

**ORIGINAL ARTICLE**

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Plasticity in multi-phase solids with incoherent interfaces and junctions

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Abstract Boundaries and junctions (both internal and external) can contribute significantly to the plastic deformation of metallic solids, especially when the average size of the grains (phases) is less than hundred nanometres or when the size of the solid itself is of the order of microns. The overall permanent deformation of the solid is a result of a coupling between bulk plasticity with moving interfaces/junctions/edges and intrinsic plasticity of internal and external surfaces. We use a novel continuum thermodynamic theory of plastic evolution, with incoherent interfaces and non-splitting junctions, to derive flow rules for bulk and surface plasticity in addition to kinetic relations for interface, edge, and junction motion, all coupled to each other. We assume rate-independent associative isotropic plastic response with bulk flow stress dependent on accumulated plastic strain and an appropriate measure of inhomogeneity. The resulting theory has two internal length scales: one given by the average grain size and another associated with the material inhomogeneity.

Keywords Plasticity · Strain gradient · Incoherent interface · Junction · Multi-phase solid

1 Introduction

Multi-phase and polycrystalline solids of size of the order of microns, or having an average grain size of less than hundred nanometres, have a large volume fraction of interfaces and junctions [22]. The internal boundaries play a central role in the microstructural evolution during phase transformations, shock propagation, and plastic deformation in such solids, cf. [16, 29], Chapter 12 of [34], and Chapter 5 of [22, 26]. Boundaries and junctions provide sites of resistance for continuing plastic flow in the bulk (thereby hardening the material), but can also act as sources for initiating plastic deformation. They can have intrinsic defect content (e.g. dislocation walls) and finite mobility. Moreover, allowing for excess free energy densities over the boundaries and surface stresses, intrinsic plastic flow can exist at an interface and a free surface. The interaction of such surfaces with bulk plasticity can indeed be very complex while involving multiple dissipative mechanisms [7, 16, 21, 35]. The purpose of this work is to first develop a theoretical framework within which these couplings can be incorporated and second to derive coupled kinetic relations, governing plastic flow and interface/junction/edge dynamics, under various simplifying assumptions. We restrict our model to two-dimensional (2D) solids mainly in order to present certain theoretical results in detail without getting lost in notational complexity.

Dedicated to Prof. David Steigmann, in gratitude for his fundamental contributions to theoretical mechanics.

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The main contributions of this paper are:

- (i) Kinematics of incoherent interfaces in plastically deforming regions: The multiplicative decomposition of the total deformation at the interface into elastic and plastic components is introduced; it takes a simple yet instructive form in the 2D setting. The inhomogeneity at the interface is characterised with the incoherency tensor. A new compatibility condition at the junction is derived in terms of the incoherency tensor. Our kinematics is closely related to the framework developed in [17].
- (ii) A novel continuum thermodynamic framework incorporating incoherent interfaces, external boundary of the body, edges, and junctions: Assuming finite deformations, we consider interface energy to depend on interfacial elastic strain, incoherency tensor, and orientation. Local dissipation rates per unit area in the bulk, per unit length of the interface, and at the junction are obtained, where the latter two quantities are interpreted as excess entropy generated in the domain. Irreversible thermodynamics of incoherent interfaces has been previously studied in a deforming solid, but without considerations of plasticity, external surface, edges, and junctions [9,17]. On the other hand, junctions and edges have been incorporated in a theory of deforming solids but only for coherent interfaces and without any plasticity [8,31,32]. The present thermodynamic formalism, which follows our recent work on grain boundaries [3–5], should be seen as an alternative to the configurational mechanics formalism proposed by Gurtin and his coauthors [9,15].
- (iii) Flow rules coupled with kinetic relations: Assuming rate-independent plasticity and isotropic material response, we use maximum dissipation postulate to derive associative flow rules within the bulk and at the surfaces. Accumulation of plastic flow near the boundaries and junctions affects the material inhomogeneity distribution such that the solid hardens with an increase in the magnitude of the yield stress. We include these effects by assuming the yield loci to depend on accumulated plastic strain and appropriate measures of inhomogeneity. Incorporation of material inhomogeneities leads to two internal length scales in the theory: one given by the average grain size and another associated with the density of defects. In addition, we also propose kinetic relations governing the dynamics of interfaces, edges, and junctions. We emphasise the coupling between various flow rules and kinetic relations. Whereas the bulk flow rule is standard, although the considered yield locus is non-standard [23], the interfacial flow rules have been previously obtained only for a small deformation theory and with stationary interfaces [13,14].

The paper is organised as follows. The kinematical aspects of the 2D theory and certain mathematical preliminaries are elaborated in Sect. 2; in particular, we discuss interfacial kinematics and the nature of multiplicative decomposition of the total deformation at the interface. This is followed by a derivation of various local dissipation inequalities associated with the bulk, boundaries, and junctions in Sect. 3. The dissipation inequalities are taken as the starting point in Sect. 4 to develop flow rules for associative rate-independent isotropic plastic evolution in the bulk and at the surfaces (internal and external), as well for motivating linear kinetic relations for interface/edge/junction dynamics.

2 Preliminaries

In this section, we fix the notation, introduce the relevant kinematics in the bulk, at the interface, and at the junction, collect useful integral relations, and discuss the multiplicative decomposition in the bulk and at the interface. We also take a brief diversion on the nature of defect densities present in our theory.

Let \mathcal{V} be the translation space of a 2D Euclidean point space. We denote the space of all linear transformations from \mathcal{V} to itself (second-order tensors) by Lin , its subspace of positive definite tensors by Lin^+ , the subspace of invertible tensors by InvLin , the subspaces of symmetric and skew-symmetric tensors by Sym and Skw , respectively, and the subgroups of orthogonal and rotation tensors by Orth and Orth^+ , respectively. The determinant, transpose, and inverse of $\mathbf{A} \in \text{Lin}$ are denoted by $J_{\mathbf{A}}$, \mathbf{A}^T , and \mathbf{A}^{-1} , respectively. The identity tensor in Lin is denoted by $\mathbf{1}$. The space Lin is equipped with the Euclidean inner product and norm defined by $\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{A}\mathbf{B}^T)$ and $|\mathbf{A}|^2 = \mathbf{A} \cdot \mathbf{A}$, respectively, where $\mathbf{B} \in \text{Lin}$ and tr is the trace operator. We have used $\text{sym}(\mathbf{A})$ and $\text{skw}(\mathbf{A})$ to denote the symmetric and the skew-symmetric part of \mathbf{A} . The derivative of a scalar-valued differentiable function of tensors, say $G(\mathbf{A})$, is a tensor $\partial_{\mathbf{A}}G$ defined by

$$G(\mathbf{A} + \mathbf{B}) = G(\mathbf{A}) + \partial_{\mathbf{A}}G \cdot \mathbf{B} + o(|\mathbf{B}|), \quad (1)$$

where $o(|\mathbf{B}|)/|\mathbf{B}| \rightarrow 0$ as $|\mathbf{B}| \rightarrow 0$. Similar definitions can be made for vector- and tensor-valued differentiable functions (of scalars, vectors, and tensors).

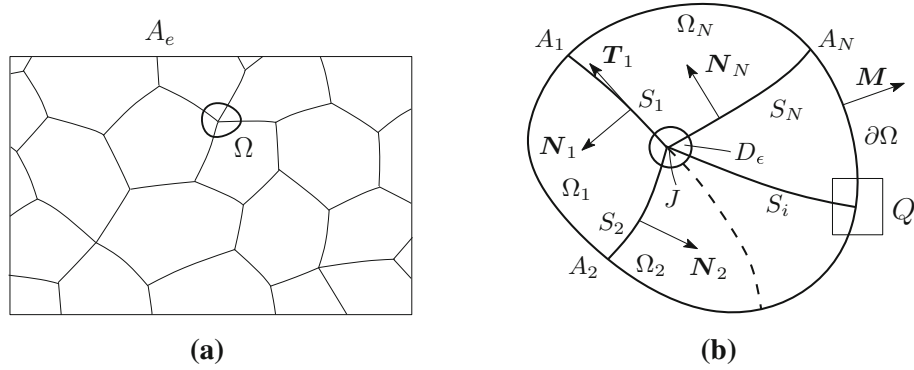


Fig. 1 **a** Schematic of a 2D multi-phase solid with an arbitrary region Ω . **b** An arbitrary region Ω of the reference configuration containing N subregions Ω_i ($i = 1, \dots, N$), N interfaces S_i , and a junction J ; points A_i denote the edge of S_i lying on $\partial\Omega$. The normals to $\partial\Omega$ and S_i are denoted by M and N_i , respectively. A circular disc D_ϵ , centred at J , is excluded from Ω to obtain the punctured region Ω_ϵ

2.1 Kinematics

Consider a 2D multi-phase solid as shown in Fig. 1a. The neighbouring grains in the body can be of the same phase or different from each other, with varying lattice orientations. Let B_0 be the reference configuration (fixed in time) associated with the body and B_t be the current configuration. The bijective mapping χ from B_0 to B_t is assumed to be continuous and piecewise differentiable map such that $\mathbf{x} = \chi(\mathbf{X}, t)$, where \mathbf{X} and \mathbf{x} denote position vectors of a particle in B_0 and B_t , respectively; the variable t represents time. The derivative of a sufficiently smooth field defined over B_0 with respect to \mathbf{X} is denoted by the gradient operator ∇ . The divergence of a smooth vector field $\mathbf{a} \in \mathcal{V}$ and a smooth tensor field $\mathbf{A} \in \text{Lin}$ are given by

$$\text{Div } \mathbf{a} = \text{tr } \nabla \mathbf{a} \text{ and } \text{Div } \mathbf{A} \cdot \mathbf{c} = \text{Div} \left(\mathbf{A}^T \mathbf{c} \right), \quad (2)$$

respectively, for any fixed $\mathbf{c} \in \mathcal{V}$. The material time derivative of a function is the derivative with respect to time for fixed \mathbf{X} ; we denote it by a superimposed dot. The particle velocity \mathbf{v} is defined as $\mathbf{v} = \dot{\chi}$. If χ is differentiable at \mathbf{X} , then the deformation gradient $\mathbf{F} \in \text{InvLin}$ exists at \mathbf{X} and is given by $\mathbf{F} = \nabla \chi$. We assume \mathbf{v} and \mathbf{F} to be piecewise continuously differentiable over B_0 ; they (and their derivatives) are allowed to be discontinuous across the interfaces and singular at the junctions.

