Chapter 5
Continuum Mechanics of the Interaction of Phase Boundaries and Dislocations in Solids

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Abstract The continuum mechanics of line defects representing singularities due to terminating discontinuities of the elastic displacement and its gradient field is developed. The development is intended for application to coupled phase transformation, grain boundary, and plasticity-related phenomena at the level of individual line defects and domain walls. The continuously distributed defect approach is developed as a generalization of the discrete, isolated defect case. Constitutive guidance for equilibrium response and dissipative driving forces respecting frame-indifference and non-negative mechanical dissipation is derived. A differential geometric interpretation of the defect kinematics is developed, and the relative simplicity of the actual adopted kinematics is pointed out. The kinematic structure of the theory strongly points to the incompatibility of dissipation with strict deformation compatibility.

5.1 Introduction

Whether due to material contrast or material instability, there are many situations in solid mechanics that necessitate the consideration of 2-d surfaces across which a distortion measure is discontinuous. By a *distortion* we refer to measures akin to a deformation 'gradient' except, in many circumstances, such a measure is not the gradient of a vector field; we refer to a 2-d surface of discontinuity of a distortion measure as a *phase boundary* (which, of course, includes a grain boundary as a special case). The more familiar situation in conventional theory (i.e. nonlinear elasticity, rate-independent macroscopic plasticity) is when the distortion field corresponds to the gradient of a continuous displacement field, but one could, and here

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we will, consider the presence of dislocations, or a discontinuity in the elastic displacement field, as well when necessary. We are particularly interested in situations where the phase boundary discontinuity actually terminates along a curve on the surface or, more generally, shows in-plane gradients along the surface. We consider such terminating curves as phase boundary *tips* and the more general case as a continuously distributed density of tips and their coupling to dislocations. We refer to the phase boundary tip curves as *generalized disclinations* (or g.disclinations; a (classical) disclination in solids corresponds to the tip constituting the termination of a pure rotation discontinuity). Concrete physical situations where the kinematic construct we have just outlined occur are commonplace. In connection to fundamental, (un)loaded, microstructure of materials, such terminating boundaries (or domain walls) occur as grain boundaries and triple junction lines in polycrystalline metals [DW72, BZB+12, LXBC10, HLL+12] or layered polymeric materials [LB06, RFL+12]. As agents of failure, some examples are weak interfaces between matrix and fiber in fiber-reinforced polymer composites, or two such phase boundaries spaced closely apart enclosing a matrix weak zone in such materials, e.g. crazed inclusions and shear bands. Of course, deformation bands (especially shear bands) are just as commonplace in the path to failure in metallic materials and granular materials. More mundane situations arise in understanding stress singularities at sharp corners of inclusions in a matrix of dissimilar material in a linear elastic context.

The conditions for the emergence of phase boundaries/localized deformation bands are by now well-understood, whether in the theory of inelastic deformation localization, e.g. [HH75, Ric76, PAN82] or solid-solid phase transformations, e.g. [KS78, Jam81, AK06]. On the other hand, there does not exist a theory today to represent the kinematics and dynamics of the terminating lines of such phase boundaries and the propagation of these boundary-tips. This can be of primary importance in understanding progressive damage, e.g. onset of debonding at fiber-matrix interfaces, extension of shear bands or crazes, or the stress concentrations produced at five-fold twin junctions, or grain boundary triple lines. It is the goal of this paper to work out the general continuum mechanics of coupled phase boundary and slip (i.e. regularized displacement-gradient and displacement discontinuities), taking into account their line defects which are g.disclinations and dislocations. The developed model is expected to be of both theoretical and practical use in the study of the coupling of the structure and motion of phase boundaries coupled to dislocation and kink-like defects e.g. [HP11, WSL+13, SKS+10].

A corresponding 'small deformation' theory has been worked out in [AF12]. It was not clear to us then whether one requires a theory with couple stress or not and both thermodynamically admissible possibilities were outlined there. We now believe that dealing with g.disclinations requires mechanics mediated by torque balance[1] and, therefore, in this paper, we only consider models where couple stresses also appear. A dissipative extension of disclination-dislocation theory due to deWit [deW70] has been developed in [FTC11, UCTF11, UCTF13] as well as the first numerical

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[1]However, a dislocation-only defect model does not require any consideration of torque balance or couple stresses, as shown in [Ach11, AF12] and in Sect. 5.5.3.

implementations for the theory with application to understanding grain-boundary mechanics [TCF+13b, TCF13a]. While we focus on continuously distributed defect densities, it is to be understood that we include in our setting the modeling of individual defect lines as non-singular localizations of these density fields along space curves.

The concept of classical disclinations and dislocations arose in the work of Weingarten and Volterra (cf. [Nab87]) from the specific question of characterizing the displacement and rotation jumps across a surface of a multiply connected region with a hole, when the displacement field is required to be consistent with a prescribed twice differentiable strain (metric) field; a well-developed static theory exists [RK09] as well as a very sophisticated topological theory, full of subtle but difficult insights, due to Klemán and Friedel [KF08]. While self-contained in itself, this question does not suffice for our purposes in understanding phase boundaries, since these can, and often necessarily, involve jumps in the strain field. Nevertheless, the differential geometry of coupled dislocations and so-called disclinations have been the subject of extensive enquiry, e.g. [Kon55, Bil60, KL92, CMB06], and therefore we show how our g.disclinations can be placed in a similar differential geometric context, while pointing out the main differences from the standard treatment. The differences arise primarily from a desire to achieve relative simplicity by capitalizing on the available Euclidean structure of the ambient space in which we do our mechanics directed towards applications.

The remainder of the paper is organized as follows. In Sect. 5.2 we provide a list of notation. In Sect. 5.3 we develop a fundamental kinematic decomposition relevant for our work. In Sect. 5.4 we develop the governing mechanical equations. In Sect. 5.5 we examine consequences of material frame-indifference (used synonymously with invariance under superposed rigid body motions) and a dissipation inequality for the theory, ingredients of which provide a critical check on the finite deformation kinematics of the proposed evolution equations for defect densities. Section 5.6 describes a small deformation version of the model. In Sect. 5.7 we provide a differential geometric interpretation of our work. Some concluding observations are recorded in Sect. 5.8.

Finally, in order to provide some physical intuition for the new kinematic objects we have introduced before launching into their continuum mechanics, we demonstrate (Fig. 5.1) a possible path to the nucleation of an edge dislocation in a lattice via the formation of a g.disclination dipole. It is then not surprising that point-wise loss of ellipticity criteria applied to continuum response generated from interatomic potentials can bear some connection to predicting the onset of dislocation nucleation [LVVZ+02, ZLJVV+04].

5.2 Notation

A superposed dot on a symbol represents a material time derivative. The statement $a := b$ indicates that a is defined to be equal to b. The summation convention is
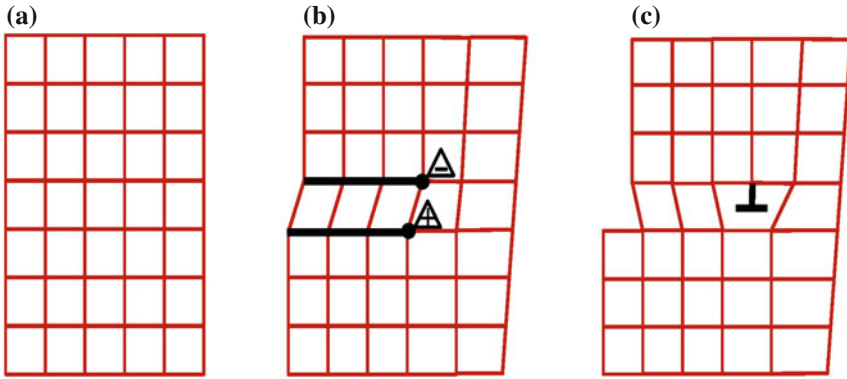
Fig. 5.1 Path to an idealized edge dislocation nucleation (**c**) involving a deformation discontinuity, achieved through the formation of a g.disclination dipole (**b**) in a continuous deformation with two surfaces of strain discontinuity of an unstretched atomic configuration (**a**). Here, a continuous deformation (**b**) of the original configuration (**a**) refers to the preservation of all nearest neighbors signified by bond connections; a discontinuous deformation (**c**) refers to a change in topology of bond connections

