Jump condition for GND evolution as a constraint on slip transmission at grain boundaries

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Abstract

The jump condition at a possibly non-material interface for geometrically-necessary dislocation density in Field Dislocation Mechanics (FDM) and its averaged approximation, Phenomenological Mesoscopic FDM (PMFDM), is derived. In the context of grain boundaries, the condition implies a tensorial constraint on all five grain boundary parameters, slip transmission at the boundary, possible grain boundary motion, and dislocation nucleation/annihilation at the grain boundary. The jump condition is physically interpreted in special cases, and the importance of understanding dislocation motion at a boundary/interface as a flux across *curves*, and not surfaces, is emphasized.

1. Introduction

The implication of balance of Burgers vector content for *arbitrary* area patches in a finitely deforming body, in the limit when such patches contract to curves on a moving surface of discontinuity in the material, is the focus of this paper. The result expresses a certain equality of generalized slipping rates, evaluated on either side of the interface. The basic areal balance statements belong to the theories of FDM [1] and PMFDM [2]; for kinematics in bulk regions with smooth fields, FDM borrows the fundamentals deduced in [3].

For other theories of slip transmission conditions at grain boundaries that do not migrate with respect to the material, we refer to [4], [5], [6], and [7]. Experimental work relevant to GND in relation to grain boundaries are [8], [9], [10].

2. Notation

The symbol $\forall$ is shorthand for 'for all'; $\cup$ stands for 'union of'(sets of points), and $\Rightarrow$ for 'implies'. A superposed dot on a symbol represents a material time derivative. The statement $a := b$ is meant to indicate that a is being defined to be equal to b. We denote by $\boldsymbol{Ab}$ the action of the second-order tensor $\boldsymbol{A}$ on the vector $\boldsymbol{b}$, producing a vector. A $\cdot$ represents the inner product of two vectors. The symbol $\boldsymbol{AB}$ represents tensor multiplication of the second-order tensors $\boldsymbol{A}$ and $\boldsymbol{B}$.

All spatial derivative operators involve differentiation with respect to the current configuration. The *curl* operation on the current configuration and the cross product of a second-

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order tensor and a vector are defined in analogy with the vectorial case and the divergence (div) of a second-order tensor on the current configuration: for a second-order tensor $\boldsymbol{A}$, a vector $\boldsymbol{v}$, and a spatially constant vector field $\boldsymbol{c}$,

$$\begin{aligned}(\boldsymbol{A}\times\boldsymbol{v})^T\boldsymbol{c} &= \left(\boldsymbol{A}^T\boldsymbol{c}\right)\times\boldsymbol{v} \quad \forall\boldsymbol{c}\\ (curl\,\boldsymbol{A})^T\boldsymbol{c} &= curl\left(\boldsymbol{A}^T\boldsymbol{c}\right) \quad \forall\boldsymbol{c}.\end{aligned} \tag{1}$$

In rectangular Cartesian components,

$$\begin{aligned}(\boldsymbol{A}\times\boldsymbol{v})_{im} &= e_{mjk}A_{ij}v_k\\ (curl\,\boldsymbol{A})_{im} &= e_{mjk}A_{ik,j},\end{aligned} \tag{2}$$

where e_{mjk} is a component of the third-order alternating tensor and the spatial derivative, for the component representation, being with respect to rectangular Cartesian coordinates on the current configuration. For all manipulations with components, we shall always use such rectangular Cartesian coordinates and spatial fields will be thought of as depending upon these coordinates as well as t, as is customary in an Eulerian setting.

Given a (unit) normal direction $\boldsymbol{N}$ (vector) and a second order tensor $\boldsymbol{A}$, we refer to

$$\begin{aligned}\boldsymbol{A}_N &= \boldsymbol{A}\boldsymbol{N}\otimes\boldsymbol{N},\\ \boldsymbol{A}_{\tan} &= \boldsymbol{A}-\boldsymbol{A}_N\end{aligned} \tag{3}$$

as the *normal* and *tangential actions* of the tensor $\boldsymbol{A}$. For a vector $\boldsymbol{v}$ we also define

$$\boldsymbol{v}_{\tan} = \boldsymbol{v}-(\boldsymbol{v}\cdot\boldsymbol{N})\boldsymbol{N} \tag{4}$$

3. The Conservation Law for Burgers vector content

Two conservation laws of similar type are considered. The first corresponds to a theory that is assumed to be valid for the situation where *all* dislocations, described by a density function, are being resolved (i.e. a very fine scale of resolution). The corresponding statement for conservation of Burgers vector content is [1]

$$\frac{d}{dt}\int_a \boldsymbol{\alpha}\boldsymbol{n}\,da = -\int_c \boldsymbol{\alpha}\times\boldsymbol{V}\,d\boldsymbol{x} + \int_a \boldsymbol{s}\boldsymbol{n}\,da \quad \forall \ a\,, \tag{5}$$

where a is any arbitrary *material* surface patch with boundary c, i.e. a bounded surface consisting of the same material particles, and $\boldsymbol{n}$ is the unit normal field on a. In (5), $\boldsymbol{\alpha}$ is the two-point tensor of dislocation density, between the current configuration and the 'intermediate'/lattice configuration, $\boldsymbol{V}$ is the dislocation velocity vector *relative to the material*, and $\boldsymbol{s}$ is the nucleation rate tensor. In regions of the body where all fields are smooth, the local form of (5) is given by [1]