Let Ω be an arbitrary interior region of B_0 such that it contains N subregions $\Omega_1, \dots, \Omega_N$ separated by N interfaces S_1, \dots, S_N , all of them intersecting at a junction J , see Fig. 1b. Each of these interfaces is a smooth one-dimensional curve with one end lying on the boundary of the region $\partial\Omega$ and the other at the junction J ; the edge point of an interface S_i , which lies on $\partial\Omega$, is denoted by A_i . The edge A_i should be differentiated from a physical edge of an interface which is the intersecting point of the interface with the external boundary of the body; we refer to the edges such as A_i as non-physical. For every interface S_i , we introduce an arc-length parameter s_i along the curve such that it starts at J and increases towards A_i . The unit normal N_i to S_i and the unit tangent T_i along it are chosen such that N_i points inside Ω_i and T_i is oriented in the direction of increasing s_i . To deal with singularities (at the junction) in various bulk fields, including stresses, strains, and strain energy, we perform the analysis in a punctured region Ω_ϵ obtained by excluding a circular disc D_ϵ of radius ϵ and centred at J from Ω ; i.e. $\Omega_\epsilon = \Omega \setminus D_\epsilon$. The boundary of D_ϵ , denoted by C_ϵ , is considered to move with a velocity \mathbf{u} such that it approaches the junction velocity, denoted by \mathbf{q} , as $\epsilon \rightarrow 0$ uniformly in time. The unit outward normal to $\partial\Omega$, as well as to C_ϵ , is denoted by M . Note that M on C_ϵ points into Ω_ϵ .

Consider a smooth interface S (such as those inside Ω) having normal N and moving with normal velocity V ; we suppress subscript ‘ i ’ here and in rest of this subsection. We take s as an arc-length parameter along S starting at J and increasing towards A . The jump and the average of a piecewise continuous bulk field f across S are defined as $\llbracket f \rrbracket = f^+ - f^-$ and $\langle f \rangle = (f^+ + f^-)/2$, where f^+ is the limiting value of f as it approaches S from the side into which N points and f^- otherwise. For two piecewise continuous bulk fields f_1 and f_2 , it can be easily shown that

$$\llbracket f_1 f_2 \rrbracket = \llbracket f_1 \rrbracket \langle f_2 \rangle + \langle f_1 \rangle \llbracket f_2 \rrbracket. \quad (3)$$

The time derivative of an interfacial fields g , continuously differentiable over S and continuous up to J , following S is given by the normal time derivative [17]

$$\dot{g} = \dot{g} + V \nabla g \cdot N. \quad (4)$$

It represents the rate of change of g noted by an observer sitting on the moving S ; see e.g. [15, 17]. This can be used to define the intrinsic material velocity of the particles lying instantaneously on S as $\mathbb{v} = \dot{\mathbf{x}}(X, t)$ for $X \in S$. Expanding it using (4), we obtain

$$\mathbb{v} = \mathbf{v}^\pm + V \mathbf{F}^\pm N = \langle \mathbf{v} \rangle + V \langle \mathbf{F} \rangle N, \quad (5)$$

where the superscript \pm indicates that either $+$ or $-$ limit of the field can be used to satisfy the equation. The compatibility equation

$$V \llbracket \mathbf{F} \rrbracket N = -\llbracket \mathbf{v} \rrbracket. \quad (6)$$

is an immediate consequence of (5)₁. Let $X_A(t)$ be the position vector of the edge A . The edge velocity is defined as

$$\mathbb{w}_A = \frac{dX_A}{dt} = V_A N_A + W_A T_A, \quad (7)$$

where $N_A(t) = N(X_A, t)$ and $T_A(t) = T(X_A, t)$; V_A and W_A are normal and tangential components of the edge velocity, respectively. The compatibility between the interface and the edge requires $V_A(t) = V(X_A, t)$. The material velocity of a particle lying instantaneously at A , given by $d\mathbf{x}(X_A(t), t)/dt$, has an intrinsic part

$$\mathbb{v}_A^{\text{int}} = \dot{\mathbf{x}}(X_A, t) = (\mathbf{v}^\pm + V \mathbf{F}^\pm N)_A = (\langle \mathbf{v} \rangle + V \langle \mathbf{F} \rangle N)_A, \quad (8)$$

where the notation $(\cdot)_A$ denotes evaluation of the bracketed field at point A , and an extrinsic part

$$\mathbb{v}_A^{\text{ext}} = \frac{d\mathbf{x}(X_A, t)}{dt} - \dot{\mathbf{x}}(X_A, t) = (W \langle \mathbf{F} \rangle T)_A. \quad (9)$$

We note from (5) and (8)₃ that $\mathbb{v}_A^{\text{int}} = (\mathbb{v})_A$.

The interfacial stretch vector, defined as $\mathbb{f} = \partial \mathbf{x}(X(s), t)/\partial s$, is related to the bulk deformation gradient as

$$\mathbb{f} = \mathbf{F}^\pm T = \langle \mathbf{F} \rangle T, \quad (10)$$

where the Hadamard compatibility relation, $\llbracket \mathbf{F} \rrbracket T = \mathbf{0}$, has been taken into account. The surface deformation gradient tensor $\mathbb{F} = \mathbf{F}^\pm T \otimes T$, where $T \otimes T$ is the projection tensor on S , is therefore related to \mathbb{f} as

$$\mathbb{F} = \mathbb{f} \otimes T. \quad (11)$$

Moreover, the definition of the stretch vector implies that we can write

$$\mathbb{f} = \lambda t, \quad (12)$$

where t is the unit tangent to the interfacial curve in the current configuration and λ , hence, can be interpreted as the measure of the local stretch of the interface. Combining above two equations, we have $\mathbb{F} = \lambda t \otimes T$.

Let ϕ be the anticlockwise angle that the normal N makes with the positive e_1 -axis of a fixed Cartesian coordinate system having a right-handed orthonormal basis $\{e_1, e_2\}$. As a result we can write $N = \cos \phi e_1 + \sin \phi e_2$ and $T = \sin \phi e_1 - \cos \phi e_2$. The curvature of S is given by $\kappa = \partial \phi / \partial s$. The identities

$$\frac{\partial N}{\partial s} = -\kappa T \quad \text{and} \quad \frac{\partial T}{\partial s} = \kappa N \quad (13)$$

follow immediately. Additionally, we have

$$\dot{\phi} = \frac{\partial V}{\partial s}; \quad (14)$$

see e.g. Section XIV of [15]. Finally, taking the normal time derivative of (10) and using (14), it can be shown that [32]

$$\dot{\mathbb{f}} = \frac{\partial}{\partial s} (\langle \mathbf{v} \rangle + V \langle \mathbf{F} \rangle N) + \kappa V \mathbb{f} = \frac{\partial \mathbb{v}}{\partial s} + \kappa V \mathbb{f}, \quad (15)$$

where the second equality follows from (5)₂.

2.2 Integral theorems

For a piecewise smooth field f defined in Ω , allowed to be discontinuous across S_i and singular at J , we assume that the limit

$$\int_{\Omega} f dA = \lim_{\epsilon \rightarrow 0} \int_{\Omega_{\epsilon}} f dA \quad (16)$$

exists, where dA is an infinitesimal area element in Ω . We will use the following transport relation for f [32]:

$$\frac{d}{dt} \int_{\Omega} f dA = \int_{\Omega} \dot{f} dA - \sum_{i=1}^N \int_{S_i} V_i \llbracket f \rrbracket dL - \lim_{\epsilon \rightarrow 0} \oint_{C_{\epsilon}} f \mathbf{u} \cdot \mathbf{M} dL, \quad (17)$$

where dL is an infinitesimal line element along a curve in Ω . For a vector field \mathbf{a} and a tensor field \mathbf{A} , both defined in Ω , sufficiently smooth within the bulk, discontinuous across S_i , and singular at J , the following divergence theorems hold [32]:

$$\int_{\Omega} \text{Div } \mathbf{a} dA = \int_{\partial\Omega} \mathbf{a} \cdot \mathbf{M} dL - \sum_{i=1}^N \int_{S_i} \llbracket \mathbf{a} \rrbracket \cdot \mathbf{N}_i dL - \lim_{\epsilon \rightarrow 0} \oint_{C_{\epsilon}} \mathbf{a} \cdot \mathbf{M} dL, \quad (18)$$

$$\int_{\Omega} \text{Div } \mathbf{A} dA = \int_{\partial\Omega} \mathbf{A} \mathbf{M} dL - \sum_{i=1}^N \int_{S_i} \llbracket \mathbf{A} \rrbracket \mathbf{N}_i dL - \lim_{\epsilon \rightarrow 0} \oint_{C_{\epsilon}} \mathbf{A} \mathbf{M} dL. \quad (19)$$

For an interfacial field g , continuously differentiable over a curve S whose one end point is on $\partial\Omega$ (labelled as A) and the other is on the junction J , we have the following transport relation [15]:

$$\frac{d}{dt} \int_S g dL = \int_S (\dot{g} - g\kappa V) dL + (gW)_A - (g\mathbf{q} \cdot \mathbf{T})_J, \quad (20)$$

where $(\cdot)_J$ denotes evaluation of the bracketed field at J .

2.3 Elastic–plastic deformation

We now introduce the multiplicative decomposition of the total deformation into elastic and plastic deformations both in the bulk and at the interface; for a related discussion in three dimensions, see [17]. Towards this end, we focus our attention on a neighbourhood $R_0 \subset \Omega$ such that it intersects only one interface S_i and is away from the junction. Let $C = R_0 \cap S_i$. We use R_t and c to denote the image of R_0 and C in the current configuration; see Fig. 2. It has been shown (in [17, 18]) that it is possible to obtain a locally stress-free configuration by cutting B_t into infinitesimally small parts. We denote such a configuration by B_r , as obtained from B_t , and R_r as its subset obtainable from R_t . If these sub-bodies cannot be made congruent in the absence of any distortion, then the body is said to be dislocated (or inhomogeneous) with no globally continuous piecewise differentiable map from B_t to the disjoint set of sub-bodies [17, 18]. At the interface, the loss of congruency requires that the tangent \mathbf{t} to the interfacial curve in B_t gets mapped to two distinct tangents in the relaxed configuration (see Fig. 2); such interfaces are called incoherent. In other words, for an incoherent interface, the surface in the current configuration splits into two distinct surfaces (locally) in the relaxed configuration. The piecewise smooth map from the local tangent space in B_r to that in B_t is represented by $\mathbf{H} \in \text{InvLin}$. Assuming the unloading to be elastic, we interpret \mathbf{H} as the elastic distortion. The absence of a globally continuous piecewise differentiable map implies that \mathbf{H} , unlike \mathbf{F} , cannot be written as gradient of a differentiable map. The defect content (or the inhomogeneity) in the bulk region, away from interfaces and junctions, is measured in terms of the curl of \mathbf{H} , while the incoherency of a singular interface is represented by the non-rank-one jump in \mathbf{H} across the interface. Whereas the former yields a continuous distribution of dislocations within the bulk of B_t , the latter gives a continuous distribution of dislocations at the interface [17].

