$
$$\mathbf{grad}\vec{\omega} = \boldsymbol{\kappa}_e + \boldsymbol{\kappa}_p \tag{28}$$

and take the **curl** of Eqs. (23), (24), to find:

$$\mathbf{curl}\,\boldsymbol{\kappa}_e = \mathbf{curl}\,\mathbf{curl}^{\mathbf{t}}\,\epsilon_e + \mathbf{curl}\,\mathbf{K} = 0 \tag{29}$$

$$\mathbf{curl}\,\boldsymbol{\kappa}_p = \mathbf{curl}\,\mathbf{curl}^{\mathbf{t}}\,\epsilon_p - \mathbf{curl}\,\mathbf{K} = 0 \tag{30}$$

Hence, in the elasto-plastic theory of dislocations, the elastic and plastic curvatures $(\boldsymbol{\kappa}_e, \boldsymbol{\kappa}_p)$ are curl-free and integrable quantities. $\mathbf{K}$ is referred to as Nye's curvature tensor (Nye, 1953). $(\boldsymbol{\kappa}_e, \boldsymbol{\kappa}_p)$ are also known as the elastic and plastic bend-twist tensors, respectively.

If $(\boldsymbol{\kappa}_e, \boldsymbol{\kappa}_p)$ are not supposed to be curl-free anymore, *i.e.* if the possibility of a rotational incompatibility is acknowledged, then the rotation vectors $(\vec{\omega}_e, \vec{\omega}_p)$ do not exist, and a non-zero tensor $\boldsymbol{\theta}$ such that

$$\boldsymbol{\theta} = -\mathbf{curl}\,\boldsymbol{\kappa}_p = \mathbf{curl}\,\boldsymbol{\kappa}_e \tag{31}$$

can be defined. $\boldsymbol{\theta}$ is the disclination density tensor, and Eq. (31) is part of the theory of crystal defects. It replaces Eqs. (29), (30), which pertain to the theory of dislocations. On the one hand, Eq. (31) means that an incompatible plastic curvature, $\boldsymbol{\kappa}_p^{\perp}$, is associated with the presence of the disclination density $\boldsymbol{\theta}$ and, on the other hand, that the incompatible elastic curvature, $\boldsymbol{\kappa}_e^{\perp}$ is needed to ensure the continuity of matter in the presence of this density. As already discussed for Eqs. (14), (15) in the case of translational incompatibility, to ensure that the incompatible parts $(\boldsymbol{\kappa}_e^{\perp}, \boldsymbol{\kappa}_p^{\perp})$ vanish identically throughout the body when $\boldsymbol{\theta} = 0$, Eq. (31) must be replaced with:

$$\boldsymbol{\theta} = -\mathbf{curl}\,\boldsymbol{\kappa}_p^{\perp} = \mathbf{curl}\,\boldsymbol{\kappa}_e^{\perp} \tag{32}$$

augmented with the side conditions $\mathbf{div}\,\boldsymbol{\kappa}_e^{\perp} = \mathbf{div}\,\boldsymbol{\kappa}_p^{\perp} = 0$ and $\boldsymbol{\kappa}_{\mathbf{e}}^{\perp}\cdot\mathbf{n} = \boldsymbol{\kappa}_{\mathbf{p}}^{\perp}\cdot\mathbf{n} = \mathbf{0}$ on the boundary with unit normal $\mathbf{n}$. These conditions ensure uniqueness of the solution to Eq. (32), while solutions to Eq. (31) are known up to a gradient. The continuity condition for disclinations:

$$\mathbf{div}\,\boldsymbol{\theta} = 0 \tag{33}$$

follows directly from Eqs. (31), (32). Since the rotation vectors $(\vec{\omega}_e, \vec{\omega}_p)$ do not exist in the theory of crystal defects, the corresponding elastic and plastic distortion tensors $\mathbf{U}_e$ and $\mathbf{U}_p$ are also undefined. Substituting the elastic and plastic curvatures $(\boldsymbol{\kappa}_e, \boldsymbol{\kappa}_p)$, which now include an incompatible part, for $(\mathbf{grad}\,\vec{\omega}_e, \mathbf{grad}\,\vec{\omega}_p)$ in Eqs. (20), (21), leads to the modified equations:

$$\mathbf{curl}\,\epsilon_e = +\boldsymbol{\alpha} + \boldsymbol{\kappa}_e^t - tr(\boldsymbol{\kappa}_e)\mathbf{I} \tag{34}$$

$$\mathbf{curl}\,\epsilon_p = -\boldsymbol{\alpha} + \boldsymbol{\kappa}_p^t - tr(\boldsymbol{\kappa}_p)\mathbf{I} \tag{35}$$

Eq. (35) defines the incompatible plastic strain associated with the dislocation density tensor $\boldsymbol{\alpha}$ in the concurrent presence of plastic curvature, while Eq. (34) specifies the incompatible elastic strain needed to ensure the continuity of matter in the presence of dislocations and disclinations. In the theory of crystal defects, the Frank's and Burgers vectors for a close circuit C bounding a surface S are defined as (de Wit, 1970):

$$\boldsymbol{\Omega} = \int_C \boldsymbol{\kappa}_e \cdot \mathbf{dr} \tag{36}$$

$$\mathbf{b} = \int_C (\epsilon_e - \boldsymbol{\kappa}_e \times \mathbf{r}) \cdot \mathbf{dr} \tag{37}$$

They can be related to the dislocation and disclination density tensors $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$ by applying Stokes' theorem to the surface S (de Wit, 1970):

$$\boldsymbol{\Omega} = \int_S \boldsymbol{\theta} \cdot \mathbf{n}dS \tag{38}$$

$$\mathbf{b} = \int_S (\boldsymbol{\alpha} - \boldsymbol{\theta} \times \mathbf{r}) \cdot \mathbf{n}dS \tag{39}$$

