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Kinetics of phase boundaries with edges and junctions in a three-dimensional multi-phase body

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Abstract

The propagation of phase boundaries that intersect other phase boundaries at junctions and physical boundaries at edges in a three-dimensional multi-phase body is examined. The driving forces that govern the propagation of these phase boundaries, edges and junctions are calculated, and kinetic relations consistent with the second law of thermodynamics are proposed. This work extends the two-dimensional situation discussed previously (Simha, N.K., Bhattacharya, K., 1998. J. Mech. Phys. Solids, 46, 2323–2359). © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The propagation of phase boundaries is of great interest in a variety of phenomena and has been studied extensively (see, for example, Abeyaratne and Knowles, 1990; Eshelby, 1970; Larche and Cahn, 1973; Gurtin, 1995; Heidug and Lehner, 1985; Leo and Sekerka, 1989; Mullins, 1956; Truskinovsky, 1982 and references therein).

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In a recent paper (Simha and Bhattacharya, 1998), we studied this problem with particular attention to the *edge* where a phase boundary meets the physical boundary of the specimen and the *junction* where two or more phase boundaries meet. Two issues are important at edges and junctions:

- The evolution of an isolated or an infinite phase boundary is completely determined by its normal velocity. However, we need *additional information* to uniquely determine the evolution of a finite phase boundary that ends at an edge or a junction: in Simha and Bhattacharya (1998) we describe a simple example where two interfaces starting from the same initial position and with the same normal velocity evolve quite differently due to an edge. In the setting of curvature-driven propagation, this additional information is usually provided using a 'contact-angle or triple-junction condition' (Herring's or Young's condition), which is obtained from a balance of surface tensions (see, for example, Murr, 1975). However, this is not completely satisfactory since careful experiments in fluids show that the contact angle can change with the velocity of the interface (Hoffman, 1975)[1]. Further, this condition is derived from equilibrium, but phase boundaries propagate exactly when they are not in equilibrium.
- The elastic moduli of the different phases or variants can be different. Consequently, the stress and strain can be *singular* at the edge. This singularity may play a significant role in determining the kinetics of the entire interface. In Simha and Bhattacharya (1998) we show, using an example, that this singularity depends on the contact angle and can be severe enough to contribute to the kinetics.

We discuss these issues in detail in Simha and Bhattacharya (1998). We then show that it is necessary to prescribe an evolution law for the edge and the junction in addition to the evolution law of the interface, and we derive thermodynamically consistent forms for these laws. We point out the profound influence that these laws can have on the propagation of the phase boundaries through detailed numerical computations.

The analysis in that paper, however, is limited to two-dimensional bodies where phase boundaries are lines and edges/junctions are points. The current paper generalizes the analysis to three dimensions; this extension is non-trivial in view of the significant difference in the kinematics of two and three dimensions. The scope of this paper is limited to the essential calculations, and the reader is referred to Simha and Bhattacharya (1998) for further discussion.

Our main result is a framework for prescribing a physically meaningful and thermodynamically consistent evolution law for a junction of k interfaces (or phase

[1] There are some indirect experimental indications even in martensites (see, for example, Fig. 2(a) of Chiao and Chen, 1990).

boundaries) in a multi-phase elastic body shown in Fig. 1. We first identify a *thermodynamic driving force* on the junction, Eq. (69). It has k+2 contributions: one contribution from the elastic singularity in the bulk, one contribution each from the k interfaces and a final contribution from the junction line. We then relate this driving force to the corresponding *velocity* using a *kinetic relation* (74) which satisfies the thermodynamic restriction (75). We obtain similar results [Eq. (70)] for an edge by observing that an edge can be regarded as a special (constrained) case of a triple junction.

We follow the framework developed by Abeyaratne and Knowles (1990) and Gur-

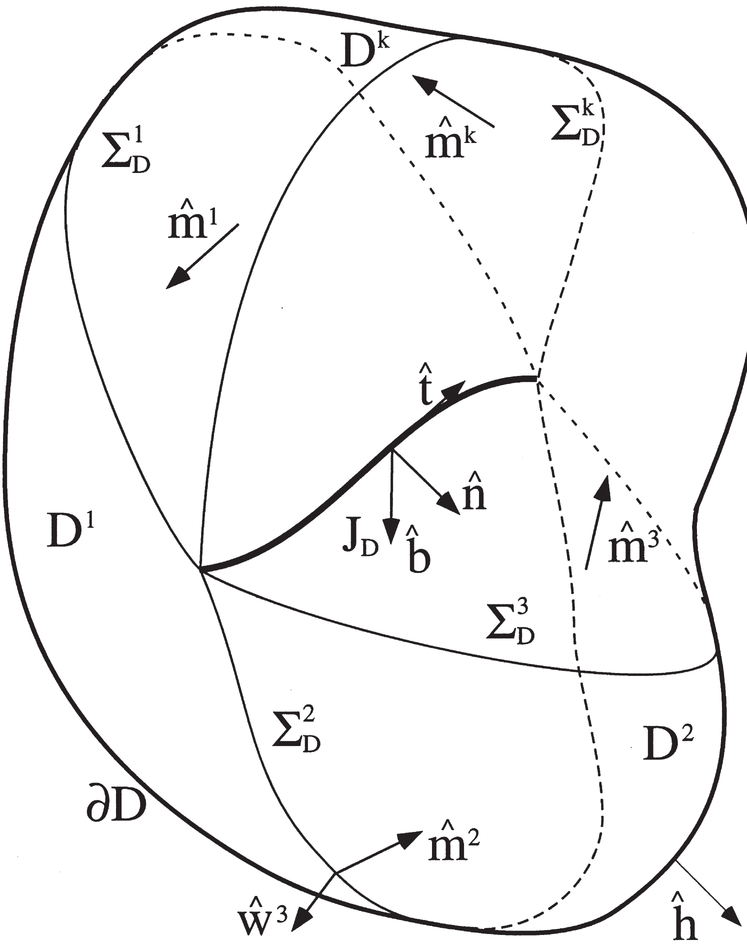

Fig. 1. The multi-phase body Ω contains k interfaces Σ^i, i=1, 2, …, k that intersect at the junction J, and a part $\mathcal{D}\subset\Omega$ is shown in the reference configuration. The part of the interface Σ^i inside $\mathcal{D}$ is Σ^i_D, while the part of the junction J within $\mathcal{D}$ is J_D. The external normal to the boundary ∂D is $\hat{\mathbf{h}}$. The normal to the interface Σ^i is $\hat{\mathbf{m}}^i$, while the external normal to the boundary curve $\partial\Sigma^i_D$ is $\hat{\mathbf{w}}^i$. The tangent $\hat{\mathbf{t}}$, normal $\hat{\mathbf{n}}$ and binormal $\hat{\mathbf{b}}$ to the junction curve are also shown.

tin (1995), amongst others, to identify the driving force. We calculate the energy dissipated by a propagating interface, and show that the dissipation per unit length of the junction may be written as $\tilde{\mathbf{d}}_J \cdot \tilde{\mathbf{v}}_p$, where $\tilde{\mathbf{v}}_p$ is the velocity of the junction and $\tilde{\mathbf{d}}_J$ is given by Eq. (69). We thus identify $\tilde{\mathbf{d}}_J$ as the thermodynamic driving force. The concept of 'configurational forces' introduced by Gurtin (1995)[2] plays a central role in our analysis. We note in passing that it is possible to derive the same driving force on the edge using a variational method following Eshelby (1970). We indeed have done so in the two-dimensional case in Simha and Bhattacharya (1997).

We start with a discussion of the kinematics of a multi-phase body containing k interfaces that intersect at a junction in Section 2. Balance laws are discussed in Section 3, and the energy dissipation due to propagation of finite interfaces is calculated in Section 4. We identify the driving force on the junction in Section 5 and propose appropriate kinetic relations in Section 6. Table 1 describes the notation.

2. Kinematics

Consider a body occupying the region $\Omega \in \mathbb{R}^3$ in the reference configuration. The region is divided into k sub-regions Ω^i by k interfaces Σ^i that intersect at the junction J (see Fig. 1). The unit normal $\hat{\mathbf{m}}^i$ to the interface Σ^i points into Ω^i. The body consists of k phases with the ith phase occupying the sub-region Ω^i. As one phase converts to another, the sub-regions evolve by the propagation of the interfaces.

2.1. Interface, junction and tube

Let the interface $\Sigma^i(t)$ be given by the smooth parametrization

$$\Sigma^i(t) = \{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} = \bar{\mathbf{x}}^i(\boldsymbol{\xi}, t)\}, \tag{1}$$

where $\boldsymbol{\xi}$ is a two-dimensional parameter. The interface velocity $\bar{\mathbf{v}}^i$ and its normal component $\bar{v}^i_m$ are given by

$$\bar{\mathbf{v}}^i = \frac{\partial \bar{\mathbf{x}}^i(., t)}{\partial t} \quad \text{and} \quad \bar{v}^i_m = \bar{\mathbf{v}}^i \cdot \hat{\mathbf{m}}^i, \tag{2}$$

respectively. Only the normal component of the interface velocity is independent of the parametrization (1). For any smooth scalar field ψ and smooth vector field $\mathbf{g}$ on a surface Σ, we define the surface gradient ∇_Σ through the chain rule: given any curve $\bar{\mathbf{z}}(\beta)$ on Σ,

$$\begin{aligned} &\frac{\partial \psi}{\partial \beta} = \nabla_\Sigma \psi \cdot \frac{\partial \bar{\mathbf{z}}}{\partial \beta}, \qquad \nabla_\Sigma \psi \cdot \hat{\mathbf{m}} = 0 \text{ and} \\ &\frac{\partial \mathbf{g}}{\partial \beta} = \nabla_\Sigma \mathbf{g} \frac{\partial \bar{\mathbf{z}}}{\partial \beta}, \qquad (\nabla_\Sigma \mathbf{g})\hat{\mathbf{m}} = 0. \end{aligned} \tag{3}$$

[2] The basic laws of this framework are also explained in Section 3 of Simha and Bhattacharya (1998).