implied unless otherwise mentioned. We denote by $\boldsymbol{Ab}$ the action of the second-order (third-order, fourth-order) tensor $\boldsymbol{A}$ on the vector (second-order tensor, second-order tensor) $\boldsymbol{b}$, producing a vector (vector, second-order tensor). A $\cdot$ represents the inner product of two vectors, a : represents the trace inner product of two second-order tensors (in rectangular Cartesian components, $\boldsymbol{A} : \boldsymbol{D} = A_{ij}D_{ij}$) and matrices and the contraction of the last two indices of a third-order tensor with a second order tensor. The symbol $\boldsymbol{AD}$ represents tensor multiplication of the second-order tensors $\boldsymbol{A}$ and $\boldsymbol{D}$. The notation $(\cdot)_{\text{sym}}$ and $(\cdot)_{\text{skw}}$ represent the symmetric and skew symmetric parts, respectively, of the second order tensor $(\cdot)$. We primarily think of a third-order tensor as a linear transformation on vectors to the space of second-order tensors. A *transpose* of a third-order tensor is thought of as a linear transformation on the space of second order tensors delivering a vector and defined by the following rule: for a third-order tensor $\boldsymbol{B}$

$$\left(\boldsymbol{B}^T \boldsymbol{D}\right) \cdot \boldsymbol{c} = (\boldsymbol{B}\boldsymbol{c}) : \boldsymbol{D},$$

for all second-order tensors $\boldsymbol{D}$ and vectors $\boldsymbol{c}$.

The symbol div represents the divergence, grad the gradient, and div grad the Laplacian on the current configuration. The same words beginning with a Latin uppercase letter represent the identical derivative operators on a reference configuration. The curl operation and the cross product of a second-order tensor and a vector are defined in analogy with the vectorial case and the divergence of a second-order

tensor: for a second-order tensor A, a third-order tensor B, a vector v, and spatially constant vector fields b, c, and a spatially uniform second-order tensor field D,

$$c \cdot (A \times v) b = \left[\left(A^T c\right) \times v\right] \cdot b, \quad \forall b, c,$$

$$D : (B \times v) b = \left[\left(B^T D\right) \times v\right] \cdot b, \quad \forall D, b,$$

$$(\operatorname{div} A) \cdot c = \operatorname{div}\left(A^T c\right), \quad \forall c,$$

$$(\operatorname{div} B) : D = \operatorname{div}\left(B^T D\right), \quad \forall D,$$

$$c \cdot (\operatorname{curl} A) b = \left[\operatorname{curl}\left(A^T c\right)\right] \cdot b, \quad \forall b, c,$$

$$D : (\operatorname{curl} B) b = \left[\operatorname{curl}\left(B^T D\right)\right] \cdot b, \quad \forall b, D.$$

In rectangular Cartesian components,

$$(A \times v)_{im} = e_{mjk} A_{ij} v_k,$$

$$(B \times v)_{irm} = e_{mjk} B_{irj} v_k,$$

$$(\operatorname{div} A)_i = A_{ij,j},$$

$$(\operatorname{div} B)_{ij} = B_{ijk,k},$$

$$(\operatorname{curl} A)_{im} = e_{mjk} A_{ik,j},$$

$$(\operatorname{curl} B)_{irm} = e_{mjk} B_{irk,j},$$

where e_{mjk} is a component of the third-order alternating tensor X. Also, the vector XAD is defined as

$$(XAD)_i = e_{ijk} A_{jr} D_{rk}.$$

The spatial derivative for the component representation is with respect to rectangular Cartesian coordinates on the current configuration of the body. Rectangular Cartesian coordinates on the reference configuration will be denoted by uppercase Latin indices. For manipulations with components, we shall always use such rectangular Cartesian coordinates, unless mentioned otherwise. Positions of particles are measured from the origin of this arbitrarily fixed Cartesian coordinate system.

For a second-order tensor W, a third-order tensor S and an orthonormal basis $\{e_i, i = 1, 2, 3\}$ we often use the notation

$$\left(WS^{2T}\right) = W_{lp} S_{rpk} e_r \otimes e_l \otimes e_k \; ; \; \left(WS^{2T}\right)_{rlk} := W_{lp} S_{rpk}.$$

The following list describes some of the mathematical symbols we use in this paper.

x: current position

F^e: elastic distortion tensor (2nd-order)

$W = (F^e)^{-1}$: inverse of elastic 1-distortion tensor (2nd-order)
S: eigenwall tensor (3rd-order)
Y: inverse-elastic 2-distortion tensor (3rd-order)
α: dislocation density tensor (2nd-order)
Π: g.disclination density tensor (3rd-order)
v: material velocity
L: velocity gradient
$D = L_{sym}$: rate of deformation tensor
$\Omega = L_{skw}$: spin tensor
$\omega = -\frac{1}{2}X : \Omega = \frac{1}{2}\,curl\,v$: half of the vorticity vector
$M = grad\,\omega$: vorticity gradient tensor
$J = grad\,W$: gradient of i-elastic distortion
V^{Π}: g.disclination velocity
V^{α}: dislocation velocity
V^{S}: eigenwall velocity
T: Cauchy stress tensor
Λ: couple stress tensor
K: external body moment per unit mass
b: external body force per unit mass
ρ: mass density
ψ: free energy per unit mass

5.3 Motivation for a Fundamental Kinematic Decomposition

With reference to Fig. 5.2a representing a cross-section of a body, suppose we are given a tensor field φ (0th-order and up) that can be measured unambiguously, or computed from measurements without further information, at most points of a domain $\mathcal{B}$. Assume that the field φ is smooth everywhere except having a terminated discontinuity of constant magnitude across the surface $\mathcal{S}$. Denote the terminating curve of the discontinuity on the surface $\mathcal{S}$ as $\mathcal{C}$. We think of the subset $\mathcal{P}$ of $\mathcal{S}$ across which a non-zero jump exists as a *wall* of the field φ and the curve $\mathcal{C}$ as a *line defect* of the field φ. Physical examples of walls are domain walls, grain boundaries, phase boundaries, slip boundaries and stacking faults (surfaces of displacement discontinuity); those of defect lines are vortices, disclinations, g.disclinations, and dislocations. Let ν be a unit normal field on $\mathcal{S}$, with arbitrarily chosen orientation. Let $\mathcal{B}^+$ be the subset of $\mathcal{B}$ into which ν points; similarly, let $\mathcal{B}^-$ be the subset of $\mathcal{B}$ into which $-\nu$ points. Let x be a point on $\mathcal{P}$. Let $x^+ \in \mathcal{B}^+$ and $x^- \in \mathcal{B}^-$ be points arbitrarily close to x but not x, and let $\varphi(x^+) = \varphi^+$ and $\varphi(x^-) = \varphi^-$. Join x^+ to x^- by any contour $C_{x^+}^{x^-}$ encircling $\mathcal{C}$. Then

$$\int_{C_{x^+}^{x^-}} grad\,\varphi \cdot dx = \varphi^- - \varphi^+ =: -[\![\varphi]\!]. \tag{5.1}$$