4. Tangential continuity of the elastic curvature at surfaces of discontinuity

In this Section, we assume the existence of a smooth surface of discontinuity $\mathcal{I}$, *i.e.* without discontinuities in its tangent plane orientation field, separating the body D into two domains D^+ and D^-. For the sake of simplicity, this interface $\mathcal{I}$ is assumed to remain attached to the material. At any point P on $\mathcal{I}$, the normal vector $\mathbf{n}$ to the interface is oriented from D^- toward D^+, and we denote by $\mathbf{l}$ and $\mathbf{t} = \mathbf{n} \times \mathbf{l}$ two unit vectors belonging to the tangent plane to the interface (see Fig. 1). $\mathcal{I}$ may be used to model a grain boundary in a polycrystal. In this case, the grain boundary is seen as having no width. Continuum mechanics requires that the displacement $\mathbf{u}$ and traction vector $\mathbf{T}\cdot\mathbf{n}$ be continuous across the interface. Hence, if $[x] = x^+ - x^-$ denotes a discontinuity in the variable x

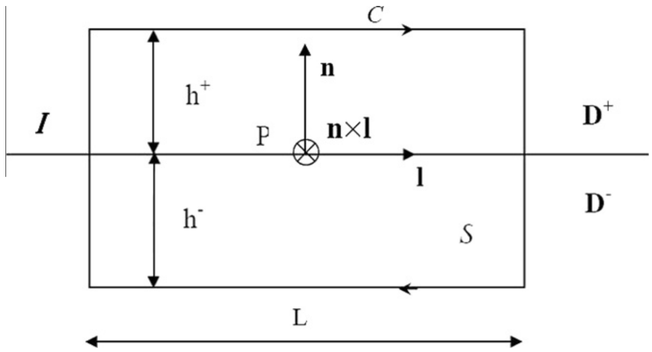

Fig. 1. Burgers circuit across an interface $\mathcal{I}$ separating the body D into domains D^-, D^+. $\mathbf{n}$ is the unit normal to the interface, and $\mathbf{t} = \mathbf{n} \times \mathbf{l}$ the normal to the bounded surface S.

through the interface $\mathcal{I}$, $[\mathbf{u}] = 0$ and $[\mathbf{T} \cdot \mathbf{n}] = 0$. The continuity of the traction vector is reflected as well by the continuity of the normal part, $\mathbf{T}_n = \mathbf{T} \cdot \mathbf{n} \otimes \mathbf{n}$, of the stress tensor: $[\mathbf{T}_n] = 0$. However, the tangential part of the stress tensor, $\mathbf{T}_t = \mathbf{T} - \mathbf{T}_n$, may be discontinuous across the interface. This discontinuity is expressed by:

$$\exists \mathbf{l} \in \mathcal{I}, \quad [\mathbf{T}] \cdot \mathbf{l} \neq 0 \tag{40}$$

which implies that:

$$[\mathbf{T}] \times \mathbf{n} \neq 0 \tag{41}$$

In contrast, the continuity of the displacement at the interface requires tangential continuity of the total distortion $\mathbf{U} = \mathbf{grad}\,\mathbf{u}$:

$$\forall \mathbf{l} \in \mathcal{I}, \quad [\mathbf{U}] \cdot \mathbf{l} = 0 \tag{42}$$

a condition also rendered as:

$$[\mathbf{U}] \times \mathbf{n} = 0 \tag{43}$$

or, in terms of the normal and tangential parts of the distortion, $[\mathbf{U}_n]$ and $[\mathbf{U}_t]$, as:

$$[\mathbf{U}_t] = [\mathbf{U}] - [\mathbf{U}_n] = [\mathbf{U}] - [\mathbf{U}] \cdot \mathbf{n} \otimes \mathbf{n} = 0 \tag{44}$$

This tangential continuity condition is known as Hadamard's compatibility condition (Hadamard, 1903). It does not impose any requirement on the normal discontinuity $[\mathbf{U}_n]$ across the interface. Of course, it is also silent on the continuity vs discontinuity of the elastic/plastic curvature and strain tensors at the interface. We show below that, if the choice is made to represent continuously the incompatibility arising from the presence of lattice defects in the interface area, additional continuity conditions on the elastic curvature and strain arise at the interface.

Indeed, let us consider a rectangular closed circuit C lying across the interface and bounding a surface S oriented by $\mathbf{t}$, in the manner shown in Fig. 1. Rewriting Eqs. (36), (38) in the present context, the net Frank vector $\boldsymbol{\Omega}$ of the disclinations threading S is such that:

$$\forall \mathbf{l} \in \mathcal{I}, \quad \Omega = \int_C \boldsymbol{\kappa}_e \cdot \mathbf{dr} = \int_S \theta \cdot \mathbf{t} dS \tag{45}$$

Provisionally, the distribution of disclinations in S is assumed to include not only a continuous distribution of disclinations $\boldsymbol{\theta}$ in each domain D^- and D^+, but also a singular distribution $\boldsymbol{\theta}(\mathcal{I})$ along the interface $\mathcal{I}$. This singular term represents "surface-disclinations" through a density of (adimensional) Frank vectors per m in the direction $\mathbf{l}$. If the circuit C is collapsed onto point P by letting h^+ and h^- tend to zero, and L shrinks along the direction $\mathbf{l}$, Eq. (45) becomes:

$$\forall \mathbf{l} \in \mathcal{I}, \quad [\boldsymbol{\kappa}_e] \cdot \mathbf{l} = \theta(\mathcal{I}) \cdot \mathbf{t} \tag{46}$$

Essentially, the bulk density $\boldsymbol{\theta}$ distributed in D^+ and D^- disappears in this limit. Thus, Eq. (46) provides the density $\boldsymbol{\theta}(\mathcal{I})$ of surface-disclinations needed to accommodate a tangential discontinuity of the elastic curvature $[\boldsymbol{\kappa}_e]$ in no width across the interface. It has no implication on its normal discontinuity. However, if the choice is made to describe the interface in a continuous manner and a small resolution length scale is used to render the fine structure of the boundary, then the surface-disclination concept must be surrendered. This modeling choice amounts to acknowledging that the accommodation of a finite variation of the tangential part of the elastic curvature takes place in a finite material layer, perhaps as thin as a few nanometers and containing a few atomic rows, but non discrete. In this case, Eq. (46) becomes:

$$\forall \mathbf{l} \in \mathcal{I}, \quad [\boldsymbol{\kappa}_e] \cdot \mathbf{l} = 0 \tag{47}$$