$$\begin{aligned}&(div\,\boldsymbol{v})\boldsymbol{\alpha}+\dot{\boldsymbol{\alpha}}-\boldsymbol{\alpha}\boldsymbol{L}^T =: \overset{\circ}{\boldsymbol{\alpha}} = -curl(\boldsymbol{\alpha}\times\boldsymbol{V})+\boldsymbol{s},\\ &\overset{\circ}{\boldsymbol{\alpha}} := (div\,\boldsymbol{v})\boldsymbol{\alpha}+\dot{\boldsymbol{\alpha}}-\boldsymbol{\alpha}\boldsymbol{L}^T,\end{aligned} \tag{6}$$

where $\boldsymbol{v}$ is the material velocity field and $\boldsymbol{L} := grad\,\boldsymbol{v}$ is the velocity gradient. It is shown in [1] that due to the fact that $\boldsymbol{\alpha}$ is a solenoidal field, i.e. divergence-free, the nucleation rate field $\boldsymbol{s}$ also has to be solenoidal and we can express $\boldsymbol{s}$ as a *curl* locally. Hence we choose to write $(6)_1$ as

$$\overset{\circ}{\boldsymbol{\alpha}} = -curl(\boldsymbol{\alpha}\times\boldsymbol{V})+curl\boldsymbol{\Omega}, \tag{7}$$

for some second-order tensor-valued nucleation rate potential field $\boldsymbol{\Omega}$, and (5) may alternatively be written as

$$\frac{d}{dt}\int_a \boldsymbol{\alpha}\boldsymbol{n}\,da = -\int_c \boldsymbol{\alpha}\times\boldsymbol{V}\,d\boldsymbol{x}+\int_a (curl\boldsymbol{\Omega})\boldsymbol{n}\,da \quad \forall \quad a. \tag{8}$$

Now

$$\left(\overset{\circ}{\boldsymbol{\alpha}}\right)_{ik} = \left\{(div\,\boldsymbol{v})\boldsymbol{\alpha}+\dot{\boldsymbol{\alpha}}-\boldsymbol{\alpha}\boldsymbol{L}^T\right\}_{ik} = \alpha_{ik,t}+\alpha_{ik,j}v_j+\alpha_{ik}v_{j,j}-\alpha_{ij}v_{k,j}, \tag{9}$$

and since $\alpha_{ij,j}=0$,

$$\left(\overset{\circ}{\boldsymbol{\alpha}}\right)_{ik} = \alpha_{ik,t}+\left(\alpha_{ik}v_j-\alpha_{ij}v_k\right)_{,j}. \tag{10}$$

If we define a second-order tensor $\boldsymbol{p}$ by the relation

$$e_{kjm}p_{im} := \alpha_{ik}v_j-\alpha_{ij}v_k, \tag{11}$$

it follows that

$$\begin{aligned}&p_{ir} = \frac{1}{2}e_{kjr}\left(\alpha_{ik}v_j-\alpha_{ij}v_k\right) = e_{rkj}\alpha_{ik}v_j,\\ &\Rightarrow \boldsymbol{p} = \boldsymbol{\alpha}\times\boldsymbol{v}.\end{aligned} \tag{12}$$

Hence (7) may be expressed as the following field equation in the Eulerian setting:

$$\frac{\partial\boldsymbol{\alpha}}{\partial t} = -curl\left\{\boldsymbol{\alpha}\times(\boldsymbol{V}+\boldsymbol{v})\right\}+curl\boldsymbol{\Omega}. \tag{13}$$

To get an idea of the type of equation that running space-time averages of the field $\boldsymbol{\alpha}$ might satisfy, we consider (13) to be defined in all of space and use the following averaging operator (cf. [2]): For a microscopic field f given as a function of space and time, we define the mesoscopic space-time averaged field $\bar{f}$ as follows:

$$\bar{f}(\boldsymbol{x},t) := \frac{1}{\int_{I(t)}\int_{\Omega(x)} w(\boldsymbol{x}-\boldsymbol{x}',t-t')\, d\boldsymbol{x}'dt'} \int_{\Im}\int_{E_3} w(\boldsymbol{x}-\boldsymbol{x}',t-t')\, f(x',t')\, d\boldsymbol{x}'dt', \qquad (14)$$

where E_3 is all of space and $\Im$ a sufficiently large interval of time. In the above, $\Omega(\boldsymbol{x})$ is a bounded region around the point $\boldsymbol{x}$ with linear dimension of the order of the spatial resolution of the macroscopic model we seek, and $I(t)$ is a bounded interval in $\Im$ containing t. The averaged field $\bar{f}$ is simply a weighted, space-time, running average of the microscopic field f. The weighting function w is non-dimensional, assumed to be smooth in the variables $\boldsymbol{x},\boldsymbol{x}',t,t'$ and, for fixed $\boldsymbol{x}$ and t, have support (i.e. to be non-zero) only in $\Omega(\boldsymbol{x})\times I(t)$ when viewed as a function of $(\boldsymbol{x}',t')$. Applying this operator to both sides of (13), and under the assumption that