(a)   **(b)**
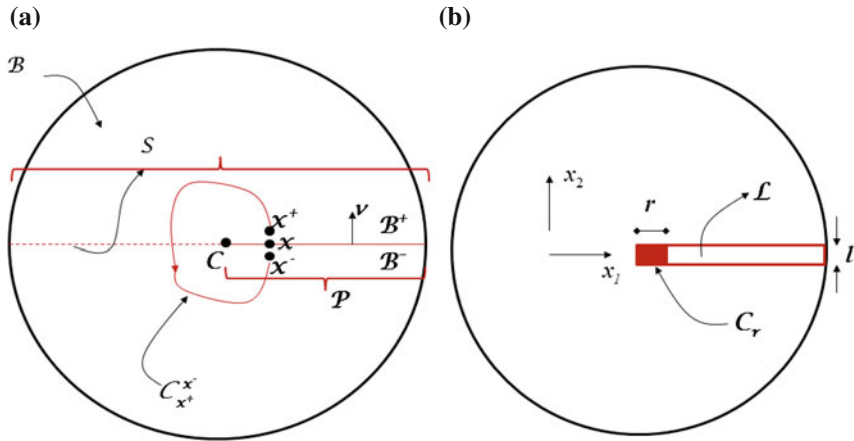

Fig. 5.2 Classical terminating discontinuity and its physical regularization

Note that by hypothesis $[\![\varphi]\!]$ is constant on $\mathcal{P}$ so that regardless of how close $\boldsymbol{x}$ is to $\mathcal{C}$, and how small the non-zero radius of a circular contour $C_{\boldsymbol{x}+}^{\boldsymbol{x}-}$ is, the contour integral takes the same value. This implies that $|grad\ \varphi(\boldsymbol{y})| \to \infty$ as $\boldsymbol{y} \to \mathcal{C}$ with $\boldsymbol{y} \in \mathcal{B}\backslash\mathcal{C}$.[2] Our goal now is to define a field $\boldsymbol{A}$ that is a physically regularized analog of $grad\ \varphi$; we require $\boldsymbol{A}$ to not have a singularity but possess the essential topological property (5.1) if $grad\ \varphi$ were to be replaced there with $\boldsymbol{A}$. For instance, this would be the task at hand if, as will be the case here, $\boldsymbol{A}$ is an ingredient of a theory and initial data for the field needs to be prescribed based on available observations on the field φ, the latter as described above.

It is a physically natural idea to regularize the discontinuity on $\mathcal{P}$ by a field on $\mathcal{B}$ that has support only on a thin layer around $\mathcal{P}$. We define such a field as follows (Fig. 5.2b). For simplicity, assume all fields to be uniform in the x_3-direction. Let the layer $\mathcal{L}$ be the set of points

$$\mathcal{L} = \{\boldsymbol{y} \in \mathcal{B} : \boldsymbol{y} = \boldsymbol{x} + h\,\boldsymbol{\nu}(\boldsymbol{x}), -l/2 \le h \le l/2, \boldsymbol{x} \in \mathcal{P}\}\,.$$

Let the x_1 coordinate of $\mathcal{C}$ be x^0. Define the *strip* field[3]

$$\boldsymbol{WV}(\boldsymbol{x}) = \begin{cases} f(x_1)\dfrac{\{\varphi^-(x_1)-\varphi^+(x_1)\}}{l} \otimes \boldsymbol{\nu}(x_1), & \text{if } \boldsymbol{x} \in \mathcal{L} \\ \boldsymbol{0}, & \text{if } \boldsymbol{x} \in \mathcal{B}\backslash\mathcal{L} \end{cases}$$

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[2]As an aside, this observation also shows why the typical assumptions made in deriving transport relations for various types of control volumes containing a shock surface do not hold when the discontinuity in question is of the 'terminating jump' type being considered here.

[3]$\boldsymbol{WV}$ is to be interpreted as the name for a single field.

where $\boldsymbol{\nu}(x_1) = \boldsymbol{e}_2$ here, and

$$f(x_1) = \begin{cases} \frac{x_1 - x^0}{r}, & \text{if } x^0 < x_1 \leq x^0 + r \\ 1, & \text{if } x^0 + r \leq x_1. \end{cases}$$

In the above, the layer width l and the defect-core width r are considered as given physical parameters. We now define A as

$$A := grad\,B + WV \quad \text{in } \mathcal{B}, \tag{5.2}$$

where B is at least a continuous and piecewise-smooth potential field in $\mathcal{B}$, to be determined from further constraints within a theoretical structure as, for example, we shall propose in this paper.

Let n be the order of the tensor field φ. A small calculation shows that the only non-vanishing component(s) of $curl\,WV$ is[4]

$$(curl\,WV)_{i_1 \cdots i_n 3} = e_{312} \frac{\partial f}{\partial x_1} \left[\frac{-[\![\varphi]\!]_{i_1 \cdots i_n}}{l} \right] = WV_{i_1 \cdots i_n 2,1}$$

and this is non-zero only in the *core cylinder* defined by

$$\mathcal{C}_r = \left\{ \boldsymbol{x} : x^0 \leq x_1 \leq x^0 + r, \, -l/2 \leq x_2 \leq l/2 \right\}.$$

Moreover, since $\frac{\partial f}{\partial x_1} = \frac{1}{r}$ in $\mathcal{C}_r$ and zero otherwise, we have

$$\int_C A \cdot d\boldsymbol{x} = \int_A curl\,WV \cdot \boldsymbol{e}_3 \, da = -\frac{[\![\varphi]\!]}{(l \cdot r)} (l \cdot r) = -[\![\varphi]\!],$$

for any *closed* curve C encircling $\mathcal{C}_r$ and A is any surface patch with boundary curve C.

Without commitment to a particular theory with constitutive assumptions, it is difficult to characterize further specific properties of the definition (5.2). However, it is important to avail of the following general intuition regarding it. Line defects are observed in the absence of applied loads. Typically, we are thinking of $grad\,\varphi$ as an elastic distortion measure that generates elastic energy, stresses, couple-stresses etc. Due to the fact that in the presence of line defects as described, $grad\,\varphi$ has non-vanishing content away from $\mathcal{P}$ in the absence of loads, if A is to serve as an analogous non-singular measure, it must have a similar property of producing *residual elastic distortion* for any choice of a $grad\,B$ field for a given WV field that contains a line defect (i.e. a non-empty subset $\mathcal{C}_r$). These possibilities can arise, for

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[4]Here it is understood that if $n = 0$ then the symbol $i_1 \cdots i_n$ correspond to the absence of any indices and the *curl* of the higher-order tensor field is understood as the natural analog of the second-order case defined in Sect. 5.2.

instance, from a hypothesis on minimizing energy or balancing forces or moments. That such a property is in-built into the definition (5.2) can be simply understood by realizing that WV is not a gradient and therefore cannot be entirely annihilated by $grad\,B$. To characterize this a bit further, one could invoke a Stokes-Helmholtz type decomposition of the (localized-in-layer) WV field to obtain

$$WV = grad\,Z + P \quad \text{on } \mathcal{B}$$

$$div\,grad\,Z = div\,WV \quad \text{on } \mathcal{B}$$

$$grad\,Zn = WVn \quad \text{on } \partial\mathcal{B}$$

$$curl\,P = curl\,WV \quad \text{on } \mathcal{B} \tag{5.3}$$

$$div\,P = 0 \quad \text{on } \mathcal{B}$$

$$Pn = 0 \quad \text{on } \partial\mathcal{B},$$

noting the interesting fact that $grad\,Z = -P$ in $\mathcal{B}\backslash\mathcal{L}$ because of the localized nature of WV. Thus, $grad\,B$ can at most negate the $grad\,Z$ part of WV and what remains is at least a *non-localized* field P representing some, or in some specific cases (e.g. screw dislocation in isotropic linear elasticity or Neo-Hookean elasticity, [Ach01]) all, of the off-$\mathcal{C}_r$ content of the original $grad\,\varphi$ field. Of course, it must be understood that the primary advantage, within our interpretation, of utilizing A in place of $grad\,\varphi$ is that the former is non-singular, but with the desired properties.[5]

It should be clear now that a field with many defect lines can as well be represented by a construct like (5.2) through superposition of their 'corresponding WV fields', including dipolar defect-line structures where the layer $\mathcal{L}$ has two-sided terminations within the body, without running all the way to the boundary.

As a common example we may think of classical small deformation plasticity where the plastic distortion field U^p may be interpreted as $-WV$, the displacement field u as the potential B and A as the elastic distortion U^e. In classical plasticity theory, the decomposition $U^e = grad\,u - U^p$ is introduced as a hypothesis based on phenomenology related to 1-d stress strain curves and the notion of permanent deformation produced in such a set-up. Our analysis may be construed as a fundamental kinematical and microstructural justification of such a hypothesis, whether in the presence of a single or many, many dislocations. At finite deformations, there is a similar decomposition for the i-elastic 1 distortion $F^{e-1} = W = \chi + grad\,f$ [Ach04, Ach11], where the spatial derivative is on the current configuration and we identify A with W, $Z + B$ with f, and P with χ.