The meaning of Eq. (47) is that, in the absence of surface-disclinations, tangential continuity of the elastic curvature tensor is required in a continuous model. Eq. (47) is equally transcribed as:

$$[\boldsymbol{\kappa}_e] \times \mathbf{n} = 0 \tag{48}$$

or in terms of its normal and tangential components, $[\boldsymbol{\kappa}_e]_n$ and $[\boldsymbol{\kappa}_e]_t$, as:

$$[\boldsymbol{\kappa}_e]_t = [\boldsymbol{\kappa}_e] - [\boldsymbol{\kappa}_e]_n = [\boldsymbol{\kappa}_e] - [\boldsymbol{\kappa}_e] \cdot \mathbf{n} \otimes \mathbf{n} = 0 \tag{49}$$

Continuity of the normal component of the elastic curvature tensor is not required by Eq. (48), nor is it accommodated by the surface-disclination density in Eq. (46).[2] The continuity of the tangential component of the elastic curvature implies that spatial correlations are existing between the lattice rotations of the neighboring grains, because limiting values of the curvature from the left and from the right of the interface must be equal. Since it is not accommodated at the interface by surface-disclinations, a finite variation of the tangential component of the elastic curvature over the boundary area must be accommodated by the bulk disclination density $\boldsymbol{\theta}$ in a layer across the interface. However, the width of this layer is not implied by Eq. (48). It may be derived from dynamic calculations in the framework of the nonlocal elasto-plastic model (Fressengeas et al., 2011). Experimental evidence of such a length scale was provided in various materials after diverse strain paths, in the form of the scaling range for the power law dependence of the probability density of a certain grain misorientation vs the inter-granular distance (Beausir et al., 2009).

Similar continuity constraints can be obtained for the plastic curvature and plastic curvature rate. Indeed, since the total rotation $\vec{\boldsymbol{\omega}}$ is compatible, taking the line integral of Eq. (28) along the closed circuit C shows that:

$$\forall \mathbf{l} \in \mathcal{I}, \quad \int_C \boldsymbol{\kappa}_p \cdot \mathbf{dr} = -\int_C \boldsymbol{\kappa}_e \cdot \mathbf{dr} \tag{50}$$

Hence, it is straightforward to show from Eqs. (47), (48), (50) that tangential continuity of the plastic curvature is also required:

$$[\boldsymbol{\kappa}_p] \times \mathbf{n} = 0 \tag{51}$$

when surface-disclinations are absent. For small rotations, the derivation with respect to time of Eq. (51) involves only partial time derivatives. Thus, tangential continuity also holds for the plastic curvature rate:

$$[\dot{\boldsymbol{\kappa}}_p] \times \mathbf{n} = 0 \tag{52}$$

This rate condition may also be obtained by integrating the transport equation of disclinations (Fressengeas et al., 2011) over a "pillbox" set across an arbitrary area patch, in the limit when such a patch contracts onto a surface of discontinuity in the mate-

[2] The occurrence of a normal discontinuity of the elastic curvature tensor implies that the continuity required in Eq. (31) for the calculation of the disclination density tensor may not be satisfied for three of its components. Thus, discontinuity of the involved disclination densities may occur at the interface.

rial (see a derivation in (Acharya, 2007), in the context of dislocation transport). A derivation of Eq. (48) was also proposed recently in Upadhyay et al. (2011).

The conservation of the Burgers vectors content across the interface also gives rise to additional tangential continuity conditions. Indeed, using Eqs. (37), (39), the net Burgers vector $\mathbf{b}$ of the dislocations threading S is such that:

$$\forall \mathbf{l} \in \mathcal{I}, \quad \mathbf{b} = \int_C (\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}) \cdot \mathbf{dr} = \int_S (\boldsymbol{\alpha} - \boldsymbol{\theta} \times \mathbf{r}) \cdot \mathbf{t} dS \tag{53}$$

We assume that a continuous distribution of dislocations and disclinations is existing in the domains D^- and D^+ and also, provisionally, singular distributions $\boldsymbol{\alpha}(\mathcal{I})$ and $\boldsymbol{\theta}(\mathcal{I})$ along the interface $\mathcal{I}$. The term $\boldsymbol{\alpha}(\mathcal{I})$ represents surface-dislocations through a density of Burgers vectors per m in the direction $\mathbf{l}$. When the circuit C collapses onto point P in the limit, when H^+, h^- and L tend to zero, Eq. (53) becomes

$$\forall \mathbf{l} \in \mathcal{I}, \quad [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0] \cdot \mathbf{l} = (\boldsymbol{\alpha}(\mathcal{I}) - \boldsymbol{\theta}(\mathcal{I}) \times \mathbf{r}_0) \cdot \mathbf{t} \tag{54}$$

where $\mathbf{r}_0$ denotes the location of point P in the reference frame. In a way similar to Eqs. (46), (54) provides information on the density of surface-dislocations and surface-disclinations needed to accommodate a discontinuity in the elastic displacement in no width across the interface $\mathcal{I}$. Now, if the choice is made to describe the interface in a continuous manner, the surface-defect concept must be surrendered and Eq. (54) reduces to:

$$\forall \mathbf{l} \in \mathcal{I}, \quad [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0] \cdot \mathbf{l} = 0 \tag{55}$$

Eq. (55) describes the tangential continuity of the tensor $\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0$ at the interface. An equivalent form, similar to Eq. (48), is:

$$[\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0] \times \mathbf{n} = 0 \tag{56}$$

or in terms of the normal and tangential components $[\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_n$ and $[\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_t$:

$$\begin{aligned} [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_t &= [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0] - [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_n \\ &= [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0] - [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0] \cdot \mathbf{n} \otimes \mathbf{n} = 0 \end{aligned} \tag{57}$$

The normal component $[\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_n$ is left unconstrained by Eq. (56). Note that, since the total displacement and rotation of the body are compatible, the following integral is zero:

$$\forall \mathbf{l} \in \mathcal{I}, \quad \int_C (\boldsymbol{\epsilon} - \mathbf{grad}\, \vec{\omega} \times \mathbf{r}) \cdot \mathbf{dr} = 0 \tag{58}$$