Let $\mathbf{G} \in \text{InvLin}$ be the piecewise smooth map of the local tangent space in B_0 to that in B_r . The multiplicative decomposition

$$\mathbf{F} = \mathbf{H}\mathbf{G} \quad (21)$$

is therefore admitted at all material points away from interfaces and junctions. The time evolution of \mathbf{G} essentially describes the evolution of the relaxed configuration with respect to a fixed reference configuration;

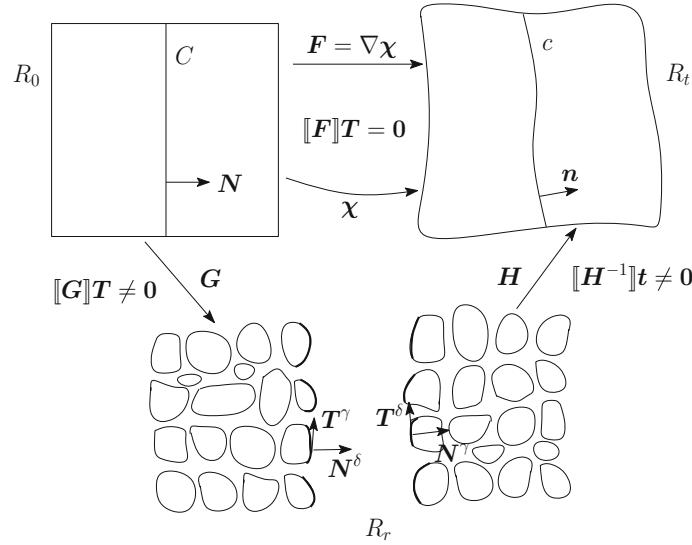


Fig. 2 Elastic–plastic decomposition in $R_0 \subset \Omega_\epsilon$

for this reason, we identify it with plastic distortion. It is clear from (21) that incompatibility of \mathbf{H} , both in the bulk as well as at the interface, is equivalent to that of \mathbf{G} [17]. Further, it is physically meaningful to assume $J_H > 0$; hence, $J_G > 0$.

To derive the multiplicative decomposition at the interface, we start by introducing \mathbf{T}^γ and \mathbf{T}^δ as two unit tangent vectors in the intermediate configuration both of which map into the tangent \mathbf{t} to c (or into tangent \mathbf{T} to C) at a fixed material point (see Fig. 2). The superscripts γ and δ are used to distinguish the two surfaces in R_r obtained by relaxing c ; for a coherent interface, the two surfaces are identical. We define (the subscript ‘ i ’ is again suppressed in this subsection)

$$\begin{aligned} \mathbb{H}^\gamma &= \mathbf{H}^+ \mathbf{T}^\gamma \otimes \mathbf{T}^\gamma, \quad \mathbb{H}^\delta = \mathbf{H}^- \mathbf{T}^\delta \otimes \mathbf{T}^\delta, \\ \mathbb{G}^\gamma &= \mathbf{G}^+ \mathbf{T} \otimes \mathbf{T}, \quad \mathbb{G}^\delta = \mathbf{G}^- \mathbf{T} \otimes \mathbf{T}. \end{aligned} \quad (22)$$

Furthermore, it is clear from an application of the Nanson’s formula that both $\mathbf{H}^+ \mathbf{T}^\gamma$ and $\mathbf{H}^- \mathbf{T}^\delta$ are parallel to \mathbf{t} [17]; we write $\mathbf{H}^+ \mathbf{T}^\gamma = v^\gamma \mathbf{t}$ and $\mathbf{H}^- \mathbf{T}^\delta = v^\delta \mathbf{t}$, where v^γ and v^δ represent the two distinct stretch values associated with the two surfaces in the relaxed configuration obtained from curve c at a fixed point. Analogously, we can write $\mathbf{G}^+ \mathbf{T} = \mu^\gamma \mathbf{T}^\gamma$ and $\mathbf{G}^- \mathbf{T} = \mu^\delta \mathbf{T}^\delta$, where μ^γ and μ^δ are the local stretch values associated with curve C with respect to the two surfaces in the relaxed configuration. As a result, we obtain from (22)

$$\mathbb{H}^\alpha = v^\alpha \mathbf{t} \otimes \mathbf{T}^\alpha \quad \text{and} \quad \mathbb{G}^\alpha = \mu^\alpha \mathbf{T}^\alpha \otimes \mathbf{T}, \quad (23)$$

where α stands for either γ or δ (no summation over repeated α here and elsewhere). Post-operating the + and the – limits of (21) with $\mathbf{T} \otimes \mathbf{T}$, while making use of (22) and (23), we obtain the following multiplicative decompositions of \mathbb{F} , cf. [17]:

$$\mathbb{F} = \mathbb{H}^\gamma \mathbb{G}^\gamma = \mathbb{H}^\delta \mathbb{G}^\delta. \quad (24)$$

In particular, after making substitutions from (11) and (23) into these relations, we are led to the decomposition

$$\lambda = v^\gamma \mu^\gamma = v^\delta \mu^\delta. \quad (25)$$

of the total stretch of the interfacial curve into an elastic and a plastic part.

The interfacial elastic strain is expressed in terms of the right Cauchy–Green tensor associated with \mathbb{H}^γ and \mathbb{H}^δ , i.e.

$$\mathbb{C}^\alpha = (\mathbb{H}^\alpha)^T \mathbb{H}^\alpha = (v^\alpha)^2 \mathbf{T}^\alpha \otimes \mathbf{T}^\alpha. \quad (26)$$

On the other hand, the incoherency of the interface is characterised by the incoherency tensor \mathbb{M} defined as [9, 17]

$$\mathbb{M} = (\mathbb{H}^\gamma)^{-1} \mathbb{H}^\delta = \mathbb{G}^\gamma (\mathbb{G}^\delta)^{-1}, \quad (27)$$

where the second equality follows from (24)₂. The inverse $(\mathbb{H}^\gamma)^{-1}$ and $(\mathbb{G}^\delta)^{-1}$ are the unique Moore-Penrose pseudo-inverse of \mathbb{H}^γ and \mathbb{G}^δ , respectively, such that $(\mathbb{H}^\gamma)^{-1}\mathbb{H}^\gamma = \mathbf{T}^\gamma \otimes \mathbf{T}^\gamma$, $\mathbb{H}^\gamma(\mathbb{H}^\gamma)^{-1} = \mathbf{t} \otimes \mathbf{t}$, $(\mathbb{G}^\delta)^{-1}\mathbb{G}^\delta = \mathbf{T} \otimes \mathbf{T}$, and $\mathbb{G}^\delta(\mathbb{G}^\delta)^{-1} = \mathbf{T}^\delta \otimes \mathbf{T}^\delta$. The incoherency tensor measures the relative distortion between the two relaxed surfaces obtained from a single interface in the reference (or the current) configuration. Based on (26) and (27)₁, we note that

$$\mathbb{C}^\delta = \mathbb{M}^T \mathbb{C}^\gamma \mathbb{M}. \quad (28)$$

We can use (23) to rewrite (27) as

$$\mathbb{M} = m \mathbf{T}^\gamma \otimes \mathbf{T}^\delta, \quad \text{where } m = \frac{\mu^\gamma}{\mu^\delta} = \frac{\nu^\delta}{\nu^\gamma} \quad (29)$$

measures the relative local elastic (or plastic) stretch of the two relaxed surfaces. The relative rotation at the interface (misorientation) is measured by the relative orientation of \mathbf{T}^γ and \mathbf{T}^δ . For a coherent interface, $m = 1$, and \mathbf{T}^γ is identical with \mathbf{T}^δ ; the incoherency tensor is then reduced to $\mathbb{M} = \mathbf{T}^\gamma \otimes \mathbf{T}^\gamma = \mathbf{T}^\delta \otimes \mathbf{T}^\delta$. We also note that \mathbb{M} is closely related to the true surface dislocation density, the latter being given by $(\mathbf{T}^\delta \otimes \mathbf{T}^\delta - \mathbb{M})$ [17], so that for a coherent interface the defect content vanishes identically.

We end this subsection by writing a compatibility condition to be satisfied at the junction. Consider N incoherent interfaces meeting at a junction J . Then, in an infinitesimally small neighbourhood of J , we have (see also [17])

$$\mathbb{M}_N \mathbb{M}_{N-1} \dots \mathbb{M}_2 \mathbb{M}_1 = \mathbf{T}_1^\delta \otimes \mathbf{T}_1^\delta, \quad (30)$$

where \mathbb{M}_i is the incoherency tensor associated with the i th interface. All the fields appearing in (30) are evaluated in the limit of approaching the junction. The above relation is easily verifiable using (27) and noting that $\mathbb{H}_i^\gamma = \mathbb{H}_{i+1}^\delta$ (at J), where subscript $N+1$ should be identified with 1. The relation (30) imposes a restriction on the dislocation densities associated with various interfaces intersecting at a junction point. A similar relation in the simplified context of plane interfaces and small strains was given by Bilby [6] and independently by Amelinckx [2] in a more specialised case of grain boundaries. The latter work used this condition to determine certain restrictions on the nature of dislocation content of the intersecting grain boundaries.

3 Balance laws and dissipation

Based on the assumptions listed in Sect. 1, we now derive local balance laws for mass and momentum. We also obtain various local dissipation inequalities starting from a mechanical version of the second law of thermodynamics. Our framework is based on Gibbs thermodynamics where all the extensive interfacial fields are understood as excess quantities. We will use the dissipation inequalities to derive flow rules for plastic evolution and kinetic laws for interfacial and junction dynamics. Throughout this subsection, we will consider an arbitrary part Ω of B_0 as introduced in the previous section and shown in Fig. 1b. The region Ω has N interfaces all intersecting at a junction point.