Table 1
List of symbols. Interface quantities are usually denoted with a bar and junction quantities with a tilde. Unit vectors are denoted with a hat

	Bulk quantities		
ϕ	Bulk energy per unit reference volume		
$\mathbf{F}$	Deformation gradient	$\mathbf{S}$	Bulk deformational stress
$\mathbf{C}$	Bulk configurational stress	$\mathbf{f}$	Bulk configurational body force
	Interface quantities		
$\bar{\mathbf{v}}^i$, $\bar{v}^i_m$	Velocity of Σ and its normal component	$\langle\cdot\rangle$, $[[\cdot]]$	Average and jump across Σ
$\bar{\mathbf{L}}$, $\bar{\kappa}$	Curvature tensor and total curvature	$\bar{\mathbf{P}}$	Projection tensor on Σ
∇_Σ	Surface gradient	$(\cdot)^\circ$	Normal time derivative following Σ
ψ	Surface energy per unit reference area	$\bar{\mathbf{F}}$	Surface deformation gradient
$\bar{\mathbf{S}}$	Surface deformational stress	$\bar{\mathbf{C}}$	Surface configurational stress
$\bar{\mathbf{f}}$	Surface configurational body force	$\bar{\mathbf{q}}$	Surface shear
$\bar{d}_\Sigma$	Interface driving force		
	Junction quantities		
$\tilde{\kappa}$, $\tilde{\tau}$	Curvature, torsion of J		
$\langle\cdot\rangle_J$	Average at J	$\tilde{\mathbf{v}}$	Velocity of J
$\tilde{v}_n$, $\tilde{v}_b$	Normal and binormal components of $\tilde{\mathbf{v}}$	$\tilde{\mathbf{v}}_p$	Projection of $\tilde{\mathbf{v}}$ to plane normal to J
$\tilde{\mathbf{P}}$	Projection tensor on J	$\tilde{v}_w$	Edge velocity
$(\cdot)^*$	Normal time derivative following J	χ	Line energy per unit reference length
$\tilde{\mathbf{F}}$	Line deformation gradient	$\tilde{\mathbf{p}}$	Tangential stretch
$\tilde{\mathbf{s}}$	Line deformation stress	$\tilde{\mathbf{c}}$	Configurational stress
$\tilde{\mathbf{f}}_J$	Line configurational body force	$\tilde{\mathbf{q}}$	Junction shear
$\tilde{\mathbf{d}}_J$	Junction driving force	$\tilde{d}_E$	Edge driving force

The surface divergence of a vector field is defined as $\nabla_\Sigma\cdot\mathbf{g}\equiv\mathrm{tr}(\nabla_\Sigma\mathbf{g})$ and of a tensor field $\bar{\mathbf{S}}$ is $\mathbf{a}\cdot\nabla_\Sigma\cdot\bar{\mathbf{S}}\equiv\nabla_\Sigma\cdot(\bar{\mathbf{S}}^T\mathbf{a})$, where $\mathbf{a}$ is some constant vector. The curvature tensor $\bar{\mathbf{L}}$ and the total curvature $\bar{\kappa}$ (twice the mean curvature) are given by

$$\bar{\mathbf{L}}=-\nabla_\Sigma\hat{\mathbf{m}} \quad \text{and} \quad \bar{\kappa}=\mathrm{tr}(\bar{\mathbf{L}})=-\nabla_\Sigma\cdot\hat{\mathbf{m}}. \tag{4}$$

The projection $\bar{\mathbf{P}}$ to the surface is defined as

$$\bar{\mathbf{P}}=\mathbf{I}-\hat{\mathbf{m}}\otimes\hat{\mathbf{m}}. \tag{5}$$

We now recall the normal time derivative following the surface defined by Gurtin and Struthers (1990). A normal trajectory to the surface $\Sigma(t)$ is a collection of points $\mathbf{z}(t)\in\Sigma(t)$ such that $\dot{\mathbf{z}}=\bar{v}_m\hat{\mathbf{m}}$. The normal time derivative $\mathbf{g}^\circ$ following the surface Σ is the time derivative of $\mathbf{g}$ taken along normal trajectories:

$$\mathbf{g}^{\circ} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{g}(\mathbf{z}(t), t) = \dot{\mathbf{g}} + \bar{v}_m (\nabla \mathbf{g})\hat{\mathbf{m}}. \tag{6}$$

The junction $J(t)$ of k interfaces is a curve in three dimensions and we describe it with an arc-length parametrization

$$J(t) = \{\mathbf{x} \in \Omega : \mathbf{x} = \tilde{\mathbf{x}}(\alpha, t)\}, \tag{7}$$

where the arc length α belongs to an interval I. The tangent $\hat{\mathbf{t}}$ is defined as

$$\hat{\mathbf{t}} = \frac{\partial \tilde{\mathbf{x}}(\alpha, \cdot)}{\partial \alpha}; \tag{8}$$

the arc-length parametrization implies that $|\hat{\mathbf{t}}| = 1$. The unit normal $\hat{\mathbf{n}}$, unit binormal $\hat{\mathbf{b}}$, curvature $\tilde{\kappa}$ and torsion $\tilde{\tau}$ are defined through the Frénet–Serret formulae as follows (also see Fig. 1)

$$\frac{\partial \hat{\mathbf{t}}}{\partial \alpha} = \tilde{\kappa}\hat{\mathbf{n}}, \quad \frac{\partial \hat{\mathbf{n}}}{\partial \alpha} = \tilde{\tau}\hat{\mathbf{b}} - \tilde{\kappa}\hat{\mathbf{t}}, \quad \frac{\partial \hat{\mathbf{b}}}{\partial \alpha} = -\tilde{\tau}\hat{\mathbf{n}}. \tag{9}$$

The projection $\tilde{\mathbf{P}}$ to the curve is defined as

$$\tilde{\mathbf{P}} = \mathbf{I} - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}} - \hat{\mathbf{b}} \otimes \hat{\mathbf{b}} = \hat{\mathbf{t}} \otimes \hat{\mathbf{t}}, \tag{10}$$

so that the projection to the plane perpendicular to the tangent is $(\mathbf{I} - \tilde{\mathbf{P}})$. The velocity of the junction $\tilde{\mathbf{v}}$ and its projection $\tilde{\mathbf{v}}_p$ to a plane perpendicular to the tangent are given respectively by

$$\tilde{\mathbf{v}}(\cdot, t) = \frac{\partial \tilde{\mathbf{x}}(\cdot, t)}{\partial t} \tag{11}$$

and

$$\tilde{\mathbf{v}}_p = (\mathbf{I} - \tilde{\mathbf{P}})\tilde{\mathbf{v}} = \tilde{v}_n \hat{\mathbf{n}} + \tilde{v}_b \hat{\mathbf{b}} \quad \text{where } \tilde{v}_n = \tilde{\mathbf{v}} \cdot \hat{\mathbf{n}},\ \tilde{v}_b = \tilde{\mathbf{v}} \cdot \hat{\mathbf{b}}. \tag{12}$$

Note that $\tilde{\mathbf{v}}_p$ is independent of the parametrization (7), but not $\tilde{\mathbf{v}}$. As on a surface, we now define a normal time derivative on the curve (Gurtin, 1993). A path $\alpha = \tilde{\alpha}(t)$ is said to be a normal arc-length trajectory, if

$$\hat{\mathbf{t}}(\tilde{\alpha}(t), t) \cdot \frac{\mathrm{d}\tilde{\mathbf{x}}(\tilde{\alpha}(t), t)}{\mathrm{d}t} = 0; \tag{13}$$

this implies the identity $\dot{\tilde{\alpha}} = -(\tilde{\mathbf{v}} \cdot \hat{\mathbf{t}})$ for normal trajectories. Then, the normal time derivative χ^* of a function $\chi(\alpha, t)$ is defined as the derivative along normal trajectories,

$$\chi^* \equiv \frac{\mathrm{d}\chi(\tilde{\alpha}(t), t)}{\mathrm{d}t}. \tag{14}$$

We have noted in the Introduction that the stresses may be singular at the junction

J. Therefore, in Sections 3 and 4 we follow the practice of classical potential theory and analyze a region obtained by removing a tubular region around the junction and then shrinking this tube to the junction. In anticipation, we introduce some notation concerning this region. Let $\mathscr{B}_\eta$ be a tube of radius η around the junction J; recalling the parametrization (7),

$$\mathscr{B}_\eta(t)=\left\{\mathbf{x}\in\mathbb{R}^3 \left\| \begin{array}{l}\mathbf{x}=\tilde{\mathbf{x}}(\alpha,t)+\rho\cos\theta\hat{\mathbf{b}}(\alpha,t)+\rho\sin\theta\hat{\mathbf{n}}(\alpha,t),\\ \alpha\in I,\ 0\le\rho<\eta,\ 0\le\theta<2\pi\end{array}\right.\right\}. \tag{15}$$

We use the notation $\partial\mathscr{B}_\eta$ to denote only the lateral boundary of the tube, which is the envelope of the circles,

$$\mathscr{C}_\eta(\alpha,t)=\left\{\mathbf{x}\in\mathbb{R}^3 \left\| \begin{array}{l}\mathbf{x}=\tilde{\mathbf{x}}(\alpha,t)+\eta\cos\theta\hat{\mathbf{b}}(\alpha,t)+\eta\sin\theta\hat{\mathbf{n}}(\alpha,t),\\ \alpha\in I,\ 0\le\theta<2\pi\end{array}\right.\right\}. \tag{16}$$

We note that

$$\lim_{\eta\to0}\int_{\partial\mathscr{B}_\eta}\mathbf{f}\,\mathrm{d}a=\lim_{\eta\to0}\int_I\int_0^{2\pi}\mathbf{f}(\alpha,\theta)(1-\eta\tilde{\kappa}\sin\theta)\eta\,\mathrm{d}\theta\,\mathrm{d}\alpha=\int_J\left[\lim_{\eta\to0}\int_{\mathscr{C}_\eta}\mathbf{f}\,\mathrm{d}l\right]\mathrm{d}l \tag{17}$$

and the velocity $\mathbf{u}$ of a point on $\partial\mathscr{B}_\eta$ satisfies

$$\mathbf{u}=\tilde{\mathbf{v}}+\eta\cos\theta\frac{\partial\hat{\mathbf{b}}}{\partial t}+\eta\sin\theta\frac{\partial\hat{\mathbf{n}}}{\partial t}\ \to\ \tilde{\mathbf{v}}\text{ and }(\mathbf{I}-\tilde{\mathbf{P}})\mathbf{u}\ \to\ \tilde{\mathbf{v}}_p\text{ as }\ \eta\to0. \tag{18}$$

Finally, for a vector field $\mathbf{a}$ defined over a region $\mathscr{D}$ containing a part of the junction, we introduce the notation

$$\int_{\mathscr{D}}\mathbf{a}\,\mathrm{d}v\equiv\lim_{\eta\to0}\int_{\mathscr{D}\backslash\mathscr{B}_\eta}\mathbf{a}\,\mathrm{d}v. \tag{19}$$

2.2. Deformation

Consider a deformation of the body $\mathbf{y}:\Omega\times T\to\mathbb{R}^3$, where T is a time interval. The deformation gradient $\mathbf{F}$ and material velocity $\dot{\mathbf{y}}$ are given by

$$\mathbf{F}(\mathbf{x},\cdot)=\nabla\mathbf{y}(\mathbf{x},\cdot)=\frac{\partial\mathbf{y}(\mathbf{x},\cdot)}{\partial\mathbf{x}}\ \text{ and }\ \dot{\mathbf{y}}(\cdot,t)=\frac{\partial\mathbf{y}(\cdot,t)}{\partial t}, \tag{20}$$

respectively. We assume that the deformation is continuous on Ω, the deformation gradient and velocity are continuously differentiable in each sub-region Ω^i with possible jumps across the interfaces and a possible singularity at the junction J. In particular, we assume that the deformation gradient and the velocity have well-defined limits (some components of which are possibly infinite) as we approach the junction from each sub-region.