$$\bar{\boldsymbol{v}} \approx \boldsymbol{v} \qquad (15)$$

implying that the fluctuations in the material velocity field are negligible (which may be justified in a setting where material-inertia forces are neglected), we obtain the equation (cf. [1])

$$\mathring{\bar{\boldsymbol{\alpha}}} = \frac{\partial\bar{\boldsymbol{\alpha}}}{\partial t} + curl(\bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{v}}) = -curl(\bar{\boldsymbol{\alpha}}\times\bar{\boldsymbol{V}} + \tilde{\boldsymbol{L}}^p) + curl\bar{\boldsymbol{\Omega}}, \qquad (16)$$

where

$$\tilde{\boldsymbol{L}}^p(\boldsymbol{x},t) := \overline{(\boldsymbol{\alpha}-\bar{\boldsymbol{\alpha}})\times\boldsymbol{V}}(\boldsymbol{x},t) = \overline{\boldsymbol{\alpha}\times\boldsymbol{V}}(\boldsymbol{x},t) - \bar{\boldsymbol{\alpha}}(\boldsymbol{x},t)\times\bar{\boldsymbol{V}}(\boldsymbol{x},t), \qquad (17)$$

and $\mathring{\bar{\boldsymbol{\alpha}}}$ is defined as in (7) for the tensor $\boldsymbol{\alpha}$. Physically, $\tilde{\boldsymbol{L}}^p$ is representative of a portion of the average slip strain rate produced by the 'microscopic' dislocation density; in particular, it can be non-vanishing even when $\bar{\boldsymbol{\alpha}} = \boldsymbol{0}$ and, as such, it is to be physically interpreted as the strain-rate produced by so-called 'statistically-stored dislocations' (SSD), as is also indicated by the extreme right-hand side of (17). The variable $\bar{V}$ has the obvious physical meaning of being a space-time average of the pointwise, microscopic dislocation velocity (relative to the material). It should be noted that only spatial gradients (in particular, the *curl*) of the SSD slipping rate affect the generation of GNDs, consistent with the physical interpretation of a dislocation being the boundary between differently slipped regions.

In a phenomenological approach to closure, the physical quantities $\bar{\boldsymbol{V}}$ and $\tilde{\boldsymbol{L}}^p$ have to be constitutively specified. Due to the physical interpretation of $\tilde{\boldsymbol{L}}^p$ as the slipping produced by SSDs within the averaging domain, it is natural to expect that it must depend weakly on $\bar{\boldsymbol{\alpha}}$, if at all; as it represents the total plastic shearing produced by spatially unresolved loops within the averaging volume, conventional plasticity representations of sums of simple shearings on individual slip systems driven by stress and resisted by strength would be appropriate as a first-order approximation. On the other hand, accepting (5) as a fundamental balance law along with the averaging operator (14) does not naturally allow for the definition of slip-system averaged GND densities and corresponding velocities. It should be noted, however, that the latter fact does not prevent slip system like behavior to be displayed, e.g. consider a fine scale α distribution of the same sign on a single slip system. Then, by definition $\bar{\alpha}$ would mimic the characteristics of the fine-scale distribution, as it should.

If we now imagine a body moving with a material velocity field $\bar{\boldsymbol{v}}$ and for regions within the body where all fields are smooth, (16) may alternatively be written as

$$\frac{d}{dt}\int_a \boldsymbol{\alpha n}\, da = -\int_c \left(\bar{\boldsymbol{\alpha}} \times \bar{\boldsymbol{V}} + \tilde{\boldsymbol{L}}^p\right) d\boldsymbol{x} + \int_a \left(curl \bar{\boldsymbol{\Omega}}\right) \boldsymbol{n}\, da \quad \forall \;\; a, \tag{18}$$

where a is any material surface patch in the region of smoothness.

We now *postulate* that, regardless of smoothness, (18) is the conservation law for conservation of Burgers vector content in the averaged theory.

Thus, in view of (8) and (18), and dropping overhead bars for convenience, we are faced with the task of deducing jump conditions at a surface of discontinuity in the body for an equation of the type

$$\frac{d}{dt}\int_a \boldsymbol{\alpha n}\, da = \int_c \boldsymbol{f}\, d\boldsymbol{x} + \int_a \left(curl \boldsymbol{\Omega}\right) \boldsymbol{n}\, da \quad \forall \;\; a \text{ (bounded by } c\text{)}, \tag{19}$$

where $\boldsymbol{f}$ is an appropriate second-order tensor field characterizing the flux of Burgers vector (per unit length, per unit time) across arbitrary curves defined by

$$\boldsymbol{f} = \begin{cases} -\left(\bar{\boldsymbol{\alpha}} \times \bar{\boldsymbol{V}} + \tilde{\boldsymbol{L}}^p\right) & \text{PMFDM} \\ -\boldsymbol{\alpha} \times \boldsymbol{V} & \text{FDM.} \end{cases} \tag{20}$$

In the following, we shall refer to $\boldsymbol{f} \times \boldsymbol{N}$ as the *flow* of $\boldsymbol{f}$ at a surface with unit normal field $\boldsymbol{N}$. The flow physically characterizes the flux of Burgers vector carried by dislocation lines (per unit length per unit time) across any curve on the surface described by $\boldsymbol{N}$, as is shown in Section 5. In addition, the flow needs to be specified at (parts of) the boundary of 3-d spatial domains on which (16) is solved.