Substracting Eq. (37) from Eq. (58), it is found that an alternative form of the Burgers vector is:

$$\mathbf{b} = -\int_C (\boldsymbol{\epsilon}_p - \boldsymbol{\kappa}_p \times \mathbf{r}) \cdot \mathbf{dr} \tag{59}$$

Then, following the above line of reasoning, an alternative relation to Eq. (56), using the plastic strain and curvature tensors is found:

$$[\boldsymbol{\epsilon}_p - \boldsymbol{\kappa}_p \times \mathbf{r}_0] \times \mathbf{n} = 0 \tag{60}$$

At small transformations, a derivation of Eq. (60) with respect to time involves only partial time derivatives, and the following result on the plastic strain rate and curvature rate is obtained:

$$[\dot{\boldsymbol{\epsilon}}_p - \dot{\kappa}_p \times \mathbf{r}_0] \times \mathbf{n} = 0 \tag{61}$$

If the reference point is chosen in the interface, such that $\mathbf{r}_0 = 0$, Eqs. (56), (60), (61) condense into simpler relations involving only the strain component of the incompatibility. We note that Eq. (60) was given in this simplified form by Hirth as early as 1972 (Hirth, 1972), on the basis of heuristic arguments. The curvature-induced incompatible plastic displacement $\boldsymbol{\kappa}_p \times \mathbf{r}_0$ and the related disclinations were not considered in this paper, where dislocation-based modeling of grain boundaries was discussed. In such context, tangential continuity should apply not only to the symmetric part of the plastic distortion rate tensor (the plastic strain rate tensor) but also to its skew-symmetric part (the plastic rotation rate tensor) (Acharya, 2007). Indeed, the tangential continuity conditions (56), (60), (61) differ from their counterparts in the theory of dislocation fields (Acharya, 2007; Beausir et al., 2009; Mach et al., 2010), because the elastic/plastic rotation and rotation rate tensors are undefined in a theory of crystal defects involving disclinations. Stated differently, the tangential continuity conditions (48), (51), (52) do not hold in the theory of dislocation fields because the elastic/plastic curvature and curvature rate tensors are assumed to be integrable in the latter.

5. Compatibility conditions at multiple junctions

Consider a multiple junction J where N interfaces, with respective discontinuities in the elastic curvature $[\boldsymbol{\kappa}_e]_i;\ i \in (1, N)$, connect along a single line. In practice, mostly triple-junctions ($N = 3$) are observed when the interfaces represent grain boundaries. If the choice of continuous modeling is made, closure requires that the sum of all discontinuities vanish at the multiple junction:

$$\sum_{i=1}^{N} [\boldsymbol{\kappa}_e]_i = 0 \tag{62}$$

$$\sum_{i=1}^{N} [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_i = 0 \tag{63}$$

Indeed, the same grain is used to start and finish a closed circuit about a multiple junction. Summing the relations (49) for all interfaces, and using Eq. (62), it is seen that the normal discontinuities in the elastic curvature need to satisfy a Kirchhoff-like compatibility condition at the multiple junction:

$$\sum_{i=1}^{N} [\boldsymbol{\kappa}_e]_i \cdot \mathbf{n}_i \otimes \mathbf{n}_i = 0 \tag{64}$$

Similarly, for a multiple junction located at $\mathbf{r}_0$, it can be shown from Eqs. (57), (63) that the normal discontinuities $[\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_n$ must satisfy the compatibility condition:

$$\sum_{i=1}^{N} [\boldsymbol{\epsilon}_e - \boldsymbol{\kappa}_e \times \mathbf{r}_0]_i \cdot \mathbf{n}_i \otimes \mathbf{n}_i = 0 \tag{65}$$

Additional compatibility conditions are obtained for the normal discontinuities in the plastic curvature and curvature rate:

$$\sum_{i=1}^{N} [\boldsymbol{\epsilon}_p - \boldsymbol{\kappa}_p \times \mathbf{r}_0]_i \cdot \mathbf{n}_i \otimes \mathbf{n}_i = 0 \tag{66}$$

$$\sum_{i=1}^{N} [\dot{\boldsymbol{\epsilon}}_p - \dot{\boldsymbol{\kappa}}_p \times \mathbf{r}_0]_i \cdot \mathbf{n}_i \otimes \mathbf{n}_i = 0 \tag{67}$$

6. Tilt boundaries and two-dimensional triple junctions

To illustrate the above results, let us consider a distribution of pure wedge disclinations and edge dislocations, as exemplified in (Fressengeas et al., 2011). In an orthonormal reference frame $(\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3})$, let the disclination tensor be: $\boldsymbol{\theta} = \theta_{33} \mathbf{e_3} \otimes \mathbf{e_3}$, all components other than θ_{33} being zero. Hence, the Frank vector of the wedge disclination distribution is $\boldsymbol{\Omega} = \theta_{33} \mathbf{e_3}$ per unit surface, while its line vector is $\mathbf{e_3}$. In this simple setting, the continuity condition (33) implies: $\theta_{33,3} = 0$. Thus, the wedge disclination density θ_{33} depends only on the coordinates $(x_1, x_2) : \theta_{33} = \theta_{33}(x_1, x_2)$. In component form, the rotational incompatibility Equation (31) reads: $\theta_{ij} = -e_{jkl}\kappa^p_{il,k} = e_{jkl}\kappa^e_{il,k}$. In the present case, it reduces to:

$$\theta_{33} = \kappa^p_{31,2} - \kappa^p_{32,1} = \kappa^e_{32,1} - \kappa^e_{31,2} \quad (68)$$