3.1 Mass and momentum balance

Assuming that the region Ω does not exchange mass with rest of the body and that there are no excess mass densities at the interfaces and the junction, we can write the mass balance relation as

$$\frac{d}{dt} \int_{\Omega} \rho_r \, dA = 0, \quad (31)$$

where ρ_r is the mass density per unit volume of B_0 . Using the transport relation (17), while considering ρ_r to remain non-singular at the junction, and localising the result, we are led to

$$\dot{\rho}_r = 0 \quad \text{in } \Omega_i \text{ and} \quad (32)$$

$$V_i \llbracket \rho_r \rrbracket = 0 \quad \text{on } S_i, \quad (33)$$

i.e. ρ_r remains constant within the bulk and is continuous across moving interfaces in Ω . Recall that the subscript i in various terms denotes the i th interface curve in Ω .

The region Ω is subjected to traction $\mathbf{P}\mathbf{M}$ on the boundary $\partial\Omega$ where \mathbf{P} is the first Piola–Kirchhoff stress and \mathbf{M} is the unit outward normal to $\partial\Omega$. Additionally, we allow for interfacial stresses such that each interface S_i is subjected to a traction \mathbb{p}_i at the edge A_i . The interfacial first Piola–Kirchhoff stress is $\mathbb{p}_i \otimes \mathbf{T}_i$. Neglecting body forces and inertial effects both in the bulk and at the interface, the balance of linear momentum in Ω yields

$$\int_{\partial\Omega} \mathbf{P}\mathbf{M} dL + \sum_{i=1}^N \mathbb{p}_i|_{A_i} = \mathbf{0}. \quad (34)$$

This can be localised using the divergence theorem (19) to obtain (see also [32])

$$\text{Div } \mathbf{P} = \mathbf{0} \quad \text{in } \Omega_i, \quad (35)$$

$$\llbracket \mathbf{P} \rrbracket \mathbf{N}_i + \frac{\partial \mathbb{p}_i}{\partial s_i} = \mathbf{0} \quad \text{on } S_i, \quad \text{and} \quad (36)$$

$$\lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{P}\mathbf{M} dL + \sum_{i=1}^N \mathbb{p}_i|_J = \mathbf{0} \quad \text{at } J. \quad (37)$$

Equations (35) and (36) are familiar stress equilibrium relations in the bulk and across singular interfaces. According to (37), which represents stress equilibrium at the junction, the limiting value of the net force acting on C_ϵ due to the singular bulk stress is finite and balances the force exerted by the interfacial stresses at the junction.

The balance of angular momentum in Ω requires

$$\int_{\partial\Omega} (\mathbf{x} - \mathbf{x}_0) \times \mathbf{P}\mathbf{M} dL + \sum_{i=1}^N (\mathbf{x} - \mathbf{x}_0) \times \mathbb{p}_i|_{A_i} = \mathbf{0}, \quad (38)$$

where $\mathbf{x}_0 \in B_t$ is a fixed point. Applying the divergence theorem (19), and substituting equilibrium relations (35)–(37) into the result, we can obtain

$$\mathbf{F}\mathbf{P}^T = \mathbf{P}\mathbf{F}^T \quad \text{in } \Omega_i \quad \text{and} \quad \mathbf{t}_i \times \mathbb{p}_i = \mathbf{0} \quad \text{on } S_i, \quad (39)$$

where recall that \mathbf{t}_i is the unit tangent vector to the i th interface in the current configuration. Hence, $\mathbf{F}\mathbf{P}^T \in \text{Sym}$ and \mathbb{p}_i is parallel to \mathbf{t}_i at the interface.

3.2 Dissipation inequality

Under isothermal conditions, the mechanical version of the second law of thermodynamics requires the rate of change of the total free energy of Ω to be less than or equal to the total power input, i.e.

$$\underbrace{\frac{d}{dt} \left(\int_{\Omega} \Psi dA + \sum_{i=1}^N \int_{S_i} \Phi_i dL \right)}_{\text{rate of change of total free energy}} \leq \underbrace{\int_{\partial\Omega} \mathbf{P}\mathbf{M} \cdot \mathbf{v} dL + \sum_{i=1}^N (\mathbb{p}_i \cdot \mathbf{v}_i^{\text{int}})_{A_i}}_{\text{mechanical power input}} + \underbrace{\sum_{i=1}^N (\mathbf{c}_i \cdot \mathbf{w}_i)_{A_i} + \sum_{i=1}^N (\mathbb{p}_i \cdot \mathbf{v}_i^{\text{ext}})_{A_i}}_{\text{non-standard power}}, \quad (40)$$

where Ψ is the free energy per unit area of Ω and Φ_i is the free energy of S_i per unit length. The first two terms on the right-hand side of the inequality in (40) represent the power input into the region through working by traction on its outer boundary due to both bulk and interfacial stresses. It should be noted that the conjugate velocity for interfacial traction \mathbb{p}_i is $\mathbf{v}_i^{\text{int}}$ which, recall from (8), is the material velocity of the particles present instantaneously at S_i as experienced by an observer moving with S_i in its normal direction. It is clear from Fig. 3 that as an interface evolves within B_0 , its domain of intersection with Ω changes; there would be portions of the interface which, previously present outside Ω , are now inside it, and vice versa. In other words, the set of points belonging to an interface and lying within Ω changes continuously as the interface moves. This warrants incorporating additional (non-standard) power inputs included here as the last two terms in (40). The first term is considered so as to ensure that there is no excess entropy production at the edges A_i , thereby restricting the excess entropy generation to the interfaces and the junction. The second term represents a correction to

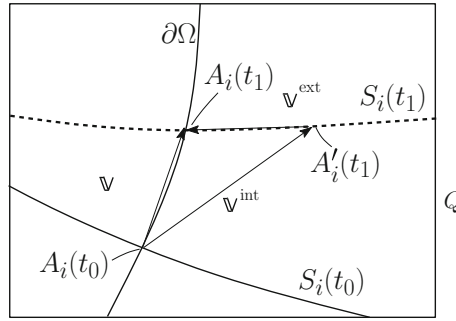


Fig. 3 A part Q of B_0 which has a non-trivial intersection with Ω , see Fig. 1b, showing the interface S_i at two time instants t_0 and t_1

the mechanical power due to interfacial traction. This is required since the intrinsic velocity v_i^{int} will move the observer, sitting at a point on the interface presently at A_i , away from $\partial\Omega$, see Fig. 3. The extrinsic velocity v_i^{ext} brings the observer back to the edge on $\partial\Omega$; this is also illustrated in Fig. 3. The exact form of c_i , however, depends on the constitutive nature of the interfacial free energy; this will be made clear in the ensuing discussion. Similar considerations as those outlined above have been made recently by the present authors [3–5] in the context of grain boundaries. Our treatment should be contrasted with the earlier works based on the concept of configurational forces [9, 15, 32], which require postulation of additional (configurational) balance laws besides the standard balance laws of continuum mechanics. Moreover, our theory is a priori invariant with respect to any change in parametrisation (of surfaces and junctions), whereas these works use this invariance to derive several important relations in their framework (for an alternate viewpoint see [25]). While leading to the same final results, our standpoint is less cumbersome both conceptually and notationally.

In rest of this section, we will use various integral theorems and balance laws to derive local dissipation inequalities in the bulk, at the interfaces, and at the junction. We will make specific constitutive choices for the free energies and make assumption on the nature of elasticity both in the bulk and at the interface. During our calculation, we will also derive an expression for c_i . We use divergence theorem (18) and transport relations (17) and (20) to rewrite (40) as

$$\sum_{l=1}^5 I_l \leq 0, \text{ where} \quad (41)$$

$$I_1 = \int_{\Omega} (\dot{\Psi} - \text{Div}(\mathbf{P}^T \mathbf{v})) \, dA, \quad (42)$$

$$I_2 = \sum_{i=1}^N \int_{S_i} \left(-V_i \llbracket \Psi \rrbracket - \llbracket \mathbf{P}^T \mathbf{v} \rrbracket \cdot \mathbf{N}_i + \dot{\Phi}_i - \Phi_i \kappa_i V_i - \frac{\partial \mathbb{P}_i}{\partial s_i} \cdot \mathbf{v}_i - \mathbb{P}_i \cdot (\dot{\mathbb{F}}_i - V_i \kappa_i \mathbb{F}_i) \right) dL, \quad (43)$$

$$I_3 = - \lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} (\Psi \mathbf{u} \cdot \mathbf{M} + \mathbf{P}^T \mathbf{v} \cdot \mathbf{M}) \, dL, \quad (44)$$

$$I_4 = - \sum_{i=1}^N (\Phi_i \mathbf{T}_i \cdot \mathbf{q} + \mathbb{P}_i \cdot \mathbf{v}_i)_J, \text{ and} \quad (45)$$

$$I_5 = \sum_{i=1}^N (W_i (\Phi_i - \mathbb{P}_i \cdot \mathbb{F}_i) - \mathbf{c}_i \cdot \mathbf{w}_i)_{A_i}. \quad (46)$$

We have also used (8) and (15) in (43), and (9) in (46).