4. The jump condition

The jump condition is derived using established methods of continuum mechanics (see, e.g., Sec. 192, [11]). To the author's knowledge, there are three different techniques by which the same jump condition may be derived. The first is the method employed in this paper, working directly with the 3-d conservation law in integral form. The second is to use a weak formulation of the governing differential equation on arbitrary 4-d domains, along with some assumptions about the geometric structure of space-time; we do not prefer this here, as the hypothesis of the weak statement being valid on arbitrary domains (possibly containing a surface of discontinuity) as well as the geometric assumptions appear to be extraneous. A possible third method involves conservation laws in space-time within the framework of world-invariant kinematics ([11], Secs. 152, 273, 277, 278), again requiring added geometric assumptions about the structure of 4-d Euclidean space-time.

With reference to Fig. 1, we consider a moving surface of discontinuity s with unit normal field $\boldsymbol{N}$, traversing through a pill box volume of *fixed material particles* deforming and moving with the material velocity field $\boldsymbol{v}$. The velocity field $\boldsymbol{u}$ of the surface of discontinuity is defined as

$$\boldsymbol{u} := u_N \boldsymbol{N}, \tag{21}$$

where u_N is the normal speed of the interface.

The material volume $V(t)$ is the union of two generally non-material volumes $V_1(t)$ and $V_2(t)$ separated by $s(t)$. This is because the interface moves relative to the material. By a non-material volume we mean a (generally time-varying) set of points in space that does not consist of the same material particles with the progress of time. Similarly, $a(t)$ is an arbitrarily oriented, materially deforming, area patch contained in $V(t)$, consisting of an identical set of material particles with the progress of time. The intersection of $a(t)$ and $s(t)$ is denoted by the curve $c(t)$ that forms the boundary of the non-material area patches $a_1(t)$ and $a_2(t)$, for all instants in at least some interval of time. At any instant in this interval, the union of the non-material area patches a_1 and a_2 is the material area patch a.

Let $\boldsymbol{n}$ be the unit normal field on a. Then

$$\frac{d}{dt}\int_{a(t)} \alpha \boldsymbol{n}\, da = \frac{d}{dt}\left[\int_{a_1(t)} \alpha \boldsymbol{n}\, da + \int_{a_2(t)} \alpha \boldsymbol{n}\, da\right]. \tag{22}$$

We now consider the time-varying, non-material volumes $V_1(t)$ and $V_2(t)$ to be configurations at the time t of fictitious motions of fixed (in time) reference volumes V_{R1} and V_{R2}. This implies that $a_1(t)\left(a_2(t)\right)$ maps to a fixed area patch $a_{R1}\left(a_{R2}\right)$ contained in $V_{R1}\left(V_{R2}\right)$. Also, for such motions, say $\boldsymbol{m}_1^*\left(\boldsymbol{m}_2^*\right)$ that maps $V_{R1}\left(V_{R2}\right)$ to $V_1\left(V_2\right)$, the velocity field of the points of $V_1(t)\left(V_2(t)\right)$ coincident with $s(t)$ is $\boldsymbol{u}$ and those coincident with the top (bottom) of the pill box is $\boldsymbol{v}(t)$. Let the velocity field corresponding to the motion $\boldsymbol{m}_1^*\left(\boldsymbol{m}_2^*\right)$ be denoted by $\boldsymbol{v}_1^*\left(\boldsymbol{v}_2^*\right)$. A term like

$$\frac{d}{dt}\int_{a_1(t)} \boldsymbol{\alpha}\boldsymbol{n}\, da \tag{23}$$

may now be evaluated by transforming the area integral to an integral over a_{R1}, pushing the time derivative inside the integral, performing the time derivative, and then transforming the resulting integral back to an integral over a_1 [1]; the result, for the 1 side, is

$$\frac{d}{dt}\int_{a_1(t)} \boldsymbol{\alpha}\boldsymbol{n}\, da = \int_{a_1(t)} \overset{\circ *1}{\boldsymbol{\alpha}}\, \boldsymbol{n}\, da \tag{24}$$

where

$$\overset{\circ *1}{\boldsymbol{\alpha}} := \frac{\partial \boldsymbol{\alpha}}{\partial t} + curl\left(\boldsymbol{\alpha} \times \boldsymbol{v}_1^*\right). \tag{25}$$