The continuity of the deformation at an interface imposes the following compatibility conditions (Simha and Bhattacharya, 1998)

$$[[\mathbf{F}]]=[[\mathbf{F}]]\hat{\mathbf{m}}^i\otimes\hat{\mathbf{m}}^i \quad \text{and} \quad [[\dot{\mathbf{y}}]]=-\bar{v}^i_m[[\mathbf{F}]]\hat{\mathbf{m}}^i, \tag{21}$$

where $[[a]]=(a^+-a^-)$ denotes the jump of a across the interface; a^+ is the limit of a from the region Ω^i while a^- is the limit from the region Ω^{i-1} (or Ω^k if $i=1$). Similarly, at the junction, we have the compatibility conditions

$$(\mathbf{F}^i-\mathbf{F}^j)\hat{\mathbf{t}}=0 \quad \text{and} \quad \dot{\mathbf{y}}^i-\dot{\mathbf{y}}^j=-(\mathbf{F}^i-\mathbf{F}^j)\tilde{\mathbf{v}}_p \tag{22}$$

for each $i, j=1, \ldots, k$ where a^i denotes the limiting value of a from Ω^i at the junction J. Continuity of the deformation at the junction means $\mathbf{y}^i(\tilde{\mathbf{x}}(\alpha, t), t)=\mathbf{y}^j(\tilde{\mathbf{x}}(\alpha, t), t)$. Differentiation of this relation with respect to α gives the first identity, while differentiation with respect to t gives the second.

On an interface Σ^i, we note that $\mathbf{y}^+=\mathbf{y}^-$, and define the surface deformation gradient as

$$\bar{\mathbf{F}}^i=\nabla_\Sigma\mathbf{y}^\pm(\mathbf{x}, t) \quad \text{where } \mathbf{x}\in\Sigma^i(t). \tag{23}$$

The surface deformation gradient maps tangents to the reference interface at $\mathbf{x}\in\Sigma^i$ to tangents to the deformed interface at $\mathbf{y}(\mathbf{x})\in\mathbf{y}(\Sigma^i)$. It is related to the bulk deformation gradient through the surface projection $\bar{\mathbf{P}}^i$ defined in Eq. (5) according to

$$\bar{\mathbf{F}}^i=\langle\mathbf{F}\rangle\bar{\mathbf{P}}^i \tag{24}$$

where $\langle a\rangle=(a^++a^-)/2$ is the average of the parameter a across the interface. Note that $\bar{\mathbf{F}}^i\hat{\mathbf{m}}^i=0$, and $\bar{\mathbf{F}}^i\mathbf{m}^\perp=\langle\mathbf{F}\rangle\mathbf{m}^\perp$ for all vectors $\mathbf{m}^\perp$ perpendicular to the normal $\hat{\mathbf{m}}^i$.

We define the junction deformation gradient $\tilde{\mathbf{F}}$ as

$$\tilde{\mathbf{F}}=\tilde{\mathbf{p}}\otimes\hat{\mathbf{t}} \quad \text{where } \tilde{\mathbf{p}}=\frac{\partial\mathbf{y}(\tilde{\mathbf{x}}(\alpha, t), t)}{\partial\alpha}. \tag{25}$$

Here $\tilde{\mathbf{p}}$ is the tangential stretch of the junction. Once again, the junction deformation gradient maps tangents to the junction in the reference to tangents in the deformed configuration, and is related to the bulk deformation gradient through the projection $\tilde{\mathbf{P}}$ defined in Eq. (10):

$$\tilde{\mathbf{F}}=\langle\mathbf{F}\rangle_J\tilde{\mathbf{P}}, \tag{26}$$

where

$$\langle a\rangle_J=\frac{1}{k}\sum_{i=1}^{k}a^i.$$

Note that $\tilde{\mathbf{F}}\hat{\mathbf{n}}=0=\tilde{\mathbf{F}}\hat{\mathbf{b}}$ and $\tilde{\mathbf{p}}=\tilde{\mathbf{F}}\hat{\mathbf{t}}=\langle\mathbf{F}\rangle_J\hat{\mathbf{t}}$.

2.3. Evolving part of the body

Now consider an evolving part of the body $\mathscr{D} = \mathscr{D}(t) \subset \Omega$ which intersects the junction J as shown in Fig. 1. The external unit normal to its boundary $\partial\mathscr{D}$ is $\hat{\mathbf{h}}$ and the (reference) velocity of any point on $\partial\mathscr{D}$ is denoted as $\mathbf{u}$. The part of the junction J that lies within the part $\mathscr{D}$ is denoted as $J_D = J \cap \mathscr{D}$; the corresponding range of arc lengths is $\alpha_1 \leq \alpha \leq \alpha_2$. The velocity of the end-points of J_D in the reference configuration is denoted by $\tilde{\mathbf{V}}$. For instance, at the end-point corresponding to $\alpha_1(t)$, the velocity in the reference configuration is

$$\tilde{\mathbf{V}} = \frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathbf{x}}(\alpha_1(t), t) = \tilde{\mathbf{v}}(\alpha_1) + \dot{\alpha}_1 \hat{\mathbf{t}}(\alpha_1).$$

Consequently,

$$\tilde{\mathbf{V}}\cdot\hat{\mathbf{n}} = \tilde{\mathbf{v}}\cdot\hat{\mathbf{n}} \text{ and } \tilde{\mathbf{V}}\cdot\hat{\mathbf{b}} = \tilde{\mathbf{v}}\cdot\hat{\mathbf{b}} \text{ so that } \tilde{\mathbf{V}} = (\tilde{\mathbf{V}}\cdot\hat{\mathbf{t}})\hat{\mathbf{t}} + \tilde{\mathbf{v}}_p. \tag{27}$$

The image of this end-point in the current configuration is given by

$$\mathbf{y}(\tilde{\mathbf{x}}(\alpha_1(t), t), t) = \langle \mathbf{y}(\tilde{\mathbf{x}}(\alpha_1(t), t), t)\rangle_J,$$

and hence the velocity of image of the end-point in the current configuration is

$$\langle \dot{\mathbf{y}}\rangle_J + \langle \mathbf{F}\rangle_J \tilde{\mathbf{V}}.$$

Let $\Sigma^i_D = \Sigma^i \cap \mathscr{D}$ be the part of the interface Σ^i that intersects $\mathscr{D}$. The boundary $\partial\Sigma^i_D$ is a curve whose normal we denote as $\hat{\mathbf{w}}^i$ and it is chosen to point outward to Σ^i_D. It turns out that the binormal to the curve $\partial\Sigma^i_D$ coincides with the normal $\hat{\mathbf{m}}^i$ to the interface Σ^i_D.

We denote the velocity of a point on $\partial\Sigma^i_D$ in the reference configuration as $\bar{\mathbf{V}}^i$; it can easily be shown that

$$\bar{\mathbf{V}}^i\cdot\hat{\mathbf{m}}^i = \bar{\mathbf{v}}^i\cdot\hat{\mathbf{m}}^i. \tag{28}$$

As before, the velocity of the image in the deformed configuration of a point on $\partial\mathscr{D}$ is $(\dot{\mathbf{y}}+\mathbf{F}\mathbf{u})$ and on $\partial\Sigma^i_D$ is $(\langle\dot{\mathbf{y}}\rangle + \langle\mathbf{F}\rangle\bar{\mathbf{V}}^i)$.

3. Balance of forces and moments

A phase boundary is not a material surface, instead it moves across material points as it propagates. Hence, it has to be regarded as a change in the reference configuration. Therefore, we follow Gurtin (1995) and assume that there are two types of forces that act on our body: (1) deformational, which are the conventional forces that act against the deformation of the body; and (2) configurational, which act against changes in the reference configuration of the body (see Simha and Bhattacharya, 1998 for the motivation and discussion of this framework in this context).

Consider now an evolving part of the body $\mathscr{D}$. The conventional forces acting on it arise from the bulk stress $\mathbf{S}$ acting on the boundary $\partial\mathscr{D}$, surface stress $\bar{\mathbf{S}}^i$ acting on the boundary of an interface $\partial\Sigma_D^i$, and curve stress $\tilde{\mathbf{s}}$ acting at the end-points of J_D. We assume that all deformational body forces are zero. The balance of deformational forces requires that

$$\int_{\partial\mathscr{D}} \mathbf{S}\hat{\mathbf{h}}\,\mathrm{d}a+\sum_{i=1,2}^{k}\int_{\partial\Sigma_D^i}\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\,\mathrm{d}l+\{\tilde{\mathbf{s}}\}_{\alpha_1}^{\alpha_2}=0$$

for each time $t\in T$ and for every part $\mathscr{D}\subset\Omega$; here $\{\tilde{\mathbf{s}}\}_{\alpha_1}^{\alpha_2}=\tilde{\mathbf{s}}(\alpha_2)-\tilde{\mathbf{s}}(\alpha_1)$.

The configurational contact forces arise from the bulk stress $\mathbf{C}$ acting on boundary $\partial\mathscr{D}$, surface stress $\bar{\mathbf{C}}^i$ acting on the boundary of the interface $\partial\Sigma_D^i$, and curve stress $\tilde{\mathbf{c}}$ acting at the end-points of J_D. The configurational body forces are $\mathbf{f}$ that act on $\mathscr{D}$, $\bar{\mathbf{f}}^i$ on Σ_D^i, and $\tilde{\mathbf{f}}_J$ on J_D. The balance of configurational forces requires that

$$\int_{\mathscr{D}}\mathbf{f}\,\mathrm{d}v+\int_{\partial\mathscr{D}}\mathbf{C}\hat{\mathbf{h}}\,\mathrm{d}a+\sum_{i=1,2}^{k}\left[\int_{\Sigma_D^i}\bar{\mathbf{f}}^i\,\mathrm{d}a+\int_{\partial\Sigma_D^i}\bar{\mathbf{C}}^i\hat{\mathbf{w}}^i\,\mathrm{d}l\right]+\int_{J_D}\tilde{\mathbf{f}}_J\,\mathrm{d}l+\{\tilde{\mathbf{c}}\}_{\alpha_1}^{\alpha_2}=0$$

for each time $t\in T$ and for every part $\mathscr{D}\subset\Omega$.