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[5] It is to be noted that the decomposition (5.3) is merely *a* means to understand the definitions (5.2), (5.4), the latter being fundamental to the theory.

Based on the above motivation, for the theory that follows, we shall apply the definition (5.2) to the i-elastic 2-distortion Y to write

$$Y = grad\, W + S, \tag{5.4}$$

where W is the i-elastic 1-distortion and we refer to S (3rd-order tensor) as the *eigenwall* field.

What we have achieved above is a generalization of the *eigenstrain* concept of Kröner, Mura, and deWit. With the gained understanding, it becomes *the* natural modeling tool for dealing with the dynamics of discontinuities and line-singularities of first and higher-order deformation gradients with smooth (everywhere) fields within material and geometrically linear and nonlinear theories. The main utility of WV fields, as will be evident later, is in providing a tool for stating kinematically natural evolution equations for defect densities; while they also provide regularization of nasty singularities, such a smoothing effect can, at least in principle, also be obtained by demanding that the jump $[\![\varphi]\!]$ rise to a constant value from 0 over a short distance in $\mathcal{P}$, without introducing any new fields.

5.4 Mechanical Structure and Dissipation

5.4.1 Physical Notions

This subsection has been excerpted from [AZ14] for the sake of completeness.

The physical model we have in mind for the evolution of the body is as follows. The body consists of a fixed set of atoms. At any given time each atom occupies a well defined region of space and the collection of these regions (at that time) is well-approximated by a connected region of space called a configuration. We *assume* that any two of these configurations can necessarily be connected to each other by a continuous mapping. The temporal sequence of configurations occupied by the set of atoms are further considered as parametrized by increasing time to yield a *motion* of the body. A fundamental assumption in what follows is that the mass and momentum of the set of atoms constituting the body are transported in space by this continuous motion. For simplicity, we think of each spatial point of the configuration corresponding to the body in the as-received state for any particular analysis as a set of 'material particles,' a particle generically denoted by X.

Another fundamental assumption related to the motion of the atomic substructure is as follows. Take a spatial point x of a configuration at a given time t. Take a collection of atoms around that point in a spatial volume of fixed extent, the latter independent of x and with size related to the spatial scale of resolution of the model we have in mind. Denote this region as $\mathcal{D}_c(x, t)$; this represents the 'box' around the base point x at time t. We now think of relaxing the set of atoms in $\mathcal{D}_c(x, t)$ from the constraints placed on it by the rest of the atoms of the whole body, the latter possibly externally loaded. This may be achieved, in principle at least, by removing the rest of the atoms of the body or, in other words, by ignoring the forces exerted by

them on the collection within $\mathcal{D}_c(\boldsymbol{x}, t)$. This (thought) procedure generates a unique placement of the atoms in $\mathcal{D}_c(\boldsymbol{x}, t)$ denoted by $\mathsf{A}_{\boldsymbol{x}}$ with no forces in each of the atomic bonds in the collection.

We now imagine immersing $\mathsf{A}_{\boldsymbol{x}}$ in a larger collection of atoms (without superimposing any rigid body rotation), ensuring that the entire collection is in a zero-energy ground state (this may require the larger collection to be 'large enough' but not space-filling, as in the case of amorphous materials (cf. [KS79]). Let us assume that as $\boldsymbol{x}$ varies over the entire body, these larger collections, one for each $\boldsymbol{x}$, can be made to contain identical numbers of atoms. Within the larger collection corresponding to the point $\boldsymbol{x}$, let the region of space occupied by $\mathsf{A}_{\boldsymbol{x}}$ be approximated by a connected domain $\mathcal{D}_r^{pre}(\boldsymbol{x}, t)$, containing the same number of atoms as in $\mathcal{D}_c(\boldsymbol{x}, t)$. The spatial configuration $\mathcal{D}_r^{pre}(\boldsymbol{x}, t)$ may correctly be thought of as stress-free. Clearly, a deformation can be defined mapping the set of points $\mathcal{D}_c(\boldsymbol{x}, t)$ to $\mathcal{D}_r^{pre}(\boldsymbol{x}, t)$. We now *assume* that this deformation is well approximated by a homogeneous deformation.

Next, we assume that the set of these larger collections of relaxed atoms, one collection corresponding to each $\boldsymbol{x}$ of the body, differ from each other only in orientation, if distinguishable at all. We choose one such larger collection arbitrarily, say C, and impose the required rigid body rotation to each of the other collections to orient them identically to C. Let the obtained configuration after the rigid rotation of $\mathcal{D}_r^{pre}(\boldsymbol{x}, t)$ be denoted by $\mathcal{D}_r(\boldsymbol{x}, t)$.

We denote the *gradient of the homogeneous deformation mapping $\mathcal{D}_c(\boldsymbol{x}, t)$ to $\mathcal{D}_r(\boldsymbol{x}, t)$ by $\boldsymbol{W}(\boldsymbol{x}, t)$, the i-elastic 1-distortion at $\boldsymbol{x}$ at time t.

What we have described above is an embellished version of the standard fashion of thinking about the problem of defining elastic distortion in the classical theory of finite elastoplasticity [Lee69], with an emphasis on making a connection between the continuum mechanical ideas and discrete atomistic ideas as well as emphasizing that no ambiguities related to spatially inhomogeneous rotations need be involved in defining the field $\boldsymbol{W}$.[6] However, our physical construct requires no choice of a reference configuration or a 'multiplicative decomposition' of it into elastic and plastic parts to be invoked [Ach04]. In fact, *there is no notion of a plastic deformation $\boldsymbol{F}^p$ invoked in our model*. Instead, as we show in Sect. 5.4.4 (5.14), an additive decomposition of the velocity gradient into elastic and plastic parts emerges naturally in this model from the kinematics of dislocation motion representing conservation of Burgers vector content in the body.

Clearly, the field $\boldsymbol{W}$ need not be a gradient of a vector field at any time. Thinking of this ielastic 1-distortion field $\boldsymbol{W}$ on the current configuration at any given time as the $\boldsymbol{\varphi}$ field of Sect. 5.3, the i-elastic 2-distortion field $\boldsymbol{Y}$ is then defined as described therein.

It is important to note that if a material particle X is tracked by an individual trajectory $\boldsymbol{x}(t)$ in the motion (with $\boldsymbol{x}(0) = X$), the family of neighborhoods $\mathcal{D}_c(\boldsymbol{x}(t), t)$ parametrized by t in general can contain vastly different sets of atoms compared to the set contained initially in $\mathcal{D}_c(\boldsymbol{x}(0), 0)$. The intuitive idea is that the connectivity, or

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[6]Note that the choice of C affects the $\boldsymbol{W}$ field at most by a superposed *spatio-temporally uniform* rotation field.

nearest neighbor identities, of the atoms that persist in $\mathcal{D}_c(\boldsymbol{x}(t), t)$ over time remains fixed only in purely elastic motions of the body.

5.4.2 The Standard Continuum Balance Laws

For any fixed set of material particles occupying the volume $B(t)$ at time t with boundary $\partial B(t)$ having outward unit normal field $\boldsymbol{n}$

$$\overline{\int_{B(t)} \rho \, dv} = 0,$$

$$\overline{\int_{B(t)} \rho \boldsymbol{v} \, dv} = \int_{\partial B(t)} \boldsymbol{Tn} \, da + \int_{B(t)} \rho \boldsymbol{b} \, dv,$$

$$\overline{\int_{B(t)} \rho \left(\boldsymbol{x} \times \boldsymbol{v}\right) \, dv} = \int_{\partial B(t)} \left(\boldsymbol{x} \times \boldsymbol{T} + \boldsymbol{\Lambda}\right) \boldsymbol{n} \, da + \int_{B(t)} \rho \left(\boldsymbol{x} \times \boldsymbol{b} + \boldsymbol{K}\right) \, dv,$$

represent the statements of balance of mass, linear and angular momentum, respectively. We re-emphasize that it is an assumption that the actual mass and momentum transport of the underlying atomic motion can be adequately represented through the material velocity and density fields governed by the above statements (with some liberty in choosing the stress and couple-stress tensors). For instance, in the case of modeling fracture, some of these assumptions may well require revision.