We now define the limits of fields approaching s from the top of the pill box with a subscript 1 and limits of fields approaching s from the bottom with a subscript 2. Equation (19) may be expressed as

$$\begin{aligned}\int_{a_1} \frac{\partial \boldsymbol{\alpha}}{\partial t}\boldsymbol{n}\, da + \int_{a_2} \frac{\partial \boldsymbol{\alpha}}{\partial t}\boldsymbol{n}\, da + \int_{a_1} curl\left(\boldsymbol{\alpha} \times \boldsymbol{v}_1^*\right)\boldsymbol{n}\, da + \int_{a_2} curl\left(\boldsymbol{\alpha} \times \boldsymbol{v}_2^*\right)\boldsymbol{n}\, da \\ = \int_{\partial a} \boldsymbol{f}\, d\boldsymbol{x} + \int_{a_1} \left(curl\boldsymbol{\Omega}\right)\boldsymbol{n}\, da + \int_{a_2} \left(curl\boldsymbol{\Omega}\right)\boldsymbol{n}\, da + \int_{c} \left(\boldsymbol{\Omega}_2 - \boldsymbol{\Omega}_1\right) d\boldsymbol{x},\end{aligned} \tag{26}$$

where ∂a is the boundary of the area patch a, and we have assumed that the field $\boldsymbol{\Omega}$ is the possibly discontinuous limit of a sequence of differentiable functions, with discontinuity concentrated on s. We also have

$$\begin{aligned}\int_{a_1} curl\left(\boldsymbol{\alpha} \times \boldsymbol{v}_1^*\right)\boldsymbol{n}\, da &= \int_{c_1} \left(\boldsymbol{\alpha} \times \boldsymbol{v}\right) d\boldsymbol{x} + \int_{l_1} \left(\boldsymbol{\alpha} \times \boldsymbol{v}_1^*\right) d\boldsymbol{x} + \int_{c} \left(\boldsymbol{\alpha}_1 \times \boldsymbol{u}\right) d\boldsymbol{x} + \int_{r_1} \left(\boldsymbol{\alpha} \times \boldsymbol{v}_1^*\right) d\boldsymbol{x}, \\ \int_{a_2} curl\left(\boldsymbol{\alpha} \times \boldsymbol{v}_2^*\right)\boldsymbol{n}\, da &= \int_{c_2} \left(\boldsymbol{\alpha} \times \boldsymbol{v}\right) d\boldsymbol{x} + \int_{r_2} \left(\boldsymbol{\alpha} \times \boldsymbol{v}_2^*\right) d\boldsymbol{x} - \int_{c} \left(\boldsymbol{\alpha}_2 \times \boldsymbol{u}\right) d\boldsymbol{x} + \int_{l_2} \left(\boldsymbol{\alpha} \times \boldsymbol{v}_2^*\right) d\boldsymbol{x}.\end{aligned} \tag{27}$$

Applying (26) to progressively thinner pill boxes, we observe that in the limit of the pill box collapsing on to s and then shrinking the curve c to a point we obtain the relationship

$$\left\{[\![\boldsymbol{\alpha} \times \boldsymbol{v}]\!] - [\![\boldsymbol{\alpha} \times \boldsymbol{u}]\!] - [\![\boldsymbol{f}]\!] - [\![\boldsymbol{\Omega}]\!]\right\} d\boldsymbol{x} = \boldsymbol{0}, \tag{28}$$

where $[\![z]\!] := z_2 - z_1$, and since the area patch could have been oriented arbitrarily, (28) must hold for all tangent directions $d\boldsymbol{x}$ on the surface s. An alternative way of stating the same fact is

$$\left\{[\![\boldsymbol{\alpha} \times (\boldsymbol{v} - \boldsymbol{u})]\!] - [\![\boldsymbol{f}]\!] - [\![\boldsymbol{\Omega}]\!]\right\} \times \boldsymbol{N} = \boldsymbol{0}, \tag{29}$$

and we obtain

$$[\![\boldsymbol{\alpha}\left(u_N - \boldsymbol{v}\cdot\boldsymbol{N}\right)]\!] = [\![\boldsymbol{f}]\!] \times \boldsymbol{N} + [\![\boldsymbol{\Omega}]\!] \times \boldsymbol{N} - [\![\boldsymbol{\alpha}\boldsymbol{N} \otimes \left(\boldsymbol{v} - u_N\boldsymbol{N}\right)]\!]. \tag{30}$$

Hence, the *jump condition* for GND evolution is given by

$$[\![\boldsymbol{f}]\!]\times\boldsymbol{N}=[\![\boldsymbol{\alpha}_{\tan}\left(u_N-\boldsymbol{v}\cdot\boldsymbol{N}\right)]\!]+[\![\boldsymbol{\alpha}\boldsymbol{N}\otimes\boldsymbol{v}_{\tan}]\!]-[\![\boldsymbol{\Omega}]\!]\times\boldsymbol{N}\,. \tag{31}$$

It is interesting to note that the jump condition does not involve, and hence leaves unconstrained, the normal actions $[\![\boldsymbol{f}]\!]_N$, $[\![\boldsymbol{\Omega}]\!]_N$.

5. Some physical implications

For practical purposes, the jump condition (31) is to be interpreted as specifying the Burgers vector flow on one (arbitrarily chosen) side of the interface. The application of the condition admits (requires) constitutive equations for the relative interface velocity $u_N-\boldsymbol{v}\cdot\boldsymbol{N}$ and for dislocation nucleation/annihilation rate at the interface characterized by $[\![\boldsymbol{\Omega}]\!]$. We now consider some simple cases to gain physical insight.