Hence the only relevant elastic and plastic curvatures are: $(\kappa^e_{31}, \kappa^e_{32})$ and $(\kappa^p_{31}, \kappa^p_{32})$. A plane dislocation distribution involving the edge densities α_{13} and $\alpha_{23} : \alpha_{13} = \alpha_{13}(x_1, x_2),\ \alpha_{23} = \alpha_{23}(x_1, x_2)$ is consistent with this disclination distribution, in the sense that it allows satisfying the equilibrium and continuity equations (Fressengeas et al., 2011). If the other dislocation densities are absent at initial time, they are also dynamically consistent, meaning that the dislocation and disclination transport equations can be consistently satisfied. Further, transport of these edge dislocations in the plane $(\mathbf{e_1}, \mathbf{e_2})$ induces a plane plastic strain state $(\epsilon^p_{11}, \epsilon^p_{12}, \epsilon^p_{22})$, with the strain rates:

$$\dot\epsilon^p_{11} = -\alpha_{13}V^\alpha_2 \quad (69)$$

$$\dot\epsilon^p_{12} = \dot\epsilon^p_{21} = \frac{1}{2}(\alpha_{13}V^\alpha_1 - \alpha_{23}V^\alpha_2) \quad (70)$$

$$\dot\epsilon^p_{22} = +\alpha_{23}V^\alpha_1 \quad (71)$$

The relations (69), (71), where the terms $V^\alpha_i\ (i = 1, 2)$ denote the components of the dislocations velocity, indicate that non-glide motion of the edge dislocations $(\alpha_{13}, \alpha_{23})$, e.g. climb, is involved in the extension rates $(\dot\epsilon^p_{11}, \dot\epsilon^p_{22})$, whereas glide is responsible for $\dot\epsilon^p_{12}$ in Eq. (70) (Fressengeas et al., 2011).

Assume now that an interface $\mathcal{I}$ is existing between the crystals (D^-, D^+), with normal $\mathbf{n} = \mathbf{e_2}$ oriented from D^- toward D^+. Provisionally, let us also allow the possible existence of surface-dislocation and surface-disclination distributions $(\boldsymbol{\alpha}(\mathcal{I}), \boldsymbol{\theta}(\mathcal{I}))$ in the interface. Then, specializing Eq. (46), any tangential discontinuity of the elastic curvature along the interface: $[\kappa^e_{31}]$ is found to be accommodated by a wedge surface-dislocation density $\theta_{33}(\mathcal{I})$:

$$[\kappa^e_{31}] = \theta_{33}(\mathcal{I}) \quad (72)$$

However, if continuous modeling of the boundary is attempted and surface-disclinations discarded, this relation transforms into the the tangential continuity condition:

$$[\kappa^e_{31}] = 0 \quad (73)$$

while, according to Eq. (48), a normal discontinuity $[\kappa^e_{32}]$ may exist:

$$[\kappa^e_{32}] = [\psi] \quad (74)$$

where $[\psi]$ sets the disorientation of the crystals (D^-, D^+) across the interface. Hence, the latter appears to be representing a tilt boundary. The discontinuity (74) implies that the continuity demanded in writing Eq. (68) does not exist at the interface. Thus, discontinuity of the disclination density θ_{33} may occur at the interface. In the presence of disclinations, Eq. (68) allows describing how the disorientation $[\psi]$ continuously evolves along the interface.

If the reference point is chosen in the interface, such that $\mathbf{r_0} = \mathbf{0}$, specializing Eq. (54) shows that any tangential discontinuity of the elastic strain across the interface is accommodated by edge surface-dislocations $\alpha_{13}(\mathcal{I})$ and $\alpha_{23}(\mathcal{I})$:

$$[\epsilon^e_{11}] = -\alpha_{13}(\mathcal{I}) \quad (75)$$

$$[\epsilon^e_{21}] = -\alpha_{23}(\mathcal{I}) \quad (76)$$

However, if continuous modeling prevails, Eqs. (75), (76) reduce to:

$$[\epsilon^e_{11}] = 0 \quad (77)$$
$$[\epsilon^e_{21}] = 0 \quad (78)$$

Analogous relations are obtained from Eq. (61) for the plastic strain rates:

$$[\dot\epsilon^p_{11}] = 0 \quad (79)$$

$$[\dot\epsilon^p_{21}] = 0 \quad (80)$$

These relations indicate that the plastic shear strain rate and extension rate along the interface must be continuous at the interface. According to Eq. (69), preventing the non-glide motion of α_{13} edges across the interface is sufficient to fulfill Eq. (79). Possible occurrence of a normal discontinuity of the plastic strain rate tensor is written as:

$$[\dot\epsilon^p_{22}] = [\dot\chi] \quad (81)$$

where $[\dot\chi]$ may be non-zero. Together with Eq. (71), this relation implies that discontinuity of the non-glide motion of α_{23} edges along the interface, e.g. by climb or atom shuffling, is consistent with the continuity conditions on the plastic strain rate.

Let us now consider a two-dimensional triple junction built from the intersection of tilt boundaries where the dihedral angles and lattice orientation angles with respect to the $\mathbf{e_1}$ axis are denoted with β_i and $\phi_i\ (i \in \{1, 3\})$, respectively (see Fig. 2). The disorientation between grain i and grain j and the orientation angle of their interface $\mathcal{I}_{ij}$ with respect to the $\mathbf{e}_1$ axis are respectively denoted with $[\psi_{ij}]$ and $\beta_{ij}\ (\forall (i,j) \in \{1, 3\})$, while the angle between the lattice orientation of grain i and the interface $\mathcal{I}_{ij}$ is taken as $r_{ij}[\psi_{ij}]$, with $0 \leqslant r_{ij} \leqslant 1$. It is seen in Fig. 2 that the orientation angles of the boundaries are:

$$\beta_{12} = r_{12}[\psi_{12}] + \phi_1 \quad (82)$$
$$\beta_{23} = r_{23}[\psi_{23}] + [\psi_{12}] + \phi_1 \quad (83)$$
$$\beta_{31} = r_{31}[\psi_{31}] + [\psi_{23}] + [\psi_{12}] + \phi_1 \quad (84)$$

while the dihedral angles are:

$$\beta_1 = (1 - r_{31})[\psi_{31}] + r_{12}[\psi_{12}] = 2\pi - (\beta_{31} - \beta_{12}) \quad (85)$$
$$\beta_2 = (1 - r_{12})[\psi_{12}] + r_{23}[\psi_{23}] = \beta_{23} - \beta_{12} \quad (86)$$
$$\beta_3 = (1 - r_{23})[\psi_{23}] + r_{31}[\psi_{31}] = \beta_{31} - \beta_{23} \quad (87)$$