We assume that the bulk deformational and configurational stresses $\mathbf{S}$ and $\mathbf{C}$ are differentiable in each sub-region Ω^i with possible jumps across the interfaces and a possible singularity at the junction J. In particular, we assume that they have well-defined limits (some components of which are possibly infinite) as we approach the junction from each sub-region. Similarly, we assume that the surface deformational and configurational stresses $\bar{\mathbf{S}}^i$ and $\bar{\mathbf{C}}^i$ are differentiable on Σ^i away from the junction J, with well-defined limits as we approach it.

To localize the balance laws, we write them on $\mathscr{D}\backslash\mathscr{B}_\eta$ where $\mathscr{B}_\eta$ is a tube of radius η, use the divergence theorem on this punctured domain and then take the limit as $\eta\to0$. Using the bulk (A3) and surface (A4) divergence theorems as well as the fundamental theorem of calculus, we obtain the following localizations of the deformational force balance:

$$\nabla\cdot\mathbf{S}=0\quad\text{in }\Omega^i(t),\ t\in T,\tag{29}$$

$$[[\mathbf{S}]]\hat{\mathbf{m}}^i+\nabla_\Sigma\cdot\bar{\mathbf{S}}^i=0\quad\text{in }\Sigma^i(t),\ t\in T\tag{30}$$

$$\lim_{\eta\to0}\int_{\mathscr{C}_\eta}\mathbf{S}\hat{\mathbf{h}}\,\mathrm{d}l-\sum_{i=1,2}^{k}\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i+\frac{\partial\tilde{\mathbf{s}}}{\partial\alpha}=0\quad\text{in }J(t),\ t\in T.\tag{31}$$

Note that the singular bulk stresses may contribute to the balance of forces at the junction [Eq. (31)].

It is important to note the notation of Eq. (31); we do not sum infinite terms as it appears, but mean

$$\lim_{\eta\to0}\left[\int_{\mathscr{C}_\eta}\mathbf{S}\hat{\mathbf{h}}\,\mathrm{d}l-\sum_{i=1,2}^{k}(\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i)|_{\Sigma_D^i\cap\mathscr{C}_\eta}\right]+\frac{\partial\tilde{\mathbf{s}}}{\partial\alpha}=0.$$

We adopt this convention in similar situations.

Localization of the configurational force balance gives

$$\nabla\cdot\mathbf{C}+\mathbf{f}=0 \quad \text{in } \Omega^i(t),\ t\in T, \tag{32}$$

$$[[\mathbf{C}]]\hat{\mathbf{m}}^i+\nabla_\Sigma\cdot\bar{\mathbf{C}}^i+\bar{\mathbf{f}}^i=0 \quad \text{in } \Sigma^i(t),\ t\in T \tag{33}$$

$$\lim_{\eta\to 0}\int_{\mathscr{C}_\eta}\mathbf{C}\hat{\mathbf{h}}\,\mathrm{d}l-\sum_{i=1,2}^{k}\bar{\mathbf{C}}^i\hat{\mathbf{w}}^i+\frac{\partial\tilde{\mathbf{c}}}{\partial\alpha}+\tilde{\mathbf{f}}_J=0 \quad \text{in } J(t),\ t\in T. \tag{34}$$

The balance of deformational moments requires that

$$\int_{\partial\mathscr{D}}\mathbf{y}\times\mathbf{S}\hat{\mathbf{h}}\,\mathrm{d}a+\sum_{i=1,2}^{k}\int_{\partial\Sigma_D^i}\mathbf{y}\times\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\,\mathrm{d}l+\{\mathbf{y}\times\tilde{\mathbf{s}}\}_{\alpha_1}^{\alpha_2}=0$$

for each time $t\in T$ and for every part $\mathscr{D}\subset\Omega$. Localizing this we obtain (Gurtin, 1996)

$$\mathbf{F}\mathbf{S}^T=\mathbf{S}\mathbf{F}^T \quad \text{in } \Omega^i(t),\ t\in T,$$

$$\bar{\mathbf{F}}\bar{\mathbf{S}}^T=\bar{\mathbf{S}}\bar{\mathbf{F}}^T \quad \text{in } \Sigma^i(t),\ t\in T$$

$$\tilde{\mathbf{s}}\times\tilde{\mathbf{p}}=0 \quad \text{in } J(T),\ t\in T.$$

Thus the Cauchy bulk and surface stresses are symmetric and the junction stress is parallel to the tangent to the junction in the deformed configuration. We omit the balance of configurational moments since we do not need it and refer the interested reader to Gurtin (1996).

4. Dissipation

In this mechanical setting, the second law of thermodynamics is the dissipation inequality

$$\Gamma(\mathscr{D})\geq 0 \quad \forall\ \mathscr{D}(t)\subset\Omega,\ \forall\ t\in T, \tag{35}$$

where the rate of energy dissipation $\Gamma(\mathscr{D})$ of a part $\mathscr{D}\subset\Omega$ is defined as

$$\Gamma(\mathscr{D})=W(\mathscr{D})-\frac{\mathrm{d}\mathscr{E}(\mathscr{D})}{\mathrm{d}t}; \tag{36}$$

here $W(\mathscr{D})$ denotes the rate of working and $\mathrm{d}\mathscr{E}/\mathrm{d}t$ is the rate of change of stored energy.

In this section we calculate the rate of energy dissipation due to the propagation of the phase boundaries. The final result is given in Eq. (67). Along the way, we also deduce that the configurational stresses are given by Eqs. (59)–(61).

4.1. Working

Deformational forces perform work on the velocities in the deformed configuration, whereas configurational forces perform work on the velocities in the reference. Thus, following Gurtin (1995), the working on part $\mathscr{D}$ is

$$W(\mathscr{D})=W_1+W_2+W_3 \tag{37}$$

where

$$W_1=\int_{\partial\mathscr{D}}[\mathbf{S}\hat{\mathbf{h}}\cdot(\dot{\mathbf{y}}+\mathbf{F}\mathbf{u})+\mathbf{C}\hat{\mathbf{h}}\cdot\mathbf{u}]\,\mathrm{d}a, \tag{38}$$

$$W_2=\sum_{i=1,2}^{k}\int_{\partial\Sigma_D^i}[\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\cdot(\langle\dot{\mathbf{y}}\rangle+\langle\mathbf{F}\rangle\bar{\mathbf{V}}^i)+\bar{\mathbf{C}}^i\hat{\mathbf{w}}^i\cdot\bar{\mathbf{V}}^i]\,\mathrm{d}l \tag{39}$$

$$W_3=\{\tilde{\mathbf{s}}\cdot(\langle\dot{\mathbf{y}}\rangle_J+\langle\mathbf{F}\rangle_J\tilde{\mathbf{V}})+\tilde{\mathbf{c}}\cdot\tilde{\mathbf{V}}\}_{\alpha_1}^{\alpha_2}. \tag{40}$$

We call W_1 the bulk working, W_2 the interface working and W_3 the junction working.

The working is required to be independent of the parameterizations chosen to describe the surface $\partial\mathscr{D}$ and the curve $\partial\Sigma^i$. It can be shown that this requires the following representations for the bulk and surface configurational stresses (Gurtin, 1995; Gurtin and Struthers, 1990)

$$\mathbf{C}=\pi\mathbf{I}-\mathbf{F}^T\mathbf{S} \tag{41}$$

$$\bar{\mathbf{C}}^i=\bar{\sigma}^i\bar{\mathbf{P}}^i+\hat{\mathbf{m}}^i\otimes\bar{\mathbf{q}}^i-(\bar{\mathbf{F}}^i)^T\bar{\mathbf{S}}^i \tag{42}$$

where π and $\bar{\sigma}^i$ are scalars and the vector $\bar{\mathbf{q}}^i := (\bar{\mathbf{C}}^i)^T\hat{\mathbf{m}}^i$ is a 'surface shear'. Further, setting $\tilde{\mu} = (\tilde{\mathbf{c}}+\tilde{\mathbf{F}}^T\tilde{\mathbf{s}})\cdot\hat{\mathbf{t}}$ and $\tilde{\mathbf{q}} = (\tilde{\mathbf{c}}+\tilde{\mathbf{F}}^T\tilde{\mathbf{s}})-\tilde{\mu}\hat{\mathbf{t}}$, we may express the configurational junction stress, $\tilde{\mathbf{c}}$, as

$$\tilde{\mathbf{c}} = \tilde{\mu}\hat{\mathbf{t}}+\tilde{\mathbf{q}}-\tilde{\mathbf{F}}^T\tilde{\mathbf{s}}. \tag{43}$$

We call $\tilde{\mathbf{q}}$ the junction shear and note that by definition it satisfies

$$\tilde{\mathbf{q}}\cdot\hat{\mathbf{t}} = 0 \text{ and } \tilde{\mathbf{c}}\cdot\hat{\mathbf{n}} = \tilde{\mathbf{q}}\cdot\hat{\mathbf{n}},\ \tilde{\mathbf{c}}\cdot\hat{\mathbf{b}} = \tilde{\mathbf{q}}\cdot\hat{\mathbf{b}}. \tag{44}$$

In the next few steps we use these representations for the configurational forces to simplify the working [Eq. (37)]. Substituting the configurational bulk stress (41) in the bulk working (38) gives

$$W_1=\int_{\partial\mathscr{D}}\mathbf{S}\hat{\mathbf{h}}\cdot\dot{\mathbf{y}}\,\mathrm{d}a+\int_{\partial\mathscr{D}}\pi\mathbf{u}\cdot\hat{\mathbf{h}}\,\mathrm{d}a.$$

We then apply the divergence theorem (A2) to the first integral and use the balance law (29) along with the compatibility condition (21) to obtain

$$
\begin{aligned}
W_1 = & \int_{\partial\mathscr{D}} \pi \mathbf{u}\cdot\hat{\mathbf{h}}\,\mathrm{d}a + \int_{\mathscr{D}} \mathbf{S}\cdot\dot{\mathbf{F}}\,\mathrm{d}v + \lim_{\eta\to 0}\int_{\partial\mathscr{B}_\eta} \mathbf{S}\hat{\mathbf{h}}\cdot\dot{\mathbf{y}}\,\mathrm{d}a \\
& + \sum_{i=1,2}^{k}\int_{\Sigma_D^i} ([[\mathbf{S}]]\hat{\mathbf{m}}^i\cdot\langle\dot{\mathbf{y}}\rangle - \vec{v}_m^i\langle\mathbf{S}\rangle\hat{\mathbf{m}}^i\cdot[[\mathbf{F}]]\hat{\mathbf{m}}^i)\,\mathrm{d}a.
\end{aligned} \tag{45}
$$