Case 1: $u_N=0$, $\boldsymbol{v}=\boldsymbol{0}$, $[\![\boldsymbol{\Omega}]\!]=\boldsymbol{0}$, i.e. no interface or material motion and no dislocation nucleation at the interface. In this case the jump condition reduces to

$$[\![\boldsymbol{f}]\!]\times\boldsymbol{N}=\boldsymbol{0}\,. \tag{32}$$

It suffices to consider the PMFDM case as the FDM case is similar (and simpler). Let $\tilde{\boldsymbol{L}}^p$ be of the form [2]

$$\tilde{\boldsymbol{L}}^p=\sum_\kappa\dot{\gamma}^\kappa\boldsymbol{m}_0^\kappa\otimes\boldsymbol{n}_0^\kappa\boldsymbol{F}^{e-1}\,, \tag{33}$$

where $\boldsymbol{F}^e$ is the elastic distortion tensor, slip systems are indexed by κ with unstretched unit slip direction $\boldsymbol{m}_0^\kappa$ and unit slip plane normal $\boldsymbol{n}_0^\kappa$, and $\dot{\gamma}^\kappa$ is the scalar slipping-rate on the system κ. The slipping rates are constitutively specified, e.g. standard power-law relationships based on slip system resolved shear stress and strength. Thus, in the case where the interface is a grain boundary,

$$[\![-\bar{\boldsymbol{\alpha}}_{\tan}\left(\bar{\boldsymbol{V}}\cdot\boldsymbol{N}\right)]\!]+[\![\bar{\boldsymbol{\alpha}}\boldsymbol{N}\otimes\bar{\boldsymbol{V}}_{\tan}]\!]+\left[\!\!\left[\sum_\kappa\dot{\gamma}^\kappa\boldsymbol{m}_0^\kappa\otimes\boldsymbol{n}_0^\kappa\boldsymbol{F}^{e-1}\right]\!\!\right]\times\boldsymbol{N}=\boldsymbol{0}\,, \tag{34}$$

and the fact that the slip system vectors on both sides of the interface as well as the interface normal appear in the jump condition implies that all five grain boundary parameters affect slip transmission at the boundary along with the GND content and the GND velocity one either side of the boundary.

Clearly, if $[\![\boldsymbol{\Omega}]\!]\neq\boldsymbol{0}$, then dislocation nucleation would also affect the slip transmission. As a practical matter, say for computation, (34) would be utilized to set boundary conditions as

$$\boldsymbol{f}_2 \times \boldsymbol{N} = \left\{ -\bar{\boldsymbol{\alpha}}_{\tan}\left(\bar{\boldsymbol{V}} \cdot \boldsymbol{N}\right) + \bar{\boldsymbol{\alpha}}\boldsymbol{N} \otimes \bar{\boldsymbol{V}}_{\tan} + \sum_{\kappa} \dot{\gamma}^{\kappa} \boldsymbol{m}_0^{\kappa} \otimes \boldsymbol{n}_0^{\kappa} \boldsymbol{F}^{e-1} \times \boldsymbol{N} \right\}\Bigg|_{\boldsymbol{1}} . \tag{35}$$

Case 2: $\boldsymbol{v} = \boldsymbol{0}$, $[\![\boldsymbol{\Omega}]\!] = \boldsymbol{0}$, i.e. no material motion and no dislocation nucleation at the interface. Following similar arguments as in Case 1, the flow on the 2-side of the interface is given by

$$\boldsymbol{f}_2 \times \boldsymbol{N} = \left\{ -\bar{\boldsymbol{\alpha}}_{\tan}\left(\bar{\boldsymbol{V}} \cdot \boldsymbol{N}\right) + \bar{\boldsymbol{\alpha}}\boldsymbol{N} \otimes \bar{\boldsymbol{V}}_{\tan} + \sum_{\kappa} \dot{\gamma}^{\kappa} \boldsymbol{m}_0^{\kappa} \otimes \boldsymbol{n}_0^{\kappa} \boldsymbol{F}^{e-1} \times \boldsymbol{N} \right\}\Bigg|_{\boldsymbol{1}} + [\![\bar{\boldsymbol{\alpha}}_{\tan}]\!] u_N . \tag{36}$$

Assuming the moving surface of discontinuity to be a moving grain boundary, this suggests that the flow on one side of the grain boundary is equal to its value on the other side plus a flow arising due to the motion of the grain boundary relative to the material and the presence of a discontinuity in the tangential action of the dislocation density tensor across the interface. The jump in $\bar{\boldsymbol{\alpha}}_{\tan}$ may be visualized as a virtual dislocation density situated on the moving boundary; since there is no material motion, this virtual dislocation density travels across material curves instantaneously coincident with the boundary, and this corresponds to a flux.

Allowing for the presence of dislocation nucleation and non-vanishing material velocity, this case may relate to a polycrystalline material under extreme shock loading.