In addition, Fig. 2 shows that:

$$\sum_{ij=12,23,31} [\psi_{ij}] = 2\pi \quad (88)$$

Eq. (88) reflects the closure relation: $\mathbf{R}_{31} \cdot \mathbf{R}_{23} \cdot \mathbf{R}_{12} = \mathbf{I}$, where $\mathbf{I}$ denotes the identity matrix, between the rotation matrices $\mathbf{R}_{ij}$ transforming grain i into grain j:

$$\mathbf{R}_{ij} = \begin{pmatrix} cos[\psi_{ij}] & -sin[\psi_{ij}] & 0 \\ sin[\psi_{ij}] & cos[\psi_{ij}] & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (89)$$

The analysis shown above in Eqs. (72)–(74) for the generic interface $\mathcal{I}$ is now reproduced in a local orthonormal frame $(\mathbf{u}_1, \mathbf{u}_2, \mathbf{e}_3)$ for each of the three interfaces $\mathcal{I}_{ij}$, with $(\mathbf{u}_1, \mathbf{e}_3)$ as the plane of the interface and $\mathbf{n} = -\mathbf{u}_2$ as its normal directed from grain i to grain j. Written in components of the elastic curvature tensor in the local frame of the interface $\mathcal{I}_{ij}$, the results corresponding to Eqs. (72), (74) are:

$$[\kappa^e_{31}]_{ij} = \theta_{33}(\mathcal{I}_{ij}) \quad (90)$$
$$[\kappa^e_{32}]_{ij} = -[\psi_{ij}] \quad (91)$$

all the other components of the matrices $[\kappa_e]$ being zero. Rotating these matrices to project Eq. (62) on the common reference frame $(\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3})$, it is found that:

$$\sum_{ij=12,23,31} [\psi_{ij}]sin\beta_{ij} + \theta_{33}(\mathcal{I}_{ij})cos\beta_{ij} = 0 \quad (92)$$

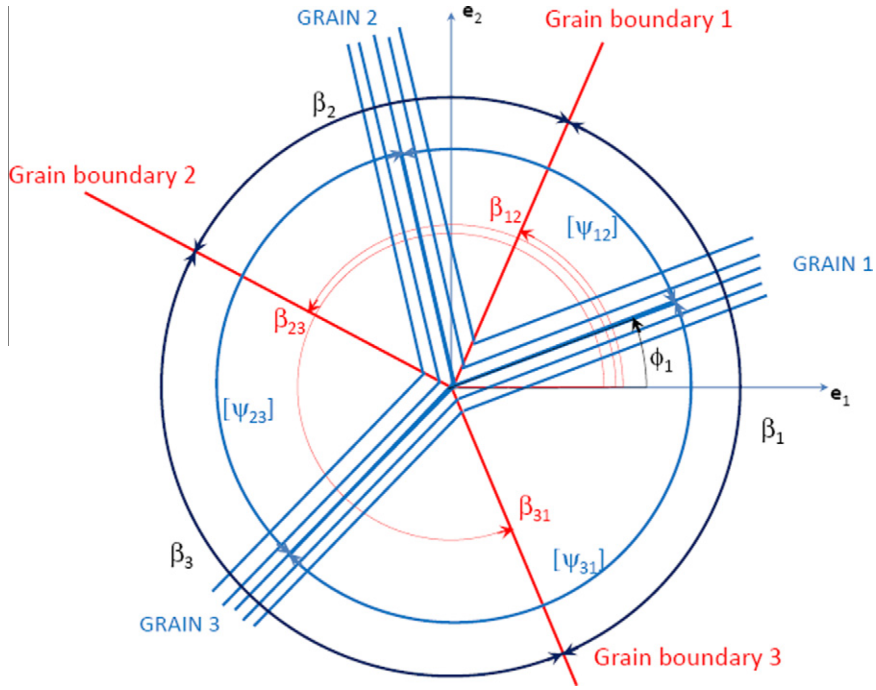

Fig. 2. Schematic of the triple junction geometry.

$$\sum_{ij=12,23,31} -[\psi_{ij}]cos\beta_{ij} + \theta_{33}(\mathcal{I}_{ij})sin\beta_{ij} = 0 \tag{93}$$

With Eqs. (88), (92), (93) set a system of algebraic linear equations for the three unknowns $[\psi_{ij}]$. As a first step in the solution of this system, assume tangential continuity of the elastic curvature at all interfaces: $\forall ij,\ \theta_{33}(\mathcal{I}_{ij}) = 0$, as required in a continuous model. With a non-zero determinant $D = sin(\beta_{23} - \beta_{31}) + sin(\beta_{31} - \beta_{12}) + sin(\beta_{12} - \beta_{23}) = -(sin\beta_1 + sin\beta_2 + sin\beta_3)$, the solutions are such that:

$$\frac{[\psi_{12}]}{sin\beta_3} = \frac{[\psi_{23}]}{sin\beta_1} = \frac{[\psi_{31}]}{sin\beta_2} = \frac{2\pi}{sin\beta_1 + sin\beta_2 + sin\beta_3} \tag{94}$$