Using Reynolds' transport theorem, the corresponding local forms for these equations are:

$$\dot{\rho} + \rho \operatorname{div} \boldsymbol{v} = 0$$
$$\rho \dot{\boldsymbol{v}} = \operatorname{div} \boldsymbol{T} + \rho \boldsymbol{b} \qquad (5.5)$$
$$\boldsymbol{0} = \operatorname{div} \boldsymbol{\Lambda} - \boldsymbol{X} : \boldsymbol{T} + \rho \boldsymbol{K}.$$

Following [MT62], the external power supplied to the body at any given time is expressed as:

$$P(t) = \int_{B(t)} \rho \boldsymbol{b} \cdot \boldsymbol{v} \, dv + \int_{\partial B(t)} (\boldsymbol{Tn}) \cdot \boldsymbol{v} \, da + \int_{\partial B(t)} (\boldsymbol{\Lambda n}) \cdot \boldsymbol{\omega} \, da + \int_{B(t)} \rho \boldsymbol{K} \cdot \boldsymbol{\omega} \, dv$$

$$= \int_{B(t)} (\rho \boldsymbol{v} \cdot \dot{\boldsymbol{v}}) \, dv + \int_{B(t)} (\boldsymbol{T} : \boldsymbol{D} + \boldsymbol{\Lambda} : \boldsymbol{M}) \, dv,$$

where Balance of linear momentum and angular momentum have been used. On defining the kinetic energy and the free energy of the body as

$$K = \int_{B(t)} \frac{1}{2} \left(\rho \boldsymbol{v} \cdot \boldsymbol{v}\right) \, dv,$$

$$F = \int_{B(t)} \rho \psi \, dv,$$

respectively, and using Reynolds' transport theorem, we obtain the mechanical dissipation

$$\mathsf{D} := P - \overline{\dot{K + F}} = \int_{B(t)} \left(\boldsymbol{T} : \boldsymbol{D} + \boldsymbol{\Lambda} : \boldsymbol{M} - \rho \dot{\psi} \right) \, dv. \tag{5.6}$$

The first equality above shows the distribution of applied mechanical power into kinetic, stored and dissipated parts. The second equality, as we show subsequently, is used to provide guidance on constitutive structure.

5.4.3 G.disclination Density and Eigenwall Evolution

The natural measure of g.disclination density is

$$curl \ (\boldsymbol{Y} - grad \, \boldsymbol{W}) = curl \, \boldsymbol{S} = \boldsymbol{\Pi}.$$

It characterizes the closure failure of integrating $\boldsymbol{Y}$ on closed contours in the body:

$$\int_a \boldsymbol{\Pi} \boldsymbol{n} da = \int_c \boldsymbol{Y} \, d\boldsymbol{x},$$

where a is any area patch with closed boundary contour c in the body. Physically, it is to be interpreted as a density of lines (threading areas) in the current configuration, carrying a tensorial attribute that reflects a jump in $\boldsymbol{W}$. As such, it is reasonable to postulate, before commitment to constitutive equations, a tautological evolution statement of balance for it in the form of "rate of change = what comes in − what goes out + what is generated." Since we are interested in nonlinear theory consistent with frame-indifference and non-negative dissipation, it is more convenient to work with the measure

$$^\star\boldsymbol{\Pi} := curl \left(\boldsymbol{W} \boldsymbol{S}^{2T} \right) \tag{5.7}$$

$$\left(\boldsymbol{W} \boldsymbol{S}^{2T} \right)_{rlk} := W_{lp} S_{rpk}$$
$$^\star\Pi_{rli} = e_{ijk} \left[W_{lp} S_{rpk} \right]_{,j} = e_{ijk} \left[W_{lp} \left(Y_{rpk} - W_{rp,k} \right) \right]_{,j},$$

(cf. [AD12]), and follow the arguments in [Ach11] to consider a conservation statement for a *density of lines* of the form

$$\overline{\int_{a(t)} {}^\star\boldsymbol{\Pi} \boldsymbol{n} \, da} = - \int_{c(t)} \boldsymbol{\Pi} \times \boldsymbol{V}^\Pi \, d\boldsymbol{x}. \tag{5.8}$$

Here, $a(t)$ is the area-patch occupied by an arbitrarily fixed set of material particles at time t and $c(t)$ is its closed bounding curve and the statement is required to hold for

all such patches. V^{Π} is the *g.disclination velocity* field, physically to be understood as responsible for transporting the g.disclination line density field in the body.

Arbitrarily fix an instant of time, say s, in the motion of a body and let F_s denote the time-dependent deformation gradient field corresponding to this motion with respect to the configuration at the time s. Denote positions on the configuration at time s as x_s and the image of the area patch $a(t)$ as $a(s)$. We similarly associate the closed curves $c(t)$ and $c(s)$. Then, using the definition (5.7), (5.8) can be written as

$$\overline{\int_{a(t)} {}^{\star}\dot{\Pi n}\, da} + \int_{c(t)} \Pi \times V^{\Pi}\, dx = \overline{\int_{c(t)} WS^{2T}\, dx} + \int_{c(t)} \Pi \times V^{\Pi}\, dx$$

$$= \int_{c(s)} \left[\overline{WS^{2T}\dot{F}_s} + \left(\Pi \times V^{\Pi} \right) F_s \right] dx_s$$

$$= \int_{c(t)} \left[\overline{WS^{2T}\dot{F}_s}F_s^{-1} + \Pi \times V^{\Pi} \right] dx = 0$$

which implies

$$\overline{WS^{2T}\dot{F}_s}F_s^{-1} = -\Pi \times V^{\Pi} + grad\,\Sigma,$$

where Σ is an arbitrary second-order tensor field with physical dimensions of strain rate (i.e. $1/Time$) that we will subsequently specify to represent grain/phase boundary motion transverse to itself. Finally, choosing $s = t$, we arrive at the following local evolution equation for S:

$$\overset{\diamond}{S}:= \dot{W}S^{2T} + W\dot{S}^{2T} + WS^{2T}L = -\Pi \times V^{\Pi} + grad\,\Sigma.$$

The local form of (5.8) is[7]

$$\overset{\circ}{{}^{\star}\Pi}:= (div\,v)\,{}^{\star}\Pi + \dot{{}^{\star}\Pi} - {}^{\star}\Pi L^T = -curl\left(\Pi \times V^{\Pi} \right). \tag{5.9}$$

---

[7]An important feature of conservation statements for signed 'topological charge' as here is that even without explicit source terms nucleation (of loops) is allowed. This fact, along with the coupling of Π to the material velocity field through the convected derivative provides an avenue for predicting homogeneous nucleation of line defects. In the dislocation-only theory, some success has been achieved with this idea in ongoing work.
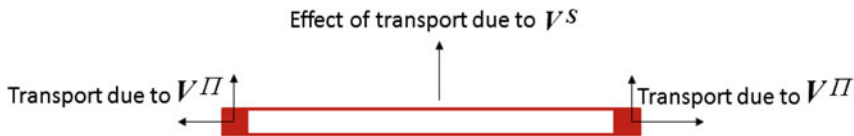
Fig. 5.3 Transport due to g.disclination and eigenwall velocities

Finally, we choose $\boldsymbol{\Sigma}$ to be

$$\boldsymbol{\Sigma} := \boldsymbol{W}\boldsymbol{S}^{2T}\boldsymbol{V}^S \ ; \ \ \Sigma_{ij} = W_{jr}S_{irk}V_k^S,$$

where $\boldsymbol{V}^S$ is the *eigenwall velocity* field that is physically to be interpreted as transporting the eigenwall field $\boldsymbol{S}$ transverse to itself. This may be heuristically justified as follows: the eigenwall field represents a gradient of i-elastic distortion in a direction normal to the phase boundary (i.e. in the notation of Sect. 5.3, normal to $\mathcal{P}$). If the band now moves with a velocity $\boldsymbol{V}^S$ relative to the material, at a material point past which the boundary moves there is change of i-elastic distortion per unit time given by $\boldsymbol{\Sigma}$. The geometrically complete local evolution equation for $\boldsymbol{S}$ is given by

$$\overset{\diamond}{\boldsymbol{S}} = -\boldsymbol{\Pi} \times \boldsymbol{V}^{\Pi} + grad\left(\boldsymbol{W}\boldsymbol{S}^{2T}\boldsymbol{V}^S\right). \tag{5.10}$$

Thus, for phase boundaries, $\boldsymbol{V}^{\Pi}$ transports in-plane gradients of $\boldsymbol{S}$ including the tips of such bands, whereas $\boldsymbol{V}^S$ transports the phase boundary transverse to itself (Fig. 5.3).