The interface working (39) can be rewritten using the representation (42) for the interface configurational stress as follows

$$
W_2 = \sum_{i=1,2}^{k}\int_{\partial\Sigma_D^i} \bar{\sigma}^i\bar{\mathbf{V}}^i\cdot\hat{\mathbf{w}}^i\,\mathrm{d}l + \sum_{i=1,2}^{k}\int_{\partial\Sigma_D^i}\left[(\bar{\mathbf{S}}^i)^T(\langle\dot{\mathbf{y}}\rangle + (\bar{\mathbf{v}}^i\cdot\hat{\mathbf{m}}^i)\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i) + (\bar{\mathbf{v}}^i\cdot\hat{\mathbf{m}}^i)\bar{\mathbf{q}}^i\right]\cdot\hat{\mathbf{w}}^i\,\mathrm{d}l,
$$

where we have used the identities $\bar{\mathbf{F}}^i\hat{\mathbf{m}}^i = 0$, $(\langle\mathbf{F}\rangle - \bar{\mathbf{F}}^i)\mathbf{m}^\perp = 0$ for vectors $\mathbf{m}^\perp$ satisfying $\mathbf{m}^\perp\cdot\hat{\mathbf{m}}^i = 0$ and Eq. (28). We then use the divergence theorem (A4) on the second term and obtain

$$
\begin{aligned}
W_2 = & \sum_{i=1,2}^{k}\int_{\partial\Sigma_D^i} \hat{\sigma}^i\bar{\mathbf{V}}^i\cdot\hat{\mathbf{w}}^i\,\mathrm{d}l - \int_{J_D}\sum_{i=1,2}^{k}\left[\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\cdot(\langle\dot{\mathbf{y}}\rangle + (\tilde{\mathbf{v}}\cdot\hat{\mathbf{m}}^i)\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i) + (\tilde{\mathbf{v}}\cdot\hat{\mathbf{m}}^i)\bar{\mathbf{q}}^i\cdot\hat{\mathbf{w}}^i\right]\mathrm{d}l \\
& + \sum_{i=1,2}^{k}\int_{\Sigma_D^i}\left[(\nabla_\Sigma\cdot\bar{\mathbf{S}}^i)\cdot\langle\dot{\mathbf{y}}\rangle + \bar{\mathbf{S}}^i\cdot\langle\mathbf{F}\rangle^\circ - [(\bar{\mathbf{S}}^i)^T\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i + \bar{\mathbf{q}}^i]\cdot(\hat{\mathbf{m}}^i)^\circ\right]\mathrm{d}a \\
& + \sum_{i=1,2}^{k}\int_{\Sigma_D^i}\left[(\nabla_\Sigma\cdot\bar{\mathbf{S}}^i)\cdot\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i + \nabla_\Sigma\cdot\bar{\mathbf{q}}^i - \langle\mathbf{F}\rangle^T\bar{\mathbf{S}}^i\cdot\bar{\mathbf{L}}^i\right]\vec{v}_m^i\,\mathrm{d}a
\end{aligned} \tag{46}
$$

where we have used the identities,

$$
\nabla_\Sigma(\langle\dot{\mathbf{y}}\rangle + v_m^i\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i) = (\langle\mathbf{F}\rangle^\circ - \langle\mathbf{F}\rangle\hat{\mathbf{m}}^i\otimes(\hat{\mathbf{m}}^i)^\circ - \vec{v}_m^i\langle\mathbf{F}\rangle\bar{\mathbf{L}}^i)\bar{\mathbf{P}}^i \tag{47}
$$

$$
(\hat{\mathbf{m}}^i)^\circ = -\nabla_\Sigma\vec{v}_m^i, \tag{48}
$$

which may be derived by differentiation and the symmetry of the second derivatives. We have also recalled the definition of the curvature tensor (4) and normal time derivative (6).

To simplify the junction working (40), we use Eq. (27) first and then Eq. (26) to obtain

$$
W_3 = \{\tilde{\mathbf{s}}\cdot(\langle\dot{\mathbf{y}}\rangle_J + \langle\mathbf{F}\rangle_J\tilde{\mathbf{v}}_p) + \tilde{\mathbf{c}}\cdot\tilde{\mathbf{v}}_p + (\tilde{\mathbf{V}}\cdot\hat{\mathbf{t}})(\tilde{\mathbf{c}} + \tilde{\mathbf{F}}^T\tilde{\mathbf{s}})\cdot\hat{\mathbf{t}}\}_{\alpha_1}^{\alpha_2}.
$$

We now use the fundamental theorem of calculus on the first two terms and the identities

$$
\frac{\partial\tilde{\mathbf{v}}_p}{\partial\alpha} = \hat{\mathbf{t}}^* - \tilde{v}_n\tilde{\kappa}\hat{\mathbf{t}} \tag{49}
$$

$$\frac{\partial}{\partial \alpha}(\langle \dot{\mathbf{y}} \rangle_J + \langle \mathbf{F} \rangle_J \tilde{\mathbf{v}}_p) = \tilde{\mathbf{p}}^* - \tilde{\kappa} \tilde{v}_n \tilde{\mathbf{p}}, \tag{50}$$

to obtain

$$\begin{aligned} W_3 = &\{(\tilde{\mathbf{V}} \cdot \hat{\mathbf{t}})(\tilde{\mathbf{c}} + \tilde{\mathbf{F}}^T \tilde{\mathbf{s}}) \cdot \hat{\mathbf{t}}\}_{\alpha_1}^{\alpha_2} + \int_{J_D} \left[\frac{\partial \tilde{\mathbf{s}}}{\partial \alpha} \cdot (\langle \dot{\mathbf{y}} \rangle_J + \langle \mathbf{F} \rangle_J \tilde{\mathbf{v}}_p) + \frac{\partial \tilde{\mathbf{c}}}{\partial \alpha} \cdot \tilde{\mathbf{v}}_p \right] \mathrm{d}l \\ &+ \int_{J_D} [\tilde{\mathbf{s}} \cdot \tilde{\mathbf{p}}^* + \tilde{\mathbf{c}} \cdot \hat{\mathbf{t}}^* - (\tilde{\mathbf{c}} + \tilde{\mathbf{F}}^T \tilde{\mathbf{s}}) \cdot \hat{\mathbf{t}} \tilde{\kappa} \tilde{v}_n] \, \mathrm{d}l. \end{aligned} \tag{51}$$

To obtain Eq. (49), we differentiate $\tilde{\mathbf{v}}_p = \tilde{\mathbf{v}} - \tilde{v}_t \hat{\mathbf{t}}$ with respect to α, and use the symmetry of the second derivative, the Frénet–Serret formula (9), the normal time derivative of $\hat{\mathbf{t}}$ and the relation

$$\frac{\partial \tilde{v}_t}{\partial \alpha} = \tilde{\kappa} \tilde{v}_n,$$

which is implied by $\hat{\mathbf{t}}^* \cdot \hat{\mathbf{t}} = 0$. To obtain the identity (50), we differentiate with respect to α, use the symmetry of the second derivative and the normal time derivative of $\tilde{\mathbf{p}} = \langle \mathbf{F} \rangle_J \hat{\mathbf{t}}$. We now recall the representation (43) in Eq. (51) and conclude that

$$\begin{aligned} W_3 = &\{\tilde{\mu}(\tilde{\mathbf{V}} \cdot \hat{\mathbf{t}})\}_{\alpha_1}^{\alpha_2} + \int_{J_D} \left[\frac{\partial \tilde{\mathbf{s}}}{\partial \alpha} \cdot (\langle \dot{\mathbf{y}} \rangle_J + \langle \mathbf{F} \rangle_J \tilde{\mathbf{v}}_p) + \frac{\partial \tilde{\mathbf{c}}}{\partial \alpha} \cdot \tilde{\mathbf{v}}_p \right] \mathrm{d}l \\ &+ \int_{J_D} [\tilde{\mathbf{s}} \cdot \tilde{\mathbf{p}}^* + \tilde{\mathbf{q}} \cdot \hat{\mathbf{t}}^* - \tilde{\mu} \tilde{\kappa} \tilde{v}_n] \, \mathrm{d}l. \end{aligned} \tag{52}$$

4.2. Energy

Let the bulk energy per unit reference volume be ϕ, the surface energy per unit reference area of the interface Σ^i be ψ^i, and the curve energy per unit reference length of the junction be χ. Then the energy of the region $\mathscr{D}$ is

$$\mathscr{E}(\mathscr{D}(t)) = \int_{\mathscr{D}(t)} \phi \, \mathrm{d}v + \sum_{i=1,2}^{k} \int_{\Sigma_D^i(t)} \psi^i \, \mathrm{d}a + \int_{J_D(t)} \chi \, \mathrm{d}l.$$

To calculate the rate of change of energy, we use the usual surface and curve transport identities (A5) and (A6) along with the bulk transport identity (A1), which is obtained by removing a tube $\mathscr{B}_\eta$ of radius η around the junction J_D, using the usual transport identity and taking the limit as $\eta \to 0$ (see Appendix A). We obtain

$$\frac{\mathrm{d}\mathscr{E}(\mathscr{D})}{\mathrm{d}t} = \int_{\mathscr{D}} \dot{\phi}\,\mathrm{d}v + \int_{\partial\mathscr{D}} \phi\mathbf{u}\cdot\hat{\mathbf{h}}\,\mathrm{d}l + \sum_{i=1,2}^{k} \int_{\partial\Sigma_D^i} \psi^i\bar{\mathbf{V}}^i\cdot\hat{\mathbf{w}}^i\,\mathrm{d}l$$
$$+ \sum_{i=1,2}^{k} \int_{\Sigma_D^i} [(\psi^i)^\circ - (\psi^i\bar{\kappa}^i + [[\phi]])\bar{v}_m^i]\,\mathrm{d}a - \lim_{\eta\to 0} \int_{\partial\mathscr{B}_\eta} \phi\mathbf{u}\cdot\hat{\mathbf{h}}\,\mathrm{d}a \tag{53}$$
$$+ \int_{J_D} \left(\chi^* - \chi\tilde{\kappa}\tilde{v}_n + \sum_{i=1,2}^{k} \psi^i\tilde{\mathbf{v}}\cdot\hat{\mathbf{w}}^i\right)\mathrm{d}l + \{\chi\tilde{\mathbf{V}}\cdot\hat{\mathbf{t}}\}_{\alpha_1}^{\alpha_2}.$$