Case 3: FDM, $\boldsymbol{v} = \boldsymbol{0}$, $u_N > 0$, $\boldsymbol{\alpha}_1 = \boldsymbol{b} \otimes \boldsymbol{t}$, $\boldsymbol{N} \cdot \boldsymbol{t} = 0$, $\boldsymbol{\alpha}_2 = \boldsymbol{0}$, $\boldsymbol{V}_1 \cdot \boldsymbol{N} = u_N$, $[\![\boldsymbol{\Omega}]\!] = \boldsymbol{0}$. This case represents a straight dislocation on the 1 side with line direction parallel to the interface, moving with identical velocity to the interface (e.g. a grain boundary traversing the material with a dislocation at fixed distance form it following it with identical velocity). There is also no material deformation. We assume $\boldsymbol{N}$ points from the 1 to the 2 side, without loss of generality. In this case,

$$\boldsymbol{f}_2 \times \boldsymbol{N} + \left(\boldsymbol{\alpha}_1 \times \boldsymbol{V}_1\right) \times \boldsymbol{N} = -\boldsymbol{\alpha}_1 u_N \Rightarrow \boldsymbol{f}_2 \times \boldsymbol{N} = -\left(-\boldsymbol{\alpha}_1 u_N\right) - \boldsymbol{\alpha}_1 u_N = \boldsymbol{0} . \tag{37}$$

Recalling the physical meaning of $\boldsymbol{f}\, d\boldsymbol{x}$ as a flux of Burgers vector per unit time carried by dislocation lines across material curves, this result makes sense since the persistent value of $\boldsymbol{f}_2\, d\boldsymbol{x}$ obtained from (37) refers to the flux across *different* material curves (parallel to the interface) on the 2-side on which no dislocations exist. Even though the dislocation on the 1-side makes forward progress, it is only by the same amount as the interface so that the curves on the 2-side on which we probe $\boldsymbol{\alpha}_2$ and $\boldsymbol{f}_2$ maintain a fixed distance from the moving dislocation. Were $\boldsymbol{f}_2\, d\boldsymbol{x}$ to be the flux across a *fixed* material curve on the 2-side, then, of course, there would be a non-vanishing flux across such a curve once the dislocation from the 1-side arrived on it. Likewise, even though the physical picture following the interface is static, there is a non-zero flux across the moving non-material curve on which the dislocation resides on the 1-side, since the velocity of the material particles instantaneously coincident with this curve at all times is zero.

Case 4: $u_N = \boldsymbol{v} \cdot \boldsymbol{N} \Rightarrow \boldsymbol{v} \cdot \boldsymbol{N}$ is continuous; $[\![\boldsymbol{\Omega}]\!] = \boldsymbol{0}$; $[\![\boldsymbol{\alpha N}]\!] = \boldsymbol{0}$; $[\![\boldsymbol{v}_{\tan}]\!] \neq \boldsymbol{0}$. This is the case where the normal action of the dislocation density tensor is continuous across the interface and the material motion corresponds to a contact discontinuity at the interface (e.g. idealized grain boundary sliding). For simplicity, we also assume $\boldsymbol{\alpha}_1 = \boldsymbol{\alpha}_2 = \boldsymbol{b} \otimes \boldsymbol{N}$. In this case,

$$\boldsymbol{f}_2 \times \boldsymbol{N} = \boldsymbol{f}_1 \times \boldsymbol{N} + \boldsymbol{b} \otimes [\![\boldsymbol{v}_{\tan}]\!], \tag{38}$$

Assuming $\boldsymbol{b}$ to be parallel to the interface so that an edge dislocation runs perpendicular through the interface, the existence of a contact discontinuity implies the production of a screw density at the interface. This is reasonable if one assumes the relative lattice displacement across the interface is of the same type as the discontinuity in the material deformation.

Case 5: Finally, we end by considering the physical interpretation of the dislocation *flow* at a boundary/interface given by

$$(\boldsymbol{\alpha} \times \boldsymbol{V}) \times \boldsymbol{N}. \tag{39}$$

Here $\boldsymbol{V}$ is the dislocation velocity and $\boldsymbol{N}$ the unit outward normal to the body. Now, the flow may be decomposed as

$$(\boldsymbol{\alpha} \times \boldsymbol{V}) \times \boldsymbol{N} = -\boldsymbol{\alpha}_{\tan} (\boldsymbol{V} \cdot \boldsymbol{N}) + \boldsymbol{\alpha N} \otimes \boldsymbol{V}_{\tan}. \tag{40}$$

In the first instance, consider $\boldsymbol{\alpha}$ at the boundary to be of the form $\boldsymbol{\alpha} = \boldsymbol{b} \otimes \boldsymbol{t}$, with $\boldsymbol{t}$ parallel to the boundary and $\boldsymbol{V}$ parallel to $\boldsymbol{N}$ so that $\boldsymbol{\alpha} = \boldsymbol{\alpha}_{\tan}$, $\boldsymbol{\alpha}_N = \boldsymbol{0}$. Fig. 2 (a) shows that in this case (39) may be interpreted both as a flux into the body through the surface s, as well as a flux into the area a through the curve c.

Next consider $\boldsymbol{\alpha} = \boldsymbol{b} \otimes \boldsymbol{t}$, with $\boldsymbol{t}$ parallel to $\boldsymbol{N}$ and $\boldsymbol{V}$ parallel to the boundary, i.e. $\boldsymbol{V} \cdot \boldsymbol{N} = 0$, so that $\boldsymbol{\alpha} = \boldsymbol{\alpha}_N$, $\boldsymbol{\alpha}_{\tan} = \boldsymbol{0}$. In this case, the flow cannot be considered as a flux into/out of the body through s; however, it is a flux through the boundary curve c into some surface patch in the body like a, as shown in Fig. 2(b), and hence it is not surprising that it appears in the jump condition.