3.2.1 Constitutive assumptions for the free energies

Before localising (41) to eventually obtain local dissipation inequalities, we need to specify the constitutive form of the free energies. The origin of both bulk and interfacial stresses is assumed to be elastic. It is then appropriate to consider strain energy densities to depend on elastic distortion. At each point on the incoherent

interface, we get two local surfaces in the relaxed configuration, as argued in the previous section. As a result, there are two independent elastic distortion tensors at the interface mapping a single unit tangent \mathbf{t}_i (corresponding to the i th surface) into two distinct unit tangents \mathbf{T}_i^γ and \mathbf{T}_i^δ . The interfacial energies are also explicitly dependent on the local orientation of the interface. Keeping all this in mind, we suppose the bulk and interface free energy densities to have the form [17, 18]

$$\Psi = J_G W(\mathbf{H}) \quad \text{and} \quad \Phi_i = \mu_i^\gamma \bar{w}_i (\mathbb{H}_i^\gamma, \mathbb{H}_i^\delta, \mathbf{N}_i^\gamma, \mathbf{N}_i^\delta), \quad (47)$$

respectively, where W is the free energy per unit area of the intermediate configuration B_r and \bar{w}_i is the interfacial energy per unit length of the local surface in B_r whose tangent is \mathbf{T}_i^γ . Invariance of \bar{w}_i under superimposed rigid body rotations requires $\bar{w}_i(\mathbb{H}_i^\gamma, \mathbb{H}_i^\delta, \mathbf{N}_i^\gamma, \mathbf{N}_i^\delta) = \tilde{w}_i(\mathbb{C}_i^\gamma, \mathbb{M}_i, \mathbf{N}_i^\gamma)$, where we have also used the fact that \mathbf{N}_i^δ can be expressed in terms of \mathbb{M}_i and \mathbf{N}_i^γ ; for a proof of both these assertions see [17]. Furthermore, we use (26)₂ and (29) to finally write Φ_i as

$$\Phi_i = \mu_i^\gamma w_i (v_i^\gamma, m_i, \theta_i^\gamma, \theta_i), \quad (48)$$

where θ_i^γ is such that $\mathbf{N}_i^\gamma = \cos \theta_i^\gamma \mathbf{e}_1 + \sin \theta_i^\gamma \mathbf{e}_2$ and θ_i is the angle between \mathbf{T}_i^γ and \mathbf{T}_i^δ . The representation (48) allows for the free energy of a general one-dimensional incoherent interface S_i to depend constitutively on (i) the local elastic stretch v_i^γ of the interface, (ii) the relative elastic (or plastic) stretch m_i between the two relaxed surfaces, (iii) the local orientation of the relaxed interface given by θ_i^γ , and (iv) the misorientation angle θ_i measuring the orientational mismatch of the adjacent lattices. The dependence on θ_i^γ characterises the anisotropic nature (interfacial orientation dependence) of the energy. For a coherent interface, the two relaxed surfaces coincide, and hence, $m_i = 1$ and $\theta_i = 0$. The interfacial energy is then a function of the local stretch and orientation. Incoherent interfacial energies without a dependency on v_i^γ and m_i are routinely considered for anisotropic grain boundaries [5].

Considering the hypothesis of hyperelastic response during elastic unloading, we assume the bulk and interfacial first Piola–Kirchhoff stresses to be given by [17, 18]

$$\mathbf{P} = J_G (\partial_{\mathbf{H}} W) \mathbf{G}^{-T} \quad \text{and} \quad \mathbb{P}_i \otimes \mathbf{T}_i = \mu_i^\gamma (\partial_{\mathbb{H}_i^\gamma} \bar{w}_i) (\mathbb{C}_i^\gamma)^{-T}, \quad (49)$$

respectively. The latter expression can be manipulated using (39)₂ and the chain rule of differentiation to derive

$$\mathbb{P}_i = \tau_i \mathbf{t}_i, \quad \text{where} \quad \tau_i = \frac{\partial w_i}{\partial v_i^\gamma}. \quad (50)$$

3.2.2 Local dissipation inequalities

We now come to the main aim of this section and derive the local dissipation inequalities in the bulk, at the interfaces, and at the junctions. The integral (42), on using compatibility relation $\nabla \mathbf{v} = \dot{\mathbf{F}}$, equilibrium (35), constitutive assumptions (47)₁ and (49)₁, and multiplicative decomposition (21), yields

$$I_1 = \int_{\Omega} \mathbf{E} \cdot \mathbf{G}^{-1} \dot{\mathbf{G}} dA, \quad \text{where} \quad (51)$$

$$\mathbf{E} = \Psi \mathbf{1} - \mathbf{F}^T \mathbf{P} \quad (52)$$

is the bulk Eshelby tensor [18].

In order to simplify (43), we start by rewriting the first two terms from its integrand as

$$V_i [\Psi] + [\mathbf{P}^T \mathbf{v}] \cdot \mathbf{N}_i = V_i [\mathbf{E}] \mathbf{N}_i \cdot \mathbf{N}_i - \frac{\partial \mathbb{P}_i}{\partial s_i} \cdot \mathbf{v}_i, \quad (53)$$

where we have used identity (3), definition of \mathbf{v}_i from (5)₂, compatibility relation (6), and equilibrium condition (36). Next, we use the chain rule to obtain the normal time derivative of Φ_i from (48) as

$$\dot{\Phi}_i = \Phi_i \frac{\dot{\mu}_i^\gamma}{\mu_i^\gamma} + \mu_i^\gamma \left(\frac{\partial w_i}{\partial v_i^\gamma} \dot{v}_i^\gamma + \frac{\partial w_i}{\partial m_i} \dot{m}_i + \frac{\partial w_i}{\partial \theta_i^\gamma} \dot{\theta}_i^\gamma + \frac{\partial w_i}{\partial \theta_i} \dot{\theta}_i \right). \quad (54)$$

Additionally, we have from (12) and (50)₁ that $\mathbb{P}_i \cdot \mathbb{f}_i = \tau_i \lambda_i$ and $\mathbb{P}_i \cdot \mathring{\mathbb{f}}_i = \tau_i \mathring{\lambda}_i$, where in the latter relation we have also used $\mathbf{t}_i \cdot \mathring{\mathbf{t}}_i = 0$. Finally, recall the multiplicative decomposition (25) and the constitutive relation (50)₂ and use the preceding equations in the integrand of (43) to obtain

$$I_2 = \sum_{i=1}^N \int_{S_i} \left(-V_i f_i + E_i \frac{\dot{\mu}_i^\gamma}{\mu_i^\gamma} + \mu_i^\gamma \left(\frac{\partial w_i}{\partial m_i} \dot{m}_i + \frac{\partial w_i}{\partial \theta_i^\gamma} \dot{\theta}_i^\gamma + \frac{\partial w_i}{\partial \theta_i} \dot{\theta}_i \right) \right) dL, \quad (55)$$

where

$$f_i = \llbracket \mathbf{E} \rrbracket \mathbf{N}_i \cdot \mathbf{N}_i + E_i \kappa_i \quad (56)$$

is the driving force for the normal velocity of the interface S_i and

$$E_i = \Phi_i - \lambda_i \tau_i \quad (57)$$

is the interfacial Eshelby tensor [15, 17, 32] for the i th interface.

Adding and subtracting $\mathbf{P}\mathbf{M} \cdot \mathbf{F}\mathbf{u}$ from the integrand in (44), we rewrite the integral I_3 as

$$I_3 = - \lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{E}\mathbf{M} \cdot \mathbf{u} dL - \lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{P}\mathbf{M} \cdot (\mathbf{v} + \mathbf{F}\mathbf{u}) dL \quad (58)$$

On the other hand, by adding and subtracting $\sum_{i=1}^N (\mathbb{F}_i^T \mathbb{P}_i \cdot \mathbf{q})$ from (45), and using the compatibility condition $V_i = \mathbf{q} \cdot \mathbf{N}_i$ (which ensures that the junction is non-splitting), we obtain

$$I_4 = - \sum_{i=1}^N (E_i \mathbf{T}_i \cdot \mathbf{q} + \mathbb{P}_i \cdot (\langle \mathbf{v} \rangle_i + \langle \mathbf{F} \rangle_i \mathbf{q}))_J, \quad (59)$$

where we have also used relations (5)₂ and (10)–(12). We assume enough smoothness of the deformation and the velocity fields such that the limiting value of both the convected velocities $(\mathbf{v} + \mathbf{F}\mathbf{u})$ and $(\langle \mathbf{v} \rangle_i + \langle \mathbf{F} \rangle_i \mathbf{q})$, as $\epsilon \rightarrow 0$ (uniformly in time), exists and is given by $\langle \mathbf{v} \rangle_J + \langle \mathbf{F} \rangle_J \mathbf{q}$, where $\langle \mathbf{v} \rangle_J = (1/N) \sum_{i=1}^N \langle \mathbf{v} \rangle_i$ and $\langle \mathbf{F} \rangle_J = (1/N) \sum_{i=1}^N \langle \mathbf{F} \rangle_i$ are average values of the velocity and deformation field at the junction [32]. The two expressions (58) and (59) can then be added to yield

$$I_3 + I_4 = - \left(\lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{E}\mathbf{M} dL + \sum_{i=1}^N E_i \mathbf{T}_i \right) \cdot \mathbf{q}, \quad (60)$$

where we have used equilibrium relation (37) to eliminate the other two terms.

We now substitute (51), (55), and (60) into (41) to obtain the reduced dissipation inequality in Ω as

$$\begin{aligned} & - \int_{\Omega} \mathbf{E} \cdot \mathbf{G}^{-1} \dot{\mathbf{G}} dA + \sum_{i=1}^N \int_{S_i} \left(V_i f_i - E_i \frac{\dot{\mu}_i^\gamma}{\mu_i^\gamma} - \mu_i^\gamma \left(\frac{\partial w_i}{\partial m_i} \dot{m}_i + \frac{\partial w_i}{\partial \theta_i^\gamma} \dot{\theta}_i^\gamma + \frac{\partial w_i}{\partial \theta_i} \dot{\theta}_i \right) \right) dL \\ & + \left(\lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{E}\mathbf{M} dL + \sum_{i=1}^N E_i \mathbf{T}_i \right) \cdot \mathbf{q} + \sum_{i=1}^N (\mathbf{c}_i \cdot \mathbb{w}_i - W_i E_i)_{A_i} \geq 0. \end{aligned} \quad (61)$$

The first term on the left-hand side of the inequality is the total dissipation rate due to bulk plasticity. The other terms represent excess entropy production within the domain. They include a group of terms with contribution from N internal interfaces, another group with contribution from the junction J , and a third group of terms representing the excess entropy contribution from N non-physical edges at which the interfaces S_i intersect with $\partial\Omega$. However, as mentioned earlier, we require our formulation to have excess entropy production only at the interfaces and the junction. The edges are in any case arbitrary as they depend on the choice of arbitrary Ω in B_0 . Consequently, in order to ensure that there is no contribution to the dissipation from the edges, we propose

$$\mathbf{c}_i = E_i \mathbf{T}_i, \quad (62)$$

where we have used (7). The global inequality (61) can then be localised, by choosing Ω appropriately, to obtain

$$\mathbf{E} \cdot \mathbf{G}^{-1} \dot{\mathbf{G}} \leq 0 \quad \text{in } \Omega_i, \quad (63)$$

$$V_i f_i - E_i \frac{\dot{\mu}_i^\gamma}{\mu_i^\gamma} - \mu_i^\gamma \left(\frac{\partial w_i}{\partial m_i} \dot{m}_i + \frac{\partial w_i}{\partial \theta_i^\gamma} \dot{\theta}_i^\gamma + \frac{\partial w_i}{\partial \theta_i} \dot{\theta}_i \right) \geq 0 \quad \text{on } S_i, \quad \text{and} \quad (64)$$

$$\mathbf{f}_J \cdot \mathbf{q} \geq 0 \quad \text{at } J, \quad (65)$$

where

$$\mathbf{f}_J = \lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{E} \mathbf{M} \, dL + \sum_{i=1}^N E_i \mathbf{T}_i \quad (66)$$

is the driving force for junction evolution; it depends on both the bulk Eshelby tensor evaluated in a close neighbourhood of J and the limiting values of the interfacial Eshelby tensors related to the interfaces which intersect at the junction. The well-known bulk dissipation inequality (63) is the starting point for deriving flow rules for finite deformation plastic evolution in the bulk [18,19]; this is done in the following section. The dissipation at the interface as governed by (64) has, on the other hand, contributions from several distinct mechanisms. These include interface motion V_i , interfacial plasticity (governed by the evolution of plastic stretch $\dot{\mu}_i^\gamma$ and orientation $\dot{\theta}_i^\gamma$), and the evolution of interfacial incompatibility or defect content (characterised by \dot{m}_i and $\dot{\theta}_i$). The inequality in (64) forms a basis for developing flow rules for interfacial plasticity and defect evolution as well as kinetic laws for interfacial dynamics; this programme is pursued in the next section. When the interface is coherent and there is no plasticity, then this inequality can be shown to reduce to a form derived earlier in [15]. For an incoherent interface, but with vanishing plasticity, it agrees with the expression obtained in [9]. For grain boundaries, where stretches are ignored and misorientation is assumed to be homogeneous, it simplifies to a form derived recently by the authors [3,5]. The dissipation inequality at the junction (65) will be used to formulate a kinetic relation for junction evolution. A similar inequality, although in the context of coherent interfaces in elastic solids, was derived in [32].