4.3. Dissipation

We evaluate the dissipation (36) from Eqs. (37), (45), (46), (52) and (53):

$$\Gamma(\mathscr{D}) = \int_{\partial\mathscr{D}} (\pi-\phi)\mathbf{u}\cdot\hat{\mathbf{h}}\,\mathrm{d}l + \sum_{i=1,2}^{k} \int_{\partial\Sigma_D^i} (\sigma^i-\psi^i)\bar{\mathbf{V}}^i\cdot\hat{\mathbf{w}}^i\,\mathrm{d}l + \{(\tilde{\mu}-\chi)\tilde{\mathbf{V}}\cdot\hat{\mathbf{t}}\}_{\alpha_1}^{\alpha_2}$$
$$+ \int_{\mathscr{D}} \{\mathbf{S}\cdot\dot{\mathbf{F}} - \dot{\phi}\}\,\mathrm{d}a + \sum_{i=1,2}^{k} \int_{\Sigma_D^i} ([[\mathbf{S}]]\hat{\mathbf{m}}^i + \nabla_\Sigma\cdot\bar{\mathbf{S}}^i)\cdot\langle\dot{\mathbf{y}}\rangle\,\mathrm{d}a$$
$$- \sum_{i=1,2}^{k} \int_{\Sigma_D^i} [(\psi^i)^\circ - \bar{\mathbf{S}}^i\cdot\langle\mathbf{F}\rangle^\circ + (\bar{\mathbf{q}}^i + (\bar{\mathbf{S}}^i)^T\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i)\cdot(\hat{\mathbf{m}}^i)^\circ]\,\mathrm{d}a \tag{54}$$
$$- \int_{J_D} [\chi^* - \tilde{\mathbf{s}}\cdot\tilde{\mathbf{p}}^* - \tilde{\mathbf{q}}\cdot\hat{\mathbf{t}}^* + (\tilde{\mu}-\chi)\tilde{\kappa}\tilde{v}_n]\,\mathrm{d}l$$
$$+ \Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4,$$

where, for future use, we collect the following terms

$$\Gamma_1 := \sum_{i=1,2}^{k} \int_{\Sigma_D^i} \Big[[[\phi]] - \langle\mathbf{S}\rangle\hat{\mathbf{m}}^i\cdot[[\mathbf{F}]]\hat{\mathbf{m}}^i + \nabla_\Sigma\cdot\bar{\mathbf{S}}^i\cdot\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i$$
$$+ (\psi^i\bar{\mathbf{P}}^i - \langle\mathbf{F}\rangle^T\bar{\mathbf{S}}^i)\cdot\bar{\mathbf{L}}^i + \nabla_\Sigma\cdot\bar{\mathbf{q}}^i \Big] \bar{v}_m^i\,\mathrm{d}a, \tag{55}$$

$$\Gamma_2 := \int_{J_D} \left[\frac{\partial\tilde{\mathbf{s}}}{\partial\alpha}\cdot(\langle\dot{\mathbf{y}}\rangle_J + \langle\mathbf{F}\rangle_J\tilde{\mathbf{v}}_p) + \frac{\partial\tilde{\mathbf{c}}}{\partial\alpha}\cdot\tilde{\mathbf{v}}_p \right] \mathrm{d}l, \tag{56}$$

$$\Gamma_3 := \lim_{\eta \to 0} \int_{\partial \mathscr{B}_\eta} [\phi \tilde{\mathbf{u}} \cdot \hat{\mathbf{h}} + \mathbf{S}\hat{\mathbf{h}} \cdot \dot{\mathbf{y}}] \, \mathrm{d}a, \tag{57}$$

$$\Gamma_4 := -\int_{J_D} \sum_{i=1,2}^{k} \left(\bar{\mathbf{S}}^i \hat{\mathbf{w}}^i \cdot [\langle \dot{\mathbf{y}} \rangle + (\tilde{\mathbf{v}} \cdot \hat{\mathbf{m}}^i) \langle \mathbf{F} \rangle \hat{\mathbf{m}}^i] + (\tilde{\mathbf{v}} \cdot \hat{\mathbf{m}}^i) \bar{\mathbf{q}}^i \cdot \hat{\mathbf{w}}^i + \psi^i \tilde{\mathbf{v}} \cdot \hat{\mathbf{w}}^i \right) \mathrm{d}l. \tag{58}$$

We can now identify the scalars in the representation for the configurational stresses [Eqs. (41)–(43)]. At any given time instant, we can consider a second control volume $\mathscr{D}'$ that coincides with the control volume $\mathscr{D}$ but whose surface has a different velocity. The dissipation (54) must be the same for both control volumes. However, the only difference in the two dissipations arises from terms on the boundary — or the first three terms of Eq. (54). Hence their sum must vanish, which implies

$$\pi = \phi, \quad \bar{\sigma}^i = \psi^i, \quad \tilde{\mu} = \chi.$$

We can now evaluate the configurational stresses:

$$\mathbf{C} = \phi \mathbf{I} - \mathbf{F}^T \mathbf{S} \quad \text{in the bulk,} \tag{59}$$

$$\bar{\mathbf{C}}^i = \psi^i \bar{\mathbf{P}}^i + \hat{\mathbf{m}}^i \otimes \bar{\mathbf{q}}^i - (\bar{\mathbf{F}}^i)^T \bar{\mathbf{S}}^i \quad \text{on an interface} \tag{60}$$

$$\tilde{\mathbf{c}} = \chi \hat{\mathbf{t}} + \tilde{\mathbf{q}} - \tilde{\mathbf{F}}^T \tilde{\mathbf{s}} \quad \text{at a junction.} \tag{61}$$

The bulk configurational stress is nothing but the Eshelby or Noether energy-momentum tensor. The first two terms of the surface configurational stress are the three-dimensional generalization of the Cahn–Hoffman vector; they account for the surface tension and the surface shear. Thus the expression (60) for the surface configurational stress generalizes the Cahn–Hoffman vector to include surface deformation and extends it to three dimensions. The curve configurational stress is the generalization of the Cahn–Hoffman vector (up to rotation) to include deformation.

We use the relations (59), (60) and (61) to rewrite the dissipation in a form that is useful to identify the driving forces. The final result is Eq. (67). We begin with Γ_1, Eq. (55). Since $\bar{\mathbf{q}}^i = (\bar{\mathbf{C}}^i)^T \hat{\mathbf{m}}^i$, it follows that $\nabla_\Sigma \cdot \bar{\mathbf{q}}^i = (\nabla_\Sigma \cdot \bar{\mathbf{C}}^i) \cdot \hat{\mathbf{m}}^i - \bar{\mathbf{C}}^i \cdot \bar{\mathbf{L}}^i$. Using this as well as Eqs. (30) and (31) results in

$$\Gamma_1 = \sum_{i=1,2}^{k} \int_{\Sigma_D^i} \left[[[\mathbf{C}]] \hat{\mathbf{m}}^i + \nabla_\Sigma \cdot \bar{\mathbf{C}}^i \right] \cdot \hat{\mathbf{m}}^i \bar{v}_m^i \, \mathrm{d}a = \sum_{i=1,2}^{k} \int_{\Sigma_D^i} -(\bar{\mathbf{f}}^i \cdot \hat{\mathbf{m}}^i) \bar{v}_m^i \, \mathrm{d}a. \tag{62}$$

Next we simplify Γ_3 [Eq. (57)]. We add and subtract $\mathbf{S}\hat{\mathbf{h}} \cdot \mathbf{F}(\mathbf{I} - \tilde{\mathbf{P}})\tilde{\mathbf{u}}$ to the integrand, note that the normal $\hat{\mathbf{h}}$ to the circle $\partial \mathscr{C}_\eta$ satisfies $\hat{\mathbf{h}} = (\mathbf{I} - \tilde{\mathbf{P}})\hat{\mathbf{h}}$, and use the decomposition (17) to obtain

$$\begin{aligned}\Gamma_3 &= \int_{\mathcal{J}_D} \left(\lim_{\eta\to 0} \int_{\partial\mathcal{C}_n} [(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{u}}\cdot(\phi\mathbf{I}-\mathbf{F}^T\mathbf{S})\hat{\mathbf{h}}+\mathbf{S}\hat{\mathbf{h}}\cdot(\dot{\mathbf{y}}+\mathbf{F}(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{u}})]\,\mathrm{d}l \right) \mathrm{d}l \\ &= \int_{\mathcal{J}_D} \left(\lim_{\eta\to 0} \int_{\partial\mathcal{C}_\eta} [(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{u}}\cdot\mathbf{C}\hat{\mathbf{h}}+\mathbf{S}\hat{\mathbf{h}}\cdot(\dot{\mathbf{y}}+\mathbf{F}(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{u}})]\,\mathrm{d}l \right) \mathrm{d}l.\end{aligned} \tag{63}$$

We now turn to Γ_4 [Eq. (58)]. At the junction $(\hat{\mathbf{m}}^i, \hat{\mathbf{w}}^i)$ are both normal to $\hat{\mathbf{t}}$ and hence they span the same subspace as $(\hat{\mathbf{n}}, \hat{\mathbf{b}})$. Therefore,

$$\tilde{\mathbf{v}}_p = (\tilde{\mathbf{v}}\cdot\hat{\mathbf{m}}^i)\hat{\mathbf{m}}^i + (\tilde{\mathbf{v}}\cdot\hat{\mathbf{w}}^i)\hat{\mathbf{w}}^i.$$

By adding and subtracting the term $(\tilde{\mathbf{v}}\cdot\hat{\mathbf{w}}^i)\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\cdot\langle\mathbf{F}\rangle\hat{\mathbf{w}}^i$ to the integrand of Γ_4, and by using the relation (60) as well as the identities $\bar{\mathbf{F}}^i\hat{\mathbf{w}}^i = \langle\mathbf{F}\rangle\hat{\mathbf{w}}^i$ and $\bar{\mathbf{F}}^i\hat{\mathbf{m}}^i = 0$, we obtain the following simplification:

$$\Gamma_4 = -\int_{\mathcal{J}_D} \sum_{i=1,2}^{k} (\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\cdot[\langle\dot{\mathbf{y}}\rangle + \langle\mathbf{F}\rangle\tilde{\mathbf{v}}_p] + \bar{\mathbf{C}}^i\hat{\mathbf{w}}^i\cdot\tilde{\mathbf{v}}_p)\,\mathrm{d}l. \tag{64}$$

We note for the convenience of the reader that it is easier to start from Eq. (64) and derive Eq. (58).