Eq. (94) is a sine law, formally similar to the Herring equation between the interfacial free energies and dihedral angles (Herring et al., 1951). However, it is not a force balance equation. Its meaning is that triple junctions with dihedral angles $\beta_i,\ i \in \{1,2,3\}$ and disorientations $[\psi_{ij}]$ fulfill rotational compatibility. In particular, when all dihedral angles are $\beta_i = 2\pi/3,\ \forall i \in \{1,2,3\}$, Eq. (94) leads to: $\forall ij,\ [\psi_{ij}] = 2\pi/3$. This case corresponds to a compatible triple junction with three-fold symmetry. In the context of singular modeling, the algebraic system of Eqs. (88), (92),(93) may be used to obtain information on the surface-disclinations needed to accommodate arbitrary disorientations $[\psi_{ij}]$ in a triple junction with dihedral angles β_i. The disorientations are, in the presence of surface-disclinations at the interfaces:

$$[\psi_{12}] = \frac{2\pi sin\beta_3 + \theta_{33}(\mathcal{I}_{12})(cos\beta_2 - cos\beta_1) + (\theta_{33}(\mathcal{I}_{23}) - \theta_{33}(\mathcal{I}_{31}))(1 - cos\beta_3)}{sin\beta_1 + sin\beta_2 + sin\beta_3} \tag{95}$$

$$[\psi_{23}] = \frac{2\pi sin\beta_1 + \theta_{33}(\mathcal{I}_{23})(cos\beta_3 - cos\beta_2) + (\theta_{33}(\mathcal{I}_{31}) - \theta_{33}(\mathcal{I}_{12}))(1 - cos\beta_1)}{sin\beta_1 + sin\beta_2 + sin\beta_3} \tag{96}$$

$$[\psi_{31}] = \frac{2\pi sin\beta_2 + \theta_{33}(\mathcal{I}_{31})(cos\beta_1 - cos\beta_3) + (\theta_{33}(\mathcal{I}_{12}) - \theta_{33}(\mathcal{I}_{23}))(1 - cos\beta_2)}{sin\beta_1 + sin\beta_2 + sin\beta_3} \tag{97}$$

However, inverting these relations for the surface-disclinations is not possible, because the involved determinant Δ:

$$\begin{aligned}\Delta = &(cos\beta_3 - cos\beta_2)(cos\beta_1 - cos\beta_3)(cos\beta_2 - cos\beta_1)\\ &+ (1 - cos\beta_1)(1 - cos\beta_3)(cos\beta_1 - cos\beta_3)\\ &+ (1 - cos\beta_2)(1 - cos\beta_3)(cos\beta_3 - cos\beta_2)\\ &+ (1 - cos\beta_1)(1 - cos\beta_2)(cos\beta_2 - cos\beta_1)\end{aligned} \tag{98}$$

is zero. As an example, consider arbitrary variations $[\delta\psi_{ij}]$ from the disorientations $[\psi_{ij}] = 2\pi/3$ obtained in the three-fold symmetric triple junction. Then, Eqs. (95)–(97) become:

$$\sqrt{3}[\delta\psi_{12}] = \theta_{33}(\mathcal{I}_{23}) - \theta_{33}(\mathcal{I}_{31}) \tag{99}$$

$$\sqrt{3}[\delta\psi_{23}] = \theta_{33}(\mathcal{I}_{31}) - \theta_{33}(\mathcal{I}_{12}) \tag{100}$$

$$\sqrt{3}[\delta\psi_{31}] = \theta_{33}(\mathcal{I}_{12}) - \theta_{33}(\mathcal{I}_{23}) \tag{101}$$

Clearly, only differences in the surface-disclination densities are available from Eqs. (99)–(101). Hence, from singular modeling analysis, any arbitrary variation from the disorientations in a compatible triple junction can be accommodated by surface-disclinations, but the densities of the latter are known up to a constant. In continuous modeling, departures from the compatible disorientations are accommodated in a finite-width layer across the interface by bulk disclination densities.

We now contemplate fulfilling the compatibility condition (67) on the normal discontinuities of the plastic strain rates at the triple junction. In the local frame of interface $\mathcal{I}_{ij}$, the relations reflecting tangential continuity and normal discontinuity of the plastic strain rate tensor, and corresponding to Eqs. (79)–(81) are:

$$[\dot{\epsilon}^p_{11}]_{ij} = 0 \tag{102}$$

$$[\dot{\epsilon}^p_{21}]_{ij} = 0 \tag{103}$$

$$[\dot{\epsilon}^p_{22}]_{ij} = -[\dot{\chi}]_{ij} \tag{104}$$

where $[\dot{\chi}]_{ij}$ may be non zero, the other components of the matrices $[\dot{\boldsymbol{\epsilon}}^p]_{ij}$ being zero in the local reference frame. Rotating these matrices to project Eq. (67) in the common reference frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, it is found that:

$$\sum_{ij=12,23,31} [\dot{\epsilon}^p_{22}]_{ij} sin^2\beta_{ij} = 0 \tag{105}$$

$$\sum_{ij=12,23,31} [\dot{\epsilon}^p_{22}]_{ij} sin\beta_{ij} cos\beta_{ij} = 0 \tag{106}$$

$$\sum_{ij=12,23,31} [\dot{\epsilon}^p_{22}]_{ij} cos^2\beta_{ij} = 0 \tag{107}$$

Choosing for convenience $\beta_{12} = 0$, without loss of generality, it is found that the determinant D of this homogeneous set of algebraic linear equations, where the unknowns are the three extension rate discontinuities $[\dot{\epsilon}^p_{22}]_{ij}, ij = 12, 23, 31$, is $D = sin\beta_1 sin\beta_2 sin\beta_3$. Since D is usually non-zero, the unique solution to Eqs. (105)–(107) is: $[\dot{\epsilon}^p_{22}]_{ij} = 0,\ ij = 12, 23, 31$. Therefore normal continuity of the plastic strain rate tensor is generally required at such triple junctions, in addition to tangential continuity. In connection with Eq. (81), the interpretation of this result in terms of dislocation mobility is that non-glide motion along the interfaces is generally not kinematically allowed at compatible triple junctions. The exception to this rule is met when one of the dihedral angles is equal to π, say $\beta_2 = \pi$. Then a non-zero solution to Eqs. (105)–(107) is existing: $[\dot{\epsilon}^p_{22}]_{31} = 0,\ [\dot{\epsilon}^p_{22}]_{12} = -[\dot{\epsilon}^p_{22}]_{23} \neq 0$, which indicates that non-glide motion of dislocations along the straight interface $(\mathcal{I}_{12}, \mathcal{I}_{23})$ is still possible at the triple junction (see Fig.2)