3.2.3 Free surfaces and edges

In this subsection, we obtain balance relations and dissipation rates at the free surface of the body and at the physical edges which are points where internal boundaries intersect the free surface. The boundary ∂B_0 is accordingly taken to be deformable and endowed with surface energy, strain fields, and stress fields. We denote a typical physical edge as A_e (see Fig. 1a). The nature of this edge can be seen analogously to a junction J in the interior of the body, except for the fact that two of the curves meeting at A_e (the surface boundaries) are non-migrating material surfaces. Moreover, the edge is constrained to move along ∂B_0 . Its velocity, denoted by \mathbf{q}_e , will therefore be of the form

$$\mathbf{q}_e = q_e \mathbf{T}', \quad (67)$$

where \mathbf{T}' denotes the tangent along ∂B_0 . Let us denote the free surface first Piola stress by $\mathbb{P}' \otimes \mathbf{T}'$. Let $\mathbf{P}^{\text{out}} \mathbf{M}$ be the applied traction on ∂B_0 (away from edges), and $\mathbb{P}^{\text{out}}|_{A_e}$ the surface traction applied along the interface at A_e . The linear momentum balance then requires

$$\mathbf{P} \mathbf{M} - \frac{\partial \mathbb{P}'}{\partial s'} = \mathbf{P}^{\text{out}} \mathbf{M} \quad (68)$$

for all points on ∂B_0 (except the edges), where s' is a local arc-length parameter (starting at A_e and increasing in the direction of the tangent \mathbf{T}') associated with B_0 , and

$$\lim_{\epsilon \rightarrow 0} \oint_{C_\epsilon} \mathbf{P} \mathbf{M} \, dL + \llbracket \mathbb{P}' \rrbracket_{A_e} + \mathbb{P} = \mathbb{P}^{\text{out}} \quad \text{at } A_e, \quad (69)$$

where C_ϵ is the boundary of a small circular disc of radius ϵ centred at A_e , and $\llbracket \mathbb{P}' \rrbracket_{A_e} = \mathbb{P}'|_{s'=0^+} - \mathbb{P}'|_{s'=0^-}$. Recall that $\mathbb{P} \otimes \mathbf{T}$ is the first Piola stress associated with the interface (with tangent \mathbf{T}) intersecting B_0 at A_e . On the other hand, the balance of angular momentum requires \mathbb{P}' to be parallel to the tangential direction \mathbf{t}' of the external surface in the deformed configuration, i.e. $\mathbf{t}' \times \mathbb{P}' = \mathbf{0}$.

Let Φ' be the energy density of the external boundary per unit length in the reference configuration such that $\Phi' = \mu' w'(v', \theta')$, where w' is the energy of the boundary per unit length in the intermediate configuration; here, v' and μ' are elastic and plastic stretches, respectively, at the boundary such that the total boundary stretch $\lambda' = v' \mu'$, and θ' denotes the orientation of the surface. The local dissipation inequalities, derived in a manner analogous to that of internal boundaries and junctions, are

$$-\left(E' \frac{\dot{\lambda}'}{\mu'} + \mu' \frac{\partial w'}{\partial \theta'}\right) \geq 0 \quad (70)$$

on the boundary ∂B_0 away from the edges, and

$$f_e q_e \geq 0 \quad \text{at } A_e, \quad (71)$$

where

$$f_e = \mathbf{T}' \cdot \left(\lim_{\epsilon \rightarrow 0} \oint_{C_e^\epsilon} \mathbf{E} \mathbf{M} \, dL + \mathbf{E} \mathbf{T} + \llbracket \mathbf{E}' \rrbracket \mathbf{T}' \right) \quad (72)$$

is the driving force for junction dynamics (see also [32]). Here, $\mathbf{E}' = \Phi' - \tau' \lambda'$ is the surface Eshelby tensor with $\tau' = \partial w' / \partial v'$.

4 Flow rules and kinetic relations

Starting with the local dissipation inequalities from the previous section, we will now derive flow rules, governing plastic evolution in the bulk, at the interfaces, and at the external boundary. We will also derive kinetic relations, which govern interfacial, edge, and junction dynamics. We will assume the material response (both elastic and plastic) to be isotropic. The rate-independent flow rules are derived with the help of maximum dissipation postulate while assuming the yield loci (both in the bulk and at the interface) to depend on the accumulated plastic strain and an appropriate measure of inhomogeneity. The latter is taken as the incompatibility tensor (which is derived from the Riemann curvature tensor) in the bulk and the relative stretch m at the interface. The interfacial energy is taken to depend only on the scalar elastic stretch v and the relative stretch m . The free boundary energy is considered to be a function of the scalar elastic stretch alone. The kinetic relations are obtained within the framework of linear irreversible thermodynamics. Our emphasis is to expose the coupling between various flow rules and kinetic relations as well as to bring out the role of interfaces, boundary, edges, and junctions in influencing overall plasticity of the solid. We will first present results in the context of a finite deformation theory and then simplify the results for small deformations, where both elastic and plastic strains will be assumed to be infinitesimal. We will conclude the discussion by relating our results to those obtained in the recent literature.

4.1 Finite deformation theory

We divide this section into four parts: obtaining the required relations separately in the bulk, at the interface, at the boundary, and at the junction/edge. A detailed treatment of the flow rules in the bulk, of the kind that are presented here and in the next subsection, is presented elsewhere [18, 19, 23].

4.1.1 Bulk plasticity

The Eshelby tensor (52), combined with relations (47)₁ and (49)₁, can be used to define [18]

$$\mathbf{E}' = J_G^{-1} \mathbf{G}^{-T} \mathbf{E} \mathbf{G}^T = \hat{W}(\mathbf{C}_H) \mathbf{1} - \mathbf{C}_H \mathbf{S}(\mathbf{C}_H), \quad (73)$$

where $\mathbf{C}_H = \mathbf{H}^T \mathbf{H}$, $\hat{W}(\mathbf{C}_H)$ is the strain energy density (with respect to B_r), and $\mathbf{S}(\mathbf{C}_H) = \partial_{\mathbf{C}_H} \hat{W}$ is the second Piola–Kirchhoff stress (relative to B_r). Note that \mathbf{E}' is the Eshelby tensor pushed forward to the relaxed configuration B_r ; it is purely elastic in origin. Using (73), we can rewrite the dissipation inequality (63) as

$$\mathbf{E}' \cdot \dot{\mathbf{G}} \mathbf{G}^{-1} \leq 0. \quad (74)$$

For isotropic response, every eigenvector of \mathbf{C}_H is an eigenvector of $\mathbf{S}(\mathbf{C}_H)$; hence, $\mathbf{E}' \in \text{Sym}$. As a result plastic spin, defined by $\text{skw}(\dot{\mathbf{G}} \mathbf{G}^{-1})$, does not contribute to the dissipation rate. In fact, it can be shown to vanish identically under the assumption of isotropy (see Ch. 97 in [20]); for an alternate viewpoint in gradient plasticity see [11, 27]. For anisotropic response, however, prescription of plastic spin leads to additional constitutive restrictions and should not be ignored [33]. The inequality (74) therefore takes the form

$$\mathbf{E}' \cdot \mathbf{D}_G \leq 0, \quad (75)$$

where $\mathbf{D}_G = \text{sym}(\dot{\mathbf{G}} \mathbf{G}^{-1})$ is the plastic stretch rate tensor.

We consider rate-independent plastic deformation. The yield locus is taken as a level set in Sym parametrised by a scalar variable (cf. [23]):

$$\mathcal{F}(\mathbf{E}', E_G) = 0, \quad (76)$$

where \mathcal{F} is assumed to be differentiable with respect to its arguments. The parameter E_G is a measure of the accumulated plastic strain whose rate $\dot{E}_G > 0$ is defined as

$$\dot{E}_G = d_G + c|\ell^2 \dot{\mathbf{\Pi}}|, \quad (77)$$

where $d_G = \sqrt{\frac{2}{3} \mathbf{D}_G \cdot \mathbf{D}_G}$ is the effective plastic strain rate, c is a phenomenological material constant, ℓ is a constant representing an internal length scale (associated with the inhomogeneity) of the material, and $\mathbf{\Pi}$ is the symmetric Einstein tensor whose components in the notation of tensor analysis are given by [36]

$$\Pi^{pq} = \mathcal{E}^{pij} \mathcal{E}^{qkl} \mathcal{R}_{ijkl}, \quad (78)$$

where $\mathcal{E}^{pij} = \mathcal{E}^{pij} / \sqrt{\det(\mathcal{M}_{mn})}$, \mathcal{E}^{pij} is the component of the alternate tensor, \mathcal{R}_{ijkl} are the components of the Riemann–Christoffel curvature tensor induced by the Riemann metric $\mathcal{M} = \mathbf{G}^T \mathbf{G}$. The Einstein tensor completely characterises the measure of material inhomogeneity in an isotropic solid [28]. In the present 2D setting, the Riemann curvature tensor reduces to one independent term given by Gaussian curvature (associated with the metric $\mathbf{G}^T \mathbf{G}$) [36]. Equation (77) generalises the classical relation for accumulated plastic strain in conventional plasticity, where it is simply equal to d_G , to include the effect of inhomogeneity. Similar extensions have been proposed in the recent literature on strain gradient plasticity, see e.g. [20].