6. Acknowledgment

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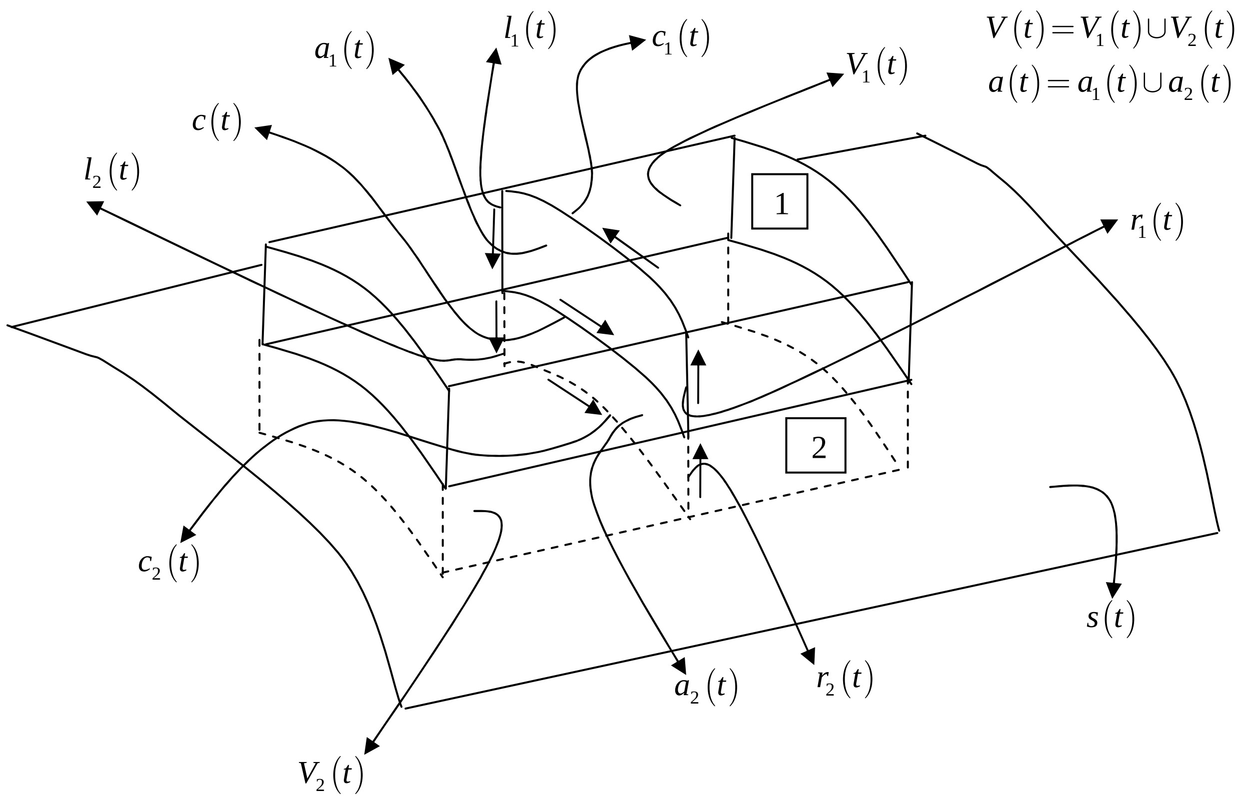

Fig. 1. Migrating surface of discontinuity in a deforming material pill box at a fixed instant of time.

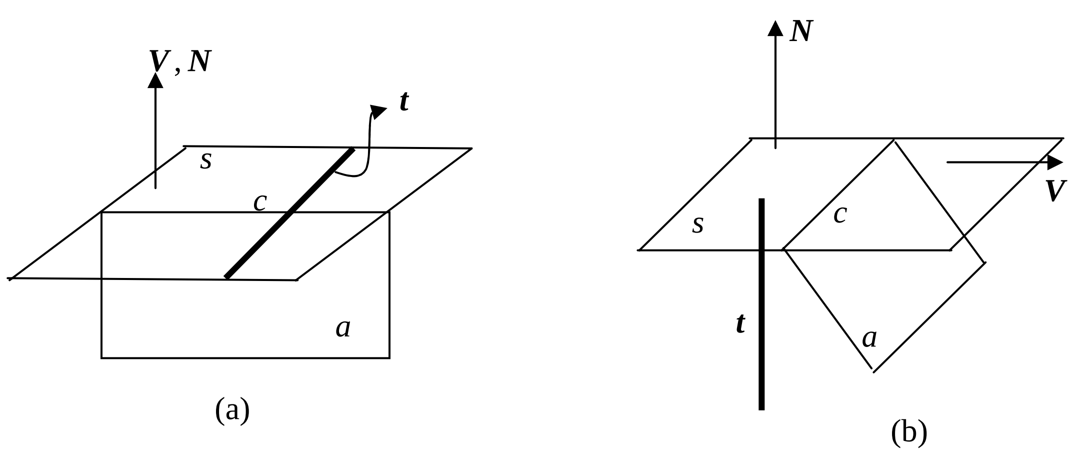

Fig. 2. Kinematics of dislocation motion at a boundary/interface.