5.4.4 Dislocation Density and I-Elastic 1-Distortion Evolution

Following tradition [deW73], we define the *dislocation density* $\boldsymbol{\alpha}$ as

$$\boldsymbol{\alpha} := \boldsymbol{Y} : \boldsymbol{X} = (\boldsymbol{S} + grad\,\boldsymbol{W}) : \boldsymbol{X} \tag{5.11}$$

and note that when $\boldsymbol{S} \equiv \boldsymbol{0}$, $\boldsymbol{\alpha} = -curl\,\boldsymbol{W}$ since for any smooth tensor field $\boldsymbol{A}$, $curl\,\boldsymbol{A} = -grad\,\boldsymbol{A} : \boldsymbol{X}$. The definition (5.11) is motivated by the displacement jump formula (5.18) corresponding to a single, isolated defect line terminating an i-elastic distortion jump in the body. In this situation, the displacement jump for an isolated defect line, measured by integrating $\boldsymbol{\alpha}$ on an area patch threaded by the defect line, is no longer a topological object independent of the area patch.

The evolution of the $\boldsymbol{S} : \boldsymbol{X}$ component of $\boldsymbol{\alpha}$ is already specified from the evolution (5.10) for $\boldsymbol{S}$. Thus, what remains to be specified for the evolution of the dislocation density field is the evolution of

$$\widetilde{\boldsymbol{\alpha}} := -curl\,\boldsymbol{W} = (\boldsymbol{Y} - \boldsymbol{S}) : \boldsymbol{X},$$

that is again an areal density of lines carrying a vectorial attribute.

When $S = 0$, then $\widetilde{\alpha} = \alpha$, and the physical arguments of finite-deformation dislocation mechanics [Ach11] yield

$$\overline{\int_{a(t)} \widetilde{\alpha}\, \boldsymbol{n}\, da} = -\int_{c(t)} \widetilde{\alpha} \times \boldsymbol{V}^{\alpha}\, d\boldsymbol{x}$$

with corresponding local form

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \widetilde{\alpha} \times \boldsymbol{V}^{\alpha},$$

(up to assuming an additive gradient of a vector field to vanish). Here, $\boldsymbol{V}^{\alpha}$ denotes the *dislocation velocity* field, to be interpreted physically as the field responsible for transporting the dislocation density field in the body.

Using identical logic, we assume as the statement of evolution of $\boldsymbol{W}$ the equation

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\alpha} \times \boldsymbol{V}^{\alpha}, \tag{5.12}$$

with a natural adjustment to reflect the change in the definition of the dislocation density field. This statement also corresponds to the following local statement for the evolution of $\widetilde{\alpha}$:

$$\overset{\circ}{\widetilde{\alpha}} := (div\, \boldsymbol{v})\, \widetilde{\alpha} + \dot{\widetilde{\alpha}} - \widetilde{\alpha}\boldsymbol{L}^{T} = -curl \left(\boldsymbol{\alpha} \times \boldsymbol{V}^{\alpha} \right). \tag{5.13}$$

It is to be noted that in this generalization of the dislocation-only case, the dislocation density is no longer necessarily divergence-free (see (5.11)) which is physically interpreted as the fact that dislocation lines may terminate at eigenwalls or phase boundaries.

We note here that (5.12) can be rewritten in the form

$$\boldsymbol{L} = \dot{\boldsymbol{F}}^{e} \boldsymbol{F}^{e-1} + \left(\boldsymbol{F}^{e} \boldsymbol{\alpha} \right) \times \boldsymbol{V}^{\alpha}, \tag{5.14}$$

where $\boldsymbol{F}^{e} := \boldsymbol{W}^{-1}$. To make contact with classical finite deformation elastoplasticity, this may be interpreted as a fundamental additive decomposition of the velocity gradient into elastic $\left(\dot{\boldsymbol{F}}^{e} \boldsymbol{F}^{e-1} \right)$ and plastic $((\boldsymbol{F}^{e} \boldsymbol{\alpha}) \times \boldsymbol{V}^{\alpha})$ parts. The latter is defined by the rate of deformation produced by the flow of dislocation lines in the current configuration, *without any reference to the notion of a total plastic deformation from some pre-assigned reference configuration*. We also note the *natural emergence of plastic spin* (i.e. a non-symmetric plastic part of $\boldsymbol{L}$), even in the absence of any assumptions of crystal structure but arising purely from the kinematics of dislocation motion (when a dislocation is interpreted as an elastic incompatibility).

5.4.5 Summary of Proposed Mechanical Structure of the Theory

To summarize, the governing equations of the proposed model are

$$\dot{\rho} = -\rho \operatorname{div} \boldsymbol{v}$$
$$\rho \dot{\boldsymbol{v}} = \operatorname{div} \boldsymbol{T} + \rho \boldsymbol{b}$$
$$\boldsymbol{0} = \operatorname{div} \boldsymbol{\Lambda} - \boldsymbol{X} : \boldsymbol{T} + \rho \boldsymbol{K} \tag{5.15}$$
$$\dot{\boldsymbol{W}} = -\boldsymbol{W}\boldsymbol{L} + \boldsymbol{\alpha} \times \boldsymbol{V}^{\alpha}$$
$$\dot{\boldsymbol{S}} = \boldsymbol{W}^{-1} \left\{ -\dot{\boldsymbol{W}} \boldsymbol{S}^{2T} - \boldsymbol{W} \boldsymbol{S}^{2T} \boldsymbol{L} - \boldsymbol{\Pi} \times \boldsymbol{V}^{\Pi} + grad \left(\boldsymbol{W} \boldsymbol{S}^{2T} \boldsymbol{V}^{S} \right) \right\}^{2T}$$
$$\boldsymbol{0} = -\boldsymbol{\alpha} + \boldsymbol{S} : \boldsymbol{X} - curl \, \boldsymbol{W}.$$

The fundamental dependent fields governed by these equations are the current position field $\boldsymbol{x}$, the i-elastic 1-distortion field $\boldsymbol{W}$, and the eigenwall field $\boldsymbol{S}$.

The relevance of the eigenwall velocity field $\boldsymbol{V}^{S}$ would seem to be greatest in the completely compatible case when there are no deformation line defects allowed (i.e. $\boldsymbol{\alpha} = \boldsymbol{0}, \boldsymbol{\Pi} = \boldsymbol{0}$). For reasons mentioned in Sect. 5.4.6, including eigenwall evolution seems to be at odds with strict compatibility. Additionally, modeling wall defects by dipolar arrays of disclinations [TCF13a] appears to be a successful, fundamental way of dealing with grain boundary motion. However, it also seems natural to consider many phase boundaries as containing no g.disclinations whatsoever, e.g. the representation of a straight phase boundary of constant strength that runs across the body without a termination (this may be physically interpreted as a consistent coarser length-scale view of a phase-boundary described by separated g.disclination-dipole units). To represent phase boundary motion in this situation of no disclinations, a construct like $\boldsymbol{V}^{S}$ is necessary, and we therefore include it for mathematical completeness.

The model requires constitutive specification for

- the stress $\boldsymbol{T}$,
- the couple-stress $\boldsymbol{\Lambda}$,
- the g.disclination velocity $\boldsymbol{V}^{\Pi}$,
- the dislocation velocity $\boldsymbol{V}^{\alpha}$, and
- the eigenwall velocity $\boldsymbol{V}^{S}$ (when not constrained to vanish).