Finally, adding Eqs. (56), (63) and (64), we get

$$\begin{aligned}\Gamma_2+\Gamma_3+\Gamma_4 &= \int_{\mathcal{J}_D} \left[\lim_{\eta\to 0} \int_{\mathcal{C}_\eta} \mathbf{C}\hat{\mathbf{h}}\cdot(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{u}}\,\mathrm{d}l + \left(\frac{\partial\tilde{\mathbf{c}}}{\partial\alpha} - \sum_{i=1,2}^{k} \bar{\mathbf{C}}^i\hat{\mathbf{w}}^i \right)\cdot\tilde{\mathbf{v}}_p \right] \mathrm{d}l \\ &+ \int_{\mathcal{J}_D} \left[\lim_{\eta\to 0} \int_{\mathcal{C}_\eta} \mathbf{S}\hat{\mathbf{h}}\cdot(\dot{\mathbf{y}}+\mathbf{F}(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{u}})\,\mathrm{d}l + \frac{\partial\tilde{\mathbf{s}}}{\partial\alpha}\cdot(\langle\dot{\mathbf{y}}\rangle_J + \langle\mathbf{F}\rangle_J\tilde{\mathbf{v}}_p) \right. \\ &\left. - \sum_{i=1,2}^{k} \bar{\mathbf{S}}^i\hat{\mathbf{w}}^i\cdot(\langle\dot{\mathbf{y}}\rangle + \langle\mathbf{F}\rangle\tilde{\mathbf{v}}_p) \right] \mathrm{d}l.\end{aligned} \tag{65}$$

Appealing to Eqs. (22) and (18), we obtain

$$\begin{aligned}\Gamma_2+\Gamma_3+\Gamma_4 &= \int_{\mathcal{J}_D} \left[\lim_{\eta\to 0} \int_{\mathcal{C}_\eta} \mathbf{C}\hat{\mathbf{h}}\,\mathrm{d}l + \frac{\partial\tilde{\mathbf{c}}}{\partial\alpha} - \sum_{i=1,2}^{k} \bar{\mathbf{C}}^i\hat{\mathbf{w}}^i \right]\cdot\tilde{\mathbf{v}}_p\,\mathrm{d}l \\ &+ \int_{\mathcal{J}_D} \left[\lim_{\eta\to 0} \int_{\mathcal{C}_\eta} \mathbf{S}\hat{\mathbf{h}}\,\mathrm{d}l + \frac{\partial\tilde{\mathbf{s}}}{\partial\alpha} - \sum_{i=1,2}^{k} \bar{\mathbf{S}}^i\hat{\mathbf{w}}^i \right]\cdot(\langle\dot{\mathbf{y}}\rangle_J + \langle\mathbf{F}\rangle_J\tilde{\mathbf{v}}_p)\,\mathrm{d}l \\ &= -\int_{\mathcal{J}_D} \tilde{\mathbf{f}}_J\cdot\tilde{\mathbf{v}}_p\,\mathrm{d}l,\end{aligned} \tag{66}$$

where we use the balances (31) and (34) to obtain the last equality.

Thus, from Eqs. (54, 62) and (66), the dissipation inequality for a region $\mathscr{D}\subset\Omega$ that contains the junction J is

$$\begin{aligned}\Gamma(\mathscr{D}) &= \int_{\mathscr{D}} \{\mathbf{S}\cdot\dot{\mathbf{F}} - \dot{\phi}\}\,\mathrm{d}a \\ &- \sum_{i=1,2}^{k} \int_{\Sigma_D^i} \left[(\psi^i)^\circ - \overline{\mathbf{S}}^i\cdot\langle\mathbf{F}\rangle^\circ + (\overline{\mathbf{q}}^i + (\overline{\mathbf{S}}^i)^T\langle\mathbf{F}\rangle\hat{\mathbf{m}}^i)\cdot(\hat{\mathbf{m}}^i)^\circ + (\overline{\mathbf{f}}^i\cdot\hat{\mathbf{m}}^i)\tilde{v}_m^i \right]\mathrm{d}a \\ &- \int_{J_D} \left[\chi^* - \tilde{\mathbf{s}}\cdot\tilde{\mathbf{p}}^* - \tilde{\mathbf{q}}\cdot\hat{\mathbf{t}}^* + \tilde{\mathbf{f}}_J\cdot\tilde{\mathbf{v}}_p \right]\mathrm{d}l \geq 0.\end{aligned} \tag{67}$$

5. Driving forces

We now identify the driving forces as the generalized forces that are conjugate to reference velocities in the dissipation inequality (67) following Abeyaratne and Knowles (1990), Gurtin (1995) and Gurtin and Struthers (1990).

5.1. Interface

The only meaningful (parametrization-free) notion of the velocity of an evolving interface is the normal velocity $\tilde{v}_m^i$. The interface driving force $\overline{d}_\Sigma^i$ is consequently a scalar. Indeed, examining Eq. (67), we find that the dissipation due to interface motion is a product of the normal velocity and $-(\overline{\mathbf{f}}_\Sigma^i\cdot\hat{\mathbf{m}}^i)$; therefore we identify $-(\overline{\mathbf{f}}_\Sigma^i\cdot\hat{\mathbf{m}}^i)$ as the interfacial driving force. Appealing to the configurational force balance (33), we conclude that the driving force on an interface is

$$\overline{d}_\Sigma^i = \hat{\mathbf{m}}^i\cdot[[\phi\mathbf{I} - \mathbf{F}^T\mathbf{S}]]\hat{\mathbf{m}}^i + (\psi^i\overline{\mathbf{P}}^i - (\overline{\mathbf{F}}^i)^T\overline{\mathbf{S}}^i)\cdot\overline{\mathbf{L}}^i + \nabla_\Sigma\cdot\overline{\mathbf{q}}^i. \tag{68}$$

This expression was obtained by Leo and Sekerka (1989), Gurtin and Struthers (1990) and Gurtin (1995).

5.2. Junction

The meaningful (parametrization-free) notion of the velocity of an evolving junction is its projection on the plane perpendicular to its tangent. Thus, the driving force $\tilde{\mathbf{d}}_J$ also lies in this plane, and by examining Eq. (67) we conclude that it is given by $-(\mathbf{I}-\tilde{\mathbf{P}})\mathbf{f}_J$, since $\mathbf{f}_J\cdot\tilde{\mathbf{v}}_p = \mathbf{f}_J\cdot(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{v}}_p = (\mathbf{I}-\tilde{\mathbf{P}})\mathbf{f}_j\cdot\tilde{\mathbf{v}}_p$. Appealing to the configuration force balance (34), we conclude that the driving force on a junction is

$$\tilde{\mathbf{d}}_J = (\mathbf{I}-\tilde{\mathbf{P}})\left[\lim_{\eta\to 0}\int_{\mathcal{C}_\eta}(\phi\mathbf{I}-\mathbf{F}^T\mathbf{S})\hat{\mathbf{h}}\,\mathrm{d}l-\sum_{i=1,2}^{k}[\psi^i\hat{\mathbf{w}}^i-(\bar{\mathbf{F}}^i)^T\bar{\mathbf{S}}^i\hat{\mathbf{w}}^i+(\bar{\mathbf{q}}^i\cdot\hat{\mathbf{w}}^i)\hat{\mathbf{m}}^i] + (\chi-\tilde{\mathbf{s}}\cdot\tilde{\mathbf{F}}\hat{\mathbf{t}})\tilde{\kappa}\hat{\mathbf{n}}+\frac{\partial\tilde{\mathbf{q}}}{\partial\alpha}\right]. \tag{69}$$

The first term (integral) is the contribution of the bulk and is reminiscent of the J integral of fracture mechanics. We note, however, that this integral is not path-independent due to the presence of the interfaces. The second term (sum) is the contribution of the interfaces, while the third is the contribution of the junction due to both line tension and shear.

5.3. Edge

Consider an interface Σ meeting the boundary of the body $\partial\Omega$ along the edge E. Fig. 2 shows the cross-sectional view. Let $\hat{\mathbf{m}}$ be the normal to the interface and $\hat{\mathbf{h}}$ the normal to the boundary $\partial\Omega$ (pointing outward from Ω). Let $\hat{\mathbf{t}}$ be the unit tangent to E (pointing into the plane of the paper in Fig. 2), $\hat{\mathbf{h}}$ be the unit binormal and define $\hat{\mathbf{w}}=\hat{\mathbf{h}}\times\hat{\mathbf{t}}$. Thus $\hat{\mathbf{w}}$ is normal to E and tangential to $\partial\Omega$. We can treat this edge as a triple junction by setting

$$\Omega^1=\Omega^-,\quad \Omega^3=\Omega^+,$$

$$\Sigma^1=\Sigma^1,\quad \Sigma^2=\partial\Omega^-,\quad \Sigma^3=\partial\Omega^+,$$

$$\hat{\mathbf{m}}^1=\hat{\mathbf{m}}^1,\quad \hat{\mathbf{m}}^2=\hat{\mathbf{h}},\quad \hat{\mathbf{m}}^3=-\hat{\mathbf{h}},$$

$$\hat{\mathbf{w}}^1=\hat{\mathbf{w}}^1,\quad \hat{\mathbf{w}}^2=\hat{\mathbf{w}},\quad \hat{\mathbf{w}}^3=-\hat{\mathbf{w}}$$

and holding $\Sigma^{2,3}$ fixed in the reference configuration. The edge is consequently constrained to move along the boundary. Thus, the velocity of the edge $\tilde{\mathbf{v}}$ satisfies $\tilde{\mathbf{v}}\cdot\hat{\mathbf{h}}=0$ and

$$\tilde{\mathbf{v}}_p=(\mathbf{I}-\tilde{\mathbf{P}})\tilde{\mathbf{v}}=v_w\hat{\mathbf{w}},\quad \text{where } v_w=\tilde{\mathbf{v}}\cdot\hat{\mathbf{w}}.$$

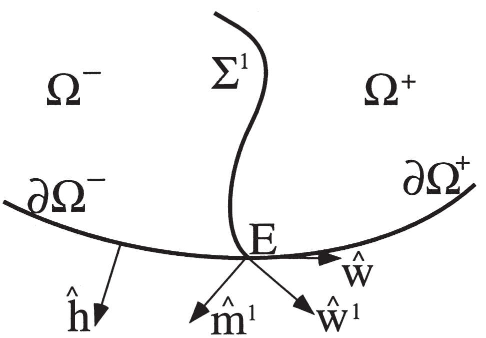

Fig. 2. An edge treated as a triple junction.

In other words, since the edge is constrained to move on a surface, the only meaningful velocity is the component normal to the curve and tangent to the surface. Consequently, the driving force is a scalar which we obtain as before from Eq. (67) to be

$$
\begin{aligned}
d_E \;&= \hat{\mathbf{w}}\cdot\Bigg[\lim_{\eta\to 0}\int_{\mathcal{C}_\eta}(\phi\mathbf{I}-\mathbf{F}^T\mathbf{S})\hat{\mathbf{h}}\,\mathrm{d}l-[\psi^1\hat{\mathbf{w}}^1-(\bar{\mathbf{F}}^1)^T\bar{\mathbf{S}}^1\hat{\mathbf{w}}^1+(\bar{\mathbf{q}}^1\cdot\hat{\mathbf{w}}^1)\hat{\mathbf{m}}^1] \\
&\quad +[[\psi\hat{\mathbf{w}}-(\bar{\mathbf{F}})^T\bar{\mathbf{S}}\hat{\mathbf{w}}+(\bar{\mathbf{q}}\cdot\hat{\mathbf{w}})\hat{\mathbf{m}}]]+(\chi-\tilde{\mathbf{s}}\cdot\tilde{\mathbf{F}}\hat{\mathbf{t}})\tilde{\kappa}\hat{\mathbf{n}}+\frac{\partial\tilde{\mathbf{q}}}{\partial\alpha}\Bigg].
\end{aligned}
\tag{70}
$$

Above, $[[a]]=a^+-a^-$ where $a^\pm$ denotes the limiting values along $\partial\Omega^\pm$. Once again, the first term is the contribution of the bulk, the second the contribution of the interface, the third the contribution of the boundary and the last two the contribution of the junction.