We assume the plastic evolution to follow maximum dissipation hypothesis according to which, for a given plastic rate \mathbf{D}_G at a fixed material point, the associated \mathbf{E}' value is the one which maximises the dissipation $-\mathbf{E}' \cdot \mathbf{D}_G$ while restricting the stress states to the elastic range given by $\mathcal{F}(\mathbf{E}', E_G) \leq 0$. The Kuhn–Tucker necessary condition associated with this optimisation problem requires \mathbf{D}_G to be parallel to the outward normal to the yield surface

$$\mathbf{D}_G = -\dot{\xi} \partial_{\mathbf{E}'} \mathcal{F}, \quad (79)$$

where $\dot{\xi} \geq 0$ is the plastic multiplier. If, for example, we consider a von Mises-type yield criterion

$$\mathcal{F}(\mathbf{E}', E_G) = \sigma_e - K(E_G), \quad (80)$$

where $\sigma_e = \left(\frac{3}{2} \mathbf{E}' \cdot \mathbf{E}'\right)^{1/2}$ is the effective Eshelby stress and $K(E_G) = K_0 + H E_G$; K_0 and H are material constants denoting the initial flow stress and hardening function, respectively. The flow rule (79) then implies that $\dot{\xi} = d_G$. Hence, the total plastic evolution \mathbf{D}_G is determined if d_G is known. The governing equation for d_G is obtained from the consistency condition $\dot{\mathcal{F}} = 0$ as $H \dot{E}_G = \dot{\sigma}_e$. Recalling (77), we note that this relation gives a highly nonlinear partial differential equation for d_G thereby furnishing a non-local evolution of plastic deformation in the bulk.

4.1.2 Interfacial flow rule and kinetic relations

For an isotropic material response, the free energy of an interface will be necessarily independent of orientation and misorientation parameters; the representation (48) for the i th interface is henceforth considered in the reduced form

$$\Phi_i = \mu_i^\gamma w_i(v_i^\gamma, m_i). \quad (81)$$

The dissipation inequality (64) can then be rewritten as

$$V_i f_i + \bar{E}_i \dot{\mu}_i^\gamma + \beta_i \dot{m}_i \geq 0, \quad (82)$$

where

$$\bar{E}_i = -\frac{E_i}{\mu_i^\gamma} = -(w_i - \tau_i v_i^\gamma) \quad \text{and} \quad \beta_i = -\mu_i^\gamma \frac{\partial w_i}{\partial m_i}. \quad (83)$$

To simplify matters at hand, we work with a sufficient condition for inequality (82) by decoupling it into two parts:

$$V_i f_i \geq 0 \quad \text{and} \quad \bar{E}_i \dot{\mu}_i^\gamma + \beta_i \dot{m}_i \geq 0. \quad (84)$$

Based on (84)₁, we assume a linear kinetic relation

$$V_i = \mathcal{M}_i f_i, \quad (85)$$

where $\mathcal{M}_i \geq 0$ is the constant mobility of the interface. We use (84)₂ to derive flow rules for plasticity at the interface. We assume the evolutions of m_i and μ_i^γ on a moving S_i to be rate-independent. The interface S_i is at a state of yield if the yield function, denoted by $\mathcal{G}_i(\zeta_i^e, e_i)$, satisfies

$$\mathcal{G}_i(\zeta_i^e, e_i) = 0, \quad (86)$$

where ζ_i^e and e_i denote effective stress and accumulated plastic deformation at S_i , defined as

$$\zeta_i^e = \sqrt{\bar{E}_i^2 + \beta_i^2}, \quad (87)$$

and

$$e_i = \int_0^t \dot{e}_i dt, \quad (88)$$

respectively. The effective plastic flow rate \dot{e}_i is taken as

$$\dot{e}_i = |\dot{\mu}_i^\gamma| + |\dot{m}_i|. \quad (89)$$

Note that the integrand in (88) implicitly depends on V_i owing to the definition of the normal time derivative. When the interface deforms elastically, the yield function $\mathcal{G}_i(\zeta_i^e, e_i) < 0$ and the effective plastic flow rate \dot{e}_i vanishes.

The postulation of maximum plastic dissipation at the interface, for dissipation given by (84)₂, subjected to $\mathcal{G}_i \leq 0$ leads to the Kuhn–Tucker necessary conditions

$$\dot{\mu}_i^\gamma = \dot{\zeta}_i \frac{\partial \mathcal{G}_i}{\partial \bar{E}_i} \quad \text{and} \quad \dot{m}_i = \dot{\zeta}_i \frac{\partial \mathcal{G}_i}{\partial \beta_i}, \quad (90)$$

where $\dot{\zeta}_i \geq 0$ is the plastic multiplier for the moving interface which is strictly positive wherever the interface is at a state of yield. If, for example, we use a von Mises type of yield function at the interface

$$\mathcal{G}_i = \zeta_i^e - k_i(e_i), \quad (91)$$

where k_i is the flow stress within S_i such that $k_i = (k_0)_i + h_i e_i$, where $(k_0)_i$ and h_i are constants. Consistency condition $\dot{\mathcal{G}}_i = 0$ yields $\dot{\zeta}_i^e = h_i \dot{e}_i$, which gives the required evolution law for effective plastic flow rate at the interface when S_i is yielding. The plastic multiplier can be obtained using (89) and (90) as

$$\dot{\zeta}_i = \frac{\dot{\zeta}_i^e \zeta_i^e}{h_i (|\bar{E}_i| + |\beta_i|)}. \quad (92)$$

The normal time derivatives include a dependence on the normal velocity V_i . This necessarily couples the plasticity flow rules as prescribed above to the moving interface. These flow rules provide boundary conditions for plastic deformation in the bulk. The evolution Eq. (90) themselves are partial differential equations (the derivatives are hidden within the normal time derivative), and they need boundary conditions. These equations are provided by the junction conditions.

4.1.3 Plastic flow at external boundary

Assuming the energy of the external boundary of the body to be isotropic (independent of crystalline orientation θ'), the dissipation inequality (70) reduces to

$$\bar{E}' \dot{\mu}' \geq 0, \quad (93)$$

where $\bar{E}' = -E'/\mu'$. We consider rate-independent isotropic elastic–plastic response and follow the same procedure of Sect. 4.1.2 to derive the necessary equations. The boundary will be in a state of yield if the yield function $\mathcal{G}'(\zeta'^e, e')$ satisfies

$$\mathcal{G}'(\zeta'^e, e') = 0, \quad (94)$$

where the effective surface stress $\zeta'^e = |\bar{E}'|$, effective plastic strain rate $\dot{e}' = |\dot{\mu}'|$, and effective plastic strain $e' = \int_0^t \dot{e}' dt$. During elastic deformation, the yield function satisfies $\mathcal{G}' < 0$ and the effective plastic flow rate \dot{e}' vanishes. Considering the postulation of maximum dissipation at the boundary subjected to $\mathcal{G}' \leq 0$, we obtain the flow rule

$$\dot{\mu}' = \dot{\zeta}' \frac{\partial \mathcal{G}'}{\partial \bar{E}'}, \quad (95)$$

where $\dot{\zeta}'$ is the plastic multiplier for the boundary. Assuming a von Mises type of yield function given by $\mathcal{G}' = \zeta'^e - k'(e)$, where the yield stress $k'(e) = k'_0 + h'e'$ (k'_0 is a constant flow stress and h' is a constant hardening function), and taking the consistence condition $\dot{\mathcal{G}}' = 0$ into account, we get $\dot{\zeta}' = h'\dot{e}'$, which can be used to obtain the effective plastic strain rate. In particular, the plastic multiplier is obtained as $\dot{\zeta}' = \dot{e}'$.

4.1.4 Junction and edge kinetics

Based on the inequalities (65) and (71), we postulate linear kinetic laws for the junction and edge dynamics as

$$\mathbf{q} = \mathcal{M}_J \mathbf{f}_J \quad \text{and} \quad q_e = \mathcal{M}_e f_e, \quad (96)$$

respectively, where $\mathcal{M}_J \geq 0$ and $\mathcal{M}_e \geq 0$ are the mobilities at the corresponding points. Note that \mathbf{f}_J depends on the instantaneous junction angles which should be determined from the compatibility relation $V_i = \mathbf{q} \cdot \mathbf{N}_i$ for $i = 1, \dots, N$ when the junction mobility is finite, see [3, 12] for details and also for the case when $\mathcal{M}_J \rightarrow \infty$.

4.2 Small deformation theory

We now specialise the above flow rules and kinetic relations assuming small deformation and small strains (both elastic and plastic). The order of smallness of all these variables is assumed to be same. The obtained results give us the simplest setting in which meaningful initial-boundary value problems can be posed. Additionally, they provide us with grounds of comparison with recent work in strain gradient plasticity.

4.2.1 Bulk plasticity

Under the assumption of small deformation and small strains, the multiplicative decomposition (21) readily reduces down to an additive decomposition given by

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}_H + \boldsymbol{\epsilon}_G, \quad (97)$$

where $\boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}_H$, and $\boldsymbol{\epsilon}_G$ denote total, elastic, and plastic infinitesimal strain, respectively, such that their norms are much less than unity (but of the same order). Therefore, we can write (to the leading-order term), $\mathbf{F} = \mathbf{1} + \boldsymbol{\omega} + \boldsymbol{\epsilon}$, $\mathbf{H} \approx \mathbf{1} + \boldsymbol{\omega} + \boldsymbol{\epsilon}_H$, and $\mathbf{G} \approx \mathbf{1} + \boldsymbol{\epsilon}_G$; here, we have ignored the infinitesimal plastic rotation (due to isotropy, see previous subsection), and hence, elastic rotation and total rotation are identical (given by $\boldsymbol{\omega} \in \text{Skw}$). We additionally assume plastic incompressibility in the bulk, i.e. $\text{tr } \boldsymbol{\epsilon}_G = 0$ or equivalently $\text{tr } \dot{\boldsymbol{\epsilon}}_G = 0$.