As a rough check on the validitiy of the mechanical structure, we would like to accommodate analogs of the following limiting model scenarios within our general theory. The first corresponds to the calculation of static stresses of disclinations in linear elasticity [deW73], assuming no dislocations are present. That is, one thinks of a terminating surface of discontinuity in the elastic rotation field, across which the elastic displacements are continuous (except at the singular tip of the terminating surface). The analog of this question in our setting would be to set $\boldsymbol{\alpha} = \boldsymbol{0}$ in (5.11) and consider $\boldsymbol{S} : \boldsymbol{X}$ as a given source for $\boldsymbol{W}$, i.e.

$$\widetilde{\boldsymbol{\alpha}} = -curl \, \boldsymbol{W} = -\boldsymbol{S} : \boldsymbol{X},$$

where W is assumed to be the only argument of the stress tensor. Thus, the S field directly affects the elastic distortion that feeds into the stress tensor. Of course, this constrained situation, i.e. $\alpha = 0$, may only be realized if the field $S : X$ is divergence-free on $\mathcal{B}$. Thus, with (5.11) as a field equation along with constitutive equations for the stress and couple stress tensor and the static versions of balance of linear and angular momentum, this problem becomes accessible within our model.

As a second validating feature of the presented model, we mention the work of [TCF13a] on the prediction of shear coupled grain boundary migration within what may be interpreted as a small-deformation, disclination-dislocation-only version of the above theory. There, the grain boundaries are modeled by an array of (stress-inducing) disclination dipoles and it is shown how the kinematic structure of the above type of system along with the presence of stresses and couple stresses allows grain boundary motion with concomitant shear-producing dislocation glide to be predicted in accord with experiments and atomistic simulations.

Finally, one would of course like to recover some regularized version of classical, compatible phase transformation theory [BJ87], i.e. classical nonlinear elasticity with a non-convex energy function and with continuous displacements, in the absence of dislocations, g.disclinations and the eigenwall field in our model, i.e. ($\alpha = 0, S = \Pi = 0$). The model reduces to a strain gradient regularization [Sle83, AK91, BK84, SLSB99] of classical nonlinear elasticity resulting from the presence of couple stresses and the dependence of the energy function on the second deformation gradient.

5.4.6 The Possibility of Additional Kinetics in the Completely Compatible Case

The question of admitting additional kinetics of phase boundary motion in the completely compatible case (i.e. no dislocations and g.disclinations) is an interesting one, raised in the works of Abeyaratne and Knowles [AK90, AK91]. In the spatially 1-d scenario considered in [AK91], it is shown that admitting higher gradient effects does provide additional conditions over classical elasticity for well-defined propagation of phase boundaries, albeit with no dissipation, while the results of [Sle83] show that a viscosity effect alone is too restrictive and does not allow propagation. The work of [AK91], that extends to 3-d [AK06], does not rule out, and in fact emphasizes, more general kinetic relations for phase boundary propagation arising from dissipative effects, demonstrating the fact through a combined viscosity-capillarity regularization of nonlinear elasticity.

Within our model, the analogous situation is to consider the g.disclination density and the dislocation density constrained to vanish ($\Pi = 0$ and $\alpha = 0$). A dissipative mechanism related to phase boundary motion may now be introduced by admitting

a generally non-vanishing V^S field. For the present purpose, it suffices then to focus on the following three kinematic equations:

$$\dot{S} = W^{-1} \left\{ -\dot{W}S^{2T} - WS^{2T}L + grad\left(WS^{2T}V^S\right) \right\}^{2T}$$

$$\dot{W} = -WL + \alpha \times V^\alpha \tag{5.16}$$

$$0 = -\alpha + S : X - curl\, W.$$

We first note from (5.16_2) that if $\alpha = 0$ then a solution for W with initial condition I would be F^{-1}, where F is the deformation gradient with respect to the fixed stress-free reference configuration. Then from (5.16_3), it can be seen that this ansatz requires the eigenwall field to be symmetric in the last two indices. In its full-blown geometric nonlinearity, it is difficult to infer from (5.16_1) that if S were to have initial conditions with the required symmetry, that such symmetry would persist on evolution.

An even more serious constraint within our setting making additional kinetics in the completely compatible case dubious is the further implication that if $\Pi = curl\, S = 0$ and $S : X = 0$ on a simply connected domain, then it is necessarily true that S can be expressed as the second gradient of a vector field say a, i.e.

$$S_{ijk} = a_{i,jk}. \tag{5.17}$$

This implies that (5.16_1) is in general a highly overdetermined system of 27 equations in 3 unknown fields, for which solutions can exist, if at all, for very special choices of the eigenwall velocity field V^S. Even in the simplest of circumstances, consider (5.16_1) under the geometrically linear assumption (i.e. all nonlinearities arising from an objective rate are ignored and we do not distinguish between a material and a spatial time derivative)

$$\dot{S} = grad\left(SV^S\right) \implies \dot{a}_{i,j} = a_{i,jk}\left(V^S\right)_k$$

(upto a spatially uniform tensor field). This is a generally over-constrained system of 9 equations for 3 fields corresponding to the evolution of the vector field a requiring, for the existence of solutions, a PDE constraint to be satisfied by the phase boundary/eigenwall velocity field, namely

$$curl\left\{(grad\, grad\, a)\, V^S\right\} = 0$$

that amounts to requiring that

$$a_{i,jk}\left(V^S_{k,l}\right) - a_{i,lk}\left(V^S_{k,j}\right) = 0.$$

While satisfied in some simple situations, e.g. $grad\,V^S = 0$ whenever $grad\,grad\,a$ is non-vanishing, or when all field-variations are in one fixed direction (as for phase boundary propagation in a 1-d bar), this is a non-trivial constraint on the V^S field in general. Of course, it is conventional wisdom that the phase boundary velocity kinetics be specifiable constitutively, and a 'nonlocal' constraint on V^S as above considerably complicates matters. On the other hand, we find it curious that a nonlocal constraint on phase transformation constitutive behavior arises naturally in our model as a consequence of enforcing strict kinematic compatibility.

If one disallows a non-local PDE constraint as above on the constitutive specification of V^S, then the kinematics suggests the choice $V^S = 0$ (and perhaps the even stronger $\dot{S} = 0$). Based on the results of Sect. 5.5.3, this *precludes dissipation in the completely compatible case*. We find it interesting that recent physical results guided by continuum mechanics theory [CCF+06, ZTY+10] point to a similar conclusion in the design of low-hysteresis phase-transforming solids.

5.4.7 Contact with the Classical View of Modeling Defects: A Weingarten Theorem for g.disclinations and Associated Dislocations

The discussion surrounding (5.17) and seeking a connection of our work to the classical tradition of the theory of isolated defects suggest the following natural question. Suppose one has a three-dimensional body with a toroidal (Fig. 5.4a) or a through-hole in it (Fig. 5.4d) (cf. [Nab87]). In both cases, the body is multiply-connected. In the first, the body can be cut by a surface of finite extent that intersects its exterior surface along a closed curve and the surface of the toroidal hole along another closed curve in such a way that the resulting body becomes simply-connected with the topology of a solid sphere (Fig. 5.4b). In more precise terminology, one thinks of isolating a surface of the original multiply-connected domain with the above properties, and the set difference of the original body and the set of points constituting the cut-surface is the resulting simply-connected domain induced by the cut. Similarly, the body with the through-hole can be cut by a surface extending from a curve on the external surface to a curve on the surface of the through-hole such that the resulting body is again simply-connected with the topology of a solid sphere (Fig. 5.4e). Finally, the body with the toroidal hole can also be cut by a surface bounded by a closed curve entirely on the surface of the toroidal hole in such a way that the resulting body is simply-connected with the topology of a solid sphere with a cavity in it. For illustration see (Fig. 5.4c).