6. Constitutive equations

We make the following constitutive assumptions:

$$\phi=\phi(\mathbf{F}),\quad \psi=\psi(\langle\mathbf{F}\rangle,\hat{\mathbf{m}}),\quad \chi=\chi(\tilde{\mathbf{p}},\hat{\mathbf{t}}), \tag{71}$$

$$\mathbf{S}=\mathbf{S}(\mathbf{F}),\quad \bar{\mathbf{S}}=\bar{\mathbf{S}}(\langle\mathbf{F}\rangle,\hat{\mathbf{m}}),\quad \tilde{\mathbf{s}}=\tilde{\mathbf{s}}(\tilde{\mathbf{p}},\hat{\mathbf{t}}), \tag{72}$$

$$\bar{\mathbf{q}}=\bar{\mathbf{q}}(\langle\mathbf{F}\rangle,\hat{\mathbf{m}}),\quad \tilde{\mathbf{q}}=\tilde{\mathbf{q}}(\tilde{\mathbf{p}},\hat{\mathbf{t}}) \tag{73}$$

and

$$d_\Sigma=\bar{d}_\Sigma(\langle\mathbf{F}\rangle,\hat{\mathbf{m}},\bar{v}_m),\quad \mathbf{d}_J=\tilde{\mathbf{d}}_J(\tilde{\mathbf{p}},\hat{\mathbf{t}},\tilde{\mathbf{v}}_p),\quad d_E=\tilde{d}_E(\tilde{\mathbf{p}},\hat{\mathbf{t}},\tilde{v}_w). \tag{74}$$

Notice that we have assumed that the energy, stress and shear of the interface, junction and edge depend on both the deformation and crystallographic orientation (through $\hat{\mathbf{m}}$ and $\hat{\mathbf{t}}$). The driving force on the interface depends on the interface deformation, the crystallographic orientation and the normal velocity of the interface. Similarly, the driving force on the junction and edge depends on the deformation, orientation and relevant velocity. These final relations between the driving force and the velocity are often known as *kinetic relations*.

We now follow Coleman and Noll (1963) to obtain restrictions on the constitutive relations by requiring that the dissipation inequality (35) hold for all motions of the interfaces and for all deformations consistent with our kinematic assumptions. Substituting Eqs. (71)–(74) in Eq. (67) and localizing appropriately, we conclude that we may replace Eqs. (72) and (73) with

$$\mathbf{S}=\frac{\mathrm{d}\phi}{\mathrm{d}\mathbf{F}},\quad \bar{\mathbf{S}}=\frac{\partial\psi}{\partial\langle\mathbf{F}\rangle},\quad \tilde{\mathbf{s}}=\frac{\partial\chi}{\partial\tilde{\mathbf{p}}},$$

$$\bar{\mathbf{q}}=\frac{\partial\psi}{\partial\hat{\mathbf{m}}}-\bar{\mathbf{S}}\cdot\langle\mathbf{F}\rangle\hat{\mathbf{m}},\quad \tilde{\mathbf{q}}=\frac{\partial\chi}{\partial\hat{\mathbf{t}}};$$

and the kinetic relations are subject to the restrictions

$$\bar{v}_m \bar{d}_\Sigma(\langle \mathbf{F} \rangle, \hat{\mathbf{m}}, \bar{v}_m,) \geq 0, \quad \tilde{\mathbf{v}}_p \cdot \tilde{\mathbf{d}}_J(\tilde{\mathbf{p}}, \hat{\mathbf{t}}, \tilde{\mathbf{v}}_p) \geq 0, \quad \tilde{v}_w \tilde{d}_E(\tilde{\mathbf{p}}, \hat{\mathbf{t}}, \tilde{v}_w) \geq 0. \tag{75}$$

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Appendix A. Integral identities

A.1. Volume integrals

The positions of the interfaces Σ^i, the boundary of the control volume $\partial\mathscr{D}$ and the tube $\partial\mathscr{B}_\eta$ change with time. Let ϕ denote a scalar field, then using the usual transport identity we can write

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathscr{D}(t)\backslash\mathscr{B}_\eta(t)} \phi \,\mathrm{d}v = \int_{\mathscr{D}(t)\backslash\mathscr{B}_\eta(t)} \dot{\phi} \,\mathrm{d}v + \int_{\partial\mathscr{D}(t)} \phi(\mathbf{u}\cdot\hat{\mathbf{h}}) \,\mathrm{d}a - \sum_{\mathrm{i}=1,\,2}^{\mathrm{k}} \int_{\Sigma^i_D\backslash\mathscr{B}_\eta(t)} [[\phi]] \vec{v}^i_m \,\mathrm{d}a$$
$$- \int_{\partial\mathscr{B}_\eta(t)\cap\mathscr{D}(t)} \phi(\mathbf{u}\cdot\hat{\mathbf{h}}) \,\mathrm{d}a,$$

where $\dot{\phi} = \partial\phi(\mathbf{x}, t)/\partial t$; the velocity of points on the boundary of the control volume $\partial\mathscr{D}$ and on the boundary of the tube $\partial\mathscr{B}_\eta$ are denoted by $\mathbf{u}$, while the normal is denoted by $\hat{\mathbf{h}}$. Appealing to the definition (19), the transport identity for a volume integral is

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathscr{D}} \phi \,\mathrm{d}v \equiv \lim_{\eta\to 0} \left[\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathscr{D}\backslash\mathscr{B}_\eta} \phi \,\mathrm{d}v \right]$$
$$= \int_{\mathscr{D}} \dot{\phi} \,\mathrm{d}v + \int_{\partial\mathscr{D}} \phi(\mathbf{u}\cdot\hat{\mathbf{h}}) \,\mathrm{d}a - \sum_{\mathrm{i}=1,\,2}^{\mathrm{k}} \int_{\Sigma^i_D} [[\phi]] \vec{v}^i_m \,\mathrm{d}a - \lim_{\eta\to 0} \int_{\partial\mathscr{B}_\eta\cap\mathscr{D}} \phi(\mathbf{u}\cdot\hat{\mathbf{h}}) \,\mathrm{d}a. \tag{A1}$$

Similarly, for a smooth vector field $\mathbf{a}$, we write the divergence theorem as

$$\int_{\mathscr{D}} \nabla\cdot\mathbf{a} \,\mathrm{d}v = \lim_{\eta\to 0} \int_{\mathscr{D}\backslash\mathscr{B}_\eta} \nabla\cdot\mathbf{a} \,\mathrm{d}v = \int_{\partial\mathscr{D}} \mathbf{a}\cdot\hat{\mathbf{h}} \,\mathrm{d}a - \lim_{\eta\to 0} \int_{\partial\mathscr{B}_\eta} \mathbf{a}\cdot\hat{\mathbf{h}} \,\mathrm{d}a - \sum_{i=1,\,2}^{k} \int_{\Sigma^i_D} [[\mathbf{a}]]\cdot\hat{\mathbf{m}}^i \,\mathrm{d}a. \tag{A2}$$

By taking $\mathbf{a}=\mathbf{A}^T\mathbf{b}$ where $\mathbf{b}$ is some constant vector, we get

$$\int_{\mathscr{D}} \nabla\cdot\mathbf{A}\,\mathrm{d}v = \int_{\partial\mathscr{D}} \mathbf{A}\hat{\mathbf{h}}\,\mathrm{d}a - \lim_{\eta\to 0}\int_{\partial\mathscr{B}_\eta} \mathbf{A}\hat{\mathbf{h}}\,\mathrm{d}a - \sum_{i=1,2}^{k}\int_{\Sigma_D^i} [[\mathbf{A}]]\hat{\mathbf{m}}^i\,\mathrm{d}a. \tag{A3}$$

A.2. Surface integrals

Let $\Sigma_D \subset \Sigma$ and $\hat{\mathbf{w}}$ be the normal to the curve $\partial\Sigma_D$. The surface divergence theorem can be written as

$$\int_{\Sigma_D} \nabla_\Sigma\cdot\mathbf{a}\,\mathrm{d}a = \int_{\partial\Sigma_D} \mathbf{a}\cdot\hat{\mathbf{w}}\,\mathrm{d}l \quad \text{and} \quad \int_{\Sigma_D} \nabla_\Sigma\cdot\mathbf{A}\,\mathrm{d}a = \int_{\partial\Sigma_D} \mathbf{A}\hat{\mathbf{w}}\,\mathrm{d}l \tag{A4}$$

for vector fields $\mathbf{a}$ satisfying $\mathbf{a}\cdot\hat{\mathbf{m}}=0$ and for tensor fields $\mathbf{A}$ satisfying $\mathbf{A}\hat{\mathbf{m}}=0$ where $\hat{\mathbf{m}}$ denotes the normal to the surface Σ.

The transport identity for a integral defined on a moving interface Σ_D is (Gurtin, 1995)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Sigma_D} \alpha\,\mathrm{d}a = \int_{\Sigma_D} (\alpha^\circ - \alpha\overline{\kappa v_m})\,\mathrm{d}a + \int_{\partial\Sigma_D} \alpha\bar{\mathbf{V}}\cdot\hat{\mathbf{w}}\,\mathrm{d}l, \tag{A5}$$

where $\bar{\kappa}$ is the total curvature and $\bar{v}_m$ is the normal velocity of Σ, α° is the normal time derivative of α following the surface Σ, and $\bar{\mathbf{V}}$ is the velocity of the boundary curve $\partial\Sigma_D$.

A.3. Curve integrals

The curve transport theorem is given by (Gurtin, 1993)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{J(t)} \chi\,\mathrm{d}l = \int_{\mathscr{J}} [\chi^* - \chi\tilde{\kappa}\tilde{v}_n]\,\mathrm{d}l + \{\chi(\tilde{\mathbf{V}}\cdot\hat{\mathbf{t}})\}_{\alpha_1}^{\alpha_2}, \tag{A6}$$

where $\tilde{v}_n$ is the normal velocity of the curve and $\tilde{\kappa}$ is its curvature, χ^* is the normal time derivative of χ following the curve and $\tilde{\mathbf{V}}$ is the velocity of its end-points.

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