The (isotropic) strain energy density \tilde{W} and the second Piola–Kirchhoff stress, with respect to the intermediate configuration, are reduced to

$$\tilde{W} \approx \frac{1}{2} c_1 (\text{tr } \boldsymbol{\epsilon}_H)^2 + c_2 \boldsymbol{\epsilon}_H \cdot \boldsymbol{\epsilon}_H \quad \text{and} \quad (98)$$

$$\mathbf{S}_H = \boldsymbol{\sigma} + o(|\boldsymbol{\epsilon}_H|), \quad \text{where} \quad \boldsymbol{\sigma} = c_1 (\text{tr } \boldsymbol{\epsilon}_H) \mathbf{1} + 2 c_2 \boldsymbol{\epsilon}_H, \quad (99)$$

where $\boldsymbol{\sigma}$ is the symmetric Cauchy stress, and c_1 and c_2 are Lamé constants. Note that the energy density is (almost) same per unit area of the reference or the intermediate configuration. The first Piola–Kirchhoff stress also reduces to $\boldsymbol{\sigma}$ to the leading order. As a result, we have from (52), $\mathbf{E} \approx -\boldsymbol{\sigma}$. Substituting this in the dissipation inequality (63) and retaining only the leading-order terms, we have

$$\boldsymbol{\sigma}_d \cdot \dot{\boldsymbol{\epsilon}}_G \geq 0, \quad (100)$$

where $\boldsymbol{\sigma}_d$ is the deviatoric part of $\boldsymbol{\sigma}$. The yield locus is accordingly taken as

$$\mathcal{F}(\boldsymbol{\sigma}_d, E_G) = 0, \quad (101)$$

where $E_G = \int_0^t \dot{E}_G dt$ and the accumulated plastic strain rate is now given by

$$\dot{E}_G = \sqrt{2/3} |\dot{\boldsymbol{\epsilon}}_G| + \ell^2 \eta, \quad (102)$$

where the rate of Gaussian curvature, here represented by the scalar incompatibility rate η (rate of the non-trivial component of the rate of curl curl $\boldsymbol{\epsilon}_G$ which is known as the Kröner's incompatibility tensor and can be obtained by linearising (78)), has a simple form

$$\eta = \left| \left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) \dot{\epsilon}_G^{11} - 2 \frac{\partial^2 \dot{\epsilon}_G^{12}}{\partial x \partial y} \right|, \quad (103)$$

where $\dot{\epsilon}_G^{ab}$ denotes the ab th component of the plastic strain $\dot{\boldsymbol{\epsilon}}_G$ in the Cartesian coordinate system (both a and b take value of either 1 or 2). Following the last subsection, we consider a yield function

$$\mathcal{F}(\boldsymbol{\sigma}_d, E_G) = \sigma_e - (K_0 + H E_G), \quad (104)$$

where $\sigma_e = \left(\frac{3}{2} \boldsymbol{\sigma}_d \cdot \boldsymbol{\sigma}_d \right)^{1/2}$ is the effective stress. The associative flow rule then implies $\dot{\boldsymbol{\epsilon}}_G = \frac{3\dot{\epsilon}}{2\sigma_e} \boldsymbol{\sigma}_d$ which when combined with the consistency condition provides a partial differential equation to solve for the plastic multiplier.

4.2.2 Interfacial flow rule and kinetic relations

The strains (total, elastic, and plastic) are infinitesimally small. As a result, we can write

$$\lambda_i \approx 1 + \Xi_i, \quad \mu_i^\alpha \approx 1 + \epsilon_i^\alpha, \quad \text{and} \quad \nu_i^\alpha \approx 1 + \epsilon_i^\alpha, \quad (105)$$

such that $|\Xi_i| \ll 1$, $|\epsilon_i^\alpha| \ll 1$, and $|\epsilon_i^\alpha| \ll 1$ (α stands for either δ or γ). The multiplicative decomposition of stretches (25) is therefore reduced to an additive decomposition given by

$$\Xi_i = \epsilon_i^\alpha + \epsilon_i^\alpha. \quad (106)$$

The relative stretch can also be approximated as $m_i \approx 1 + \kappa_i$, where κ_i can be written using (29) as

$$\kappa_i = \epsilon_i^\delta - \epsilon_i^\gamma = \epsilon_i^\gamma - \epsilon_i^\delta; \quad (107)$$

it represents the measure of incoherency at the i th interface when the strains are small and material response is isotropic. On the other hand, neglecting residual stress at the interface, we retain only the quadratic terms in the interfacial free energy:

$$\tilde{w}_i(\epsilon_i^\gamma, \kappa_i) \approx \frac{1}{2} a_i (\epsilon_i^\gamma)^2 + \frac{1}{2} b_i \kappa_i^2, \quad (108)$$

where $a_i > 0$ is the modulus of elasticity of the interface and $b_i > 0$ is another interfacial constant which we call the modulus of incoherency. The interfacial first Piola–Kirchhoff stress is approximately given by $\tau_i \mathbf{t}_i \otimes \mathbf{t}_i$, where we calculate

$$\tau_i \approx a_i \epsilon_i^\gamma \quad (109)$$

using (50)₂ and (108).

The leading-order terms in the linear momentum balance relation at the interface (36) yield

$$[[\boldsymbol{\sigma}]] \mathbf{n}_i \cdot \mathbf{n}_i + \tau_i \kappa_i = 0. \quad (110)$$

In writing the bulk and the surface Eshelby tensors, we retain terms upto quadratic order since the linear term will cancel out to give a trivial result. Under present assumptions, we have

$$\mathbf{E} \approx \tilde{W}\mathbf{1} - (\boldsymbol{\sigma} + 2\boldsymbol{\epsilon}_H\boldsymbol{\sigma} + (\boldsymbol{\epsilon}_G\boldsymbol{\sigma} - \boldsymbol{\sigma}\boldsymbol{\epsilon}_G)) \quad \text{and} \quad (111)$$

$$E_i \approx \tilde{w}_i - \tau_i(1 + \Xi_i). \quad (112)$$

The dissipation inequality at the interface is quadratic to the leading order:

$$V_i \hat{f}_i + \tau_i \dot{\hat{\epsilon}}_i^\gamma + \hat{\beta}_i \dot{\hat{\kappa}}_i \geq 0 \quad \text{on } S_i, \quad (113)$$

where

$$\hat{f}_i = \llbracket \tilde{W}\mathbf{1} - 2\boldsymbol{\epsilon}_H\boldsymbol{\sigma} \rrbracket \mathbf{n}_i \cdot \mathbf{n}_i + (\tilde{w}_i - \tau_i \Xi_i) \kappa_i \quad \text{and} \quad \hat{\beta}_i = -b_i \kappa_i. \quad (114)$$

Following Sect. 4.1.2, the interfacial dynamics is assumed to be governed by

$$V_i = \mathcal{M}_i \hat{f}_i. \quad (115)$$

The interfacial yield function is now taken as

$$\hat{\mathcal{G}}_i = \hat{\zeta}_i - k_i (\hat{e}_i), \quad (116)$$

as before, where

$$\hat{\zeta}_i = \sqrt{\tau_i^2 + \hat{\beta}_i^2} \quad \text{and} \quad \hat{e}_i = |\dot{\hat{\epsilon}}_i^\gamma| + |\dot{\hat{\kappa}}_i|. \quad (117)$$

The evolution of plastic strain and incoherency, based on the postulate of maximum plastic dissipation, can be obtained as

$$\dot{\hat{\epsilon}}_i^\gamma = \dot{\hat{\zeta}}_i \frac{\tau_i}{k_i} \quad \text{and} \quad \dot{\hat{\kappa}}_i = \dot{\hat{\zeta}}_i \frac{\hat{\beta}_i}{k_i}. \quad (118)$$

The plastic multiplier can be obtained from the consistency condition, $\dot{\hat{\mathcal{G}}}_i = 0$, as

$$\dot{\hat{\zeta}}_i = \frac{\dot{\hat{\zeta}}_i \hat{\zeta}_i}{h_i \left(|\tau_i| + |\hat{\beta}_i| \right)}. \quad (119)$$

4.2.3 Plastic flow at the external boundary

The dissipation inequality for the external boundary (93) simplifies to

$$\tau' \dot{e}' \geq 0, \quad (120)$$

where e' is the infinitesimal plastic strain along the external boundary. We consider the yield function $\hat{\mathcal{G}}' = \hat{\zeta}' - \hat{k}'(\hat{e}')$ as before, where $\hat{\zeta}' = |\tau'|$ is the effective stress, $\hat{e}' = |\dot{e}'|$ is the effective plastic strain rate, and $\hat{e}' = \int_0^t |\dot{e}'| dt$ is the effective plastic strain. Using the postulation of maximum dissipation, the flow rule is obtained as $\dot{e}' = \dot{\zeta}' \text{sign}(\tau')$, where $\text{sign}(\tau') = +1$ if $\tau' > 0$ and -1 if $\tau' < 0$, and the consistency condition $\dot{\hat{\mathcal{G}}}' = 0$ yields $\dot{\zeta}' = \dot{e}'$.

4.2.4 Comparison with the previous work

Our flow rules are comparable to those derived in [1, 13, 14] when we restrict ourselves to small deformation theory and stationary interfaces. Even then, there are several points of departure between our treatments with these recent studies. In order to incorporate the size effect, [1, 14] consider the energy of the bulk to depend on total strain, plastic strain, and gradient of the plastic strain. As a consequence, a higher-order stress called the moment stress gets introduced in the theory and the local dissipation in the bulk is due to the evolution of plastic strain and its gradient. On the other hand, [13] considers an equivalent plastic strain rate and its gradient, which contributes to the dissipation in the bulk region through respective higher-order scalar stress and its gradient. We incorporate the size effect by considering the flow stress to depend on an effective measure of material inhomogeneity which has the dimension of inverse of the square of the length. An additional length scale, denoting the size of the grain, will also appear naturally in our framework.

Secondly, [1, 13, 14] assume that the interfacial potential depends on the limiting value of the total bulk plastic strain at the interface. As a consequence, the local dissipation within the interface occurs due to the

evolution of plastic strain within it, whereas in our theory, the dissipative fluxes at the interface are due to the evolution of plastic strain on one side of the interface and difference in plastic strain on the disjoint lines of the interface in intermediate configuration. When the interface is stationary, i.e. $V = 0$, the dissipation within the interface occurs due to plastic flow on one side of the interface in the intermediate configuration aided by the evolution of incoherency.

Finally, we note that our model can be viewed as a part of a larger class of second-gradient-type theories, where the interfaces are modelled from a unified point of view as boundary-layer-type solutions, see for example recent works of dell'Isola and coworkers [10,24,30].

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