7. Conclusion

In the present paper, the continuous vs discontinuous character of the elastic/plastic curvature & curvature rate, and strain & strain rate tensors is examined at surfaces of discontinuity, typically grain boundaries in polycrystals. Tangential continuity of these tensors is derived from the conservation of the Burgers and Frank vectors over patches bridging a smooth interface, in the limit where such patches collapse onto the interface, whereas normal discontinuity is allowed. This kinematic constraint implies spatial correlation between neighbor grains on either sides of the interface and confers nonlocal character to the description of the interface, because limiting values of the tangential components from the left of the interface must equal their counterparts from the right. Using the tangential continuity condition also implies that grain boundaries are viewed as having a finite thickness. However, this condition stops short of providing a characteristic thickness, or a length scale for the extent of the spatial correlations in neighboring grains. Such a characteristic length scale may be obtained from experiments, by analyzing the spatial correlations in the misorientations between neighbor grains (Beausir et al., 2009), or from the dynamics of dislocation and disclination densities in a complete field theory (Fressengeas et al., 2011). In the numerical implementation of this theory in polycrystals, using for example the finite element method, the tangential continuity of the plastic strain rate and curvature rate tensors at grain boundaries may be seen as a penalty condition for the dynamics of the field variables. By constraining the plastic strain and curvature rates along interfaces, tangential continuity does have significant consequences on their spatial distribution and development in time. Earlier work in the (more restricted) framework of the theory of dislocation fields showed indeed that, in a rigid viscoplastic setting for the simulation of rolling textures of f.c.c. materials, similar constraints on the plastic distortion rate result in an overall texture weaker than in local models and a β fiber that is more consistent with experimental observations (Mach et al., 2010). Similarly in metal matrix composites, a Bauschinger effect and a particle size effect on particle-strengthening were demonstrated to originate solely in the tangential continuity of the plastic distortion rates at particle–matrix interfaces (Richeton et al., 2011). By incorporating disclinations in the analysis and introducing separately constraints on the plastic curvature rates and plastic strain rates, the present tangential continuity conditions address more specifically the description of grain-boundary mediated plasticity in nanocrystalline materials, through mechanisms such as dislocation emission and absorption or grain rotations. Grain boundary migration will be treated in future work by considering interfaces that can move with respect to the material.

References

Acharya, A., 2007. Jump condition for GND evolution: a connection between grain growth and slip transmission at grain boundaries. Phil. Mag. 87, 1349.
Acharya, A., Fressengeas, C., 2012. Coupled phase transformations and plasticity as a field theory of deformation incompatibility. Int. J. Fract. 174, 87–94.
Acharya, A., Roy, A., 2006. Size effects and idealized dislocation microstructure at small scales: predictions of a phenomenological model of mesoscopic field dislocation mechanics: part I. J. Mech. Phys. Solids 54, 1687–1710.
Beausir, B., Fressengeas, C., Gurao, N., Toth, L.S., Suwas, S., 2009. Spatial correlation in grain misorientation distribution. Acta Mater. 57, 5382.
Bilby, B.A. 1995. Types of dislocation source.In: Bristol Conference Report on Defects in Crystalline Solids, The Physical Society, London, pp. 124.
Cahn, J.W., Mishin, Y., Suzuki, A., 2006. Coupling grain boundary motion to shear deformation. Acta Mater. 54, 4953–4975.
de Wit, R., 1970. Linear theory of static disclinations. In: Simmons, J.A., de Wit, R., Bullough, R. (Eds.), Fundamental Aspects of Dislocation Theory. NBS Spec. Publ. 317 (1), 651–680.
de Wit, R., 1973. Theory of disclinations: IV. Straight disclinations. Journal of Research of the National Bureau of Standards – A. Physics and Chemistry 77A, 607–658.
Frank, F.C. 1950. The resultant content of dislocations in an arbitrary intercrystalline boundary. In: Symposium on The Plastic Deformation of Crystalline Solids, Mellon Institute, Pittsburgh, (NAVEXOS-P-834), pp. 150.
Fressengeas, C., Taupin, V., Capolungo, L., 2011. An elasto-plastic theory of dislocation and disclination fields. Int. J. Solids Struct. 48, 3499.
Gertsman, V. Yu., Nazarov, A.A., Romanov, A.E., Valiev, R.Z., Vladimirov, V.I., 1989. Disclination-structural unit model of grain boundaries. Phil. Mag. A 59, 1113.
Hadamard, J., 1903. Leçons sur la propagation des ondes et les équations de l'hydrodynamique. Herman, Paris.
Herring, C., 1951. Surface Tension as a Motivation for Sintering. The Physics of Powder Metallurgy. McGraw-Hill Book Co., New York, pp. 143–179.
Hirth, J.P., 1972. The influence of grain boundaries on mechanical properties. Met. Trans. 3, 3047–3067.
Huang, W., Mura, T., 1970. Elastic fields and energies of a circular edge disclination and a straight screw disclination. J. Appl. Phys. 41, 5175.
Li, J.C.M., 1972. Disclination model of high angle grain boundaries. Surf. Sci. 31, 12.
Mach, J., Beaudoin, A.J., Acharya, A., 2010. Continuity in the plastic strain rate and its influence on texture evolution. J. Mech. Phys. Solids 58, 105.
Nye, J.F., 1953. Some geometrical relations in dislocated crystals. Acta Metall. 1, 153.
Richeton, T., Wang, G.F., Fressengeas, C., 2011. Continuity constraints at interfaces and their consequences on the work hardening of metal-matrix composites. J. Mech. Phys. Solids 59, 2023.
Romanov, A.E., Kolesnikova, A.L., 2009. Application of disclination concept to solid structures. Prog. Mat. Sci. 54, 740.
Shih, K.K., Li, J.C.M., 1975. Energy of grain boundaries between cusp misorientations. Surf. Sci. 50, 109.
Sutton, A.P., Vitek, V., 1983. On the structure of tilt grain boundaries in cubic metals. I. Symmetrical tilt boundaries. Phil. Trans. R. Soc. Lond. A309 (1).
Upadhyay, M., Capolungo, L., Taupin, V., Fressengeas, C., 2011. Grain boundary and Triple line energies in crystalline media: a disclination based approach. Int. J. Solids Struct. 48, 3176.