To make contact with our development in Sect. 5.3, one conceptually associates the support of the defect core as the interior of the toroidal hole and the support of the strip field WV as a regularized cut-surface.
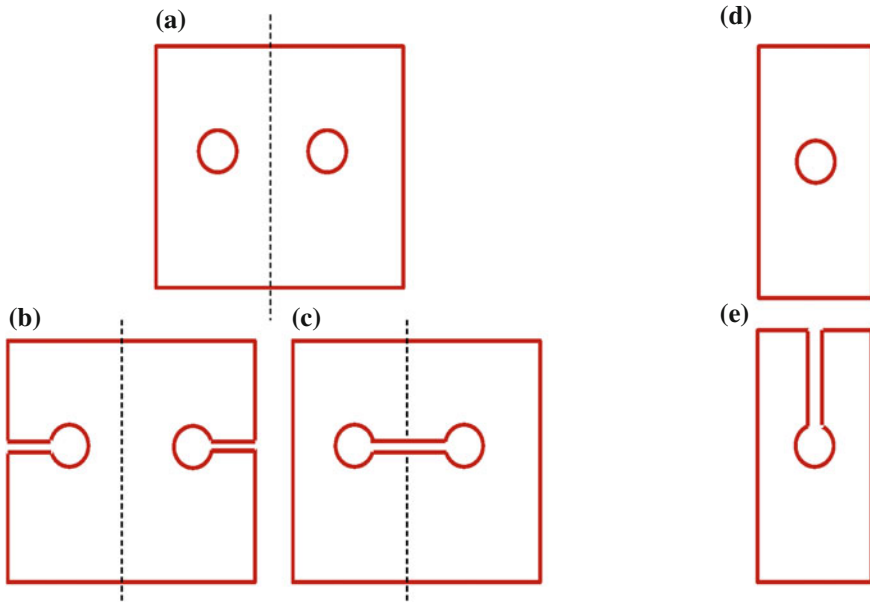
Fig. 5.4 Non simply-connected and corresponding induced simply-connected bodies. For **a–c** the bodies are obtained by rotating the planar figures by π about the axes shown; for d,e they are obtained by extruding the planar figures along the axis perpendicular to the plane of the paper

Suppose that on the original multiply-connected domain

- a continuously differentiable, 3rd-order tensor field $\tilde{Y}$ is prescribed that is
- symmetric in its last two indices ($\tilde{Y}_{ijk} = \tilde{Y}_{ikj}$) and
- whose *curl* vanishes ($\tilde{Y}_{ijk,l} = \tilde{Y}_{ijl,k}$).

Given such a field, we ask the question of whether on the corresponding simply-connected domain induced by a cut-surface as described in the previous paragraph, a vector field y can be defined such that

$$grad\, grad\, \boldsymbol{y} = \tilde{Y} \quad ; \quad y_{i,jk} = \tilde{Y}_{ijk},$$

and if the difference field of the limiting values of y, as the cut-surface is approached from the two sides of the body separated by the cut-surface, i.e. the jump $[\![\boldsymbol{y}]\!]$ of $\boldsymbol{y}$ across the cut, is arbitrary or yields to any special characterization. Here, we will refer to limits of fields approached from one (arbitrarily chosen) side of the cut-surface with a superscript '+' and limits from the corresponding other side of the cut-surface with a superscript '−' so that, for instance, $[\![\boldsymbol{y}(z)]\!] = \boldsymbol{y}^+(z) - \boldsymbol{y}^-(z)$, for z belonging to the cut-surface.

For the question of existence of y on the simply-connected domain, one first looks for a field $\tilde{W}$ such that

$$grad\,\tilde{W} = \tilde{Y} \quad ; \quad \tilde{W}_{ij,k} = \tilde{Y}_{ijk}$$

and since $\tilde{Y}$ is *curl*-free and continuously differentiable on the multiply-connected domain with the hole, on the corresponding simply-connected domain induced by a cut, the field $\tilde{W}$ can certainly be defined [Tho34]. The jump $[\![\tilde{W}]\!]$ is not to be expected to vanish on the cut surface, in general. However, by integrating $\left(grad\,\tilde{W}\right)^{+}$ and $\left(grad\,\tilde{W}\right)^{-}$ along a curve on the cut-surface joining any two arbitrarily chosen points on it, it is easy to deduce that $[\![\tilde{W}]\!]$ is constant on the surface because of the continuity of $\tilde{Y}$ on the original multiply-connected domain.

With reference to (Fig. 5.5), consider the line integral of $\tilde{Y}$ on the closed contour shown in the original multiply-connected domain without any cuts (the two oppositely-oriented adjoining parts of the contour between points A and B are intended to be overlapping). In conjunction, also consider as the 'inner' and 'outer' closed contours the closed curves that remain by ignoring the overlapping segments, the inner closed contour passing through A and the outer through B. Then, because of
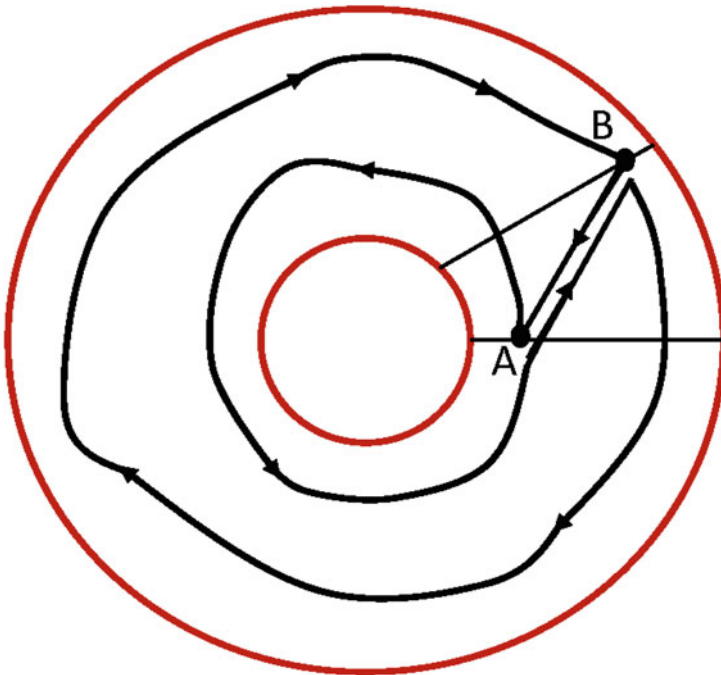

Fig. 5.5 Contour for proving independence of Δ on cut-surface. The contour need not be planar and the points A and B need not be on the same cross-sectional plane of the body

the continuity of $\tilde{Y}$ and its vanishing *curl*, the line integral of $\tilde{Y}$ on the inner and outer closed contours must be equal and this must be true for *any* closed circuit that cannot be shrunk to a point while staying within the domain. Let us denote this invariant over any such closed curve $\mathcal{C}$ as

$$\int_{\mathcal{C}} \tilde{Y}\, d\boldsymbol{x} = \boldsymbol{\Delta}.$$

If we now introduce a cut-surface passing through A and construct the corresponding $\tilde{W}$, say $\tilde{W}_1$, then the jump of $\tilde{W}_1$ at A is given by

$$[\![\tilde{W}_1]\!](A) = \int_{\mathcal{C}(A^-,A^+)} grad\,\tilde{W}_1\, d\boldsymbol{x} = \int_{\mathcal{C}(A^-,A^+)} \tilde{Y}\, d\boldsymbol{x} = \boldsymbol{\Delta},$$

where $\mathcal{C}(A^-, A^+)$ is the curve formed from the inner closed contour defined previously with the point A taken out and with start-point A^- and end-point A^+. The last equality above is due to the continuity of $\tilde{Y}$ on the original multiply-connected domain. Similarly, a different cut-surface passing through B can be introduced and an associated $\tilde{W}_2$ constructed with $[\![\tilde{W}_2]\!](B) = \boldsymbol{\Delta}$. Since A, B and the cut surfaces through them were chosen arbitrarily, it follows that the jump of any of the functions $[\![\tilde{W}]\!]$ across their corresponding cut-surface takes on the same value regardless of the cut-surface invoked to render simply-connected the multiply-connected body.

On a cut-induced simply-connected domain, since $\tilde{W}$ exists and its *curl* vanishes (due to the symmetry of $\tilde{Y}$ in its last two indices), clearly a vector field $\boldsymbol{y}$ can be defined such that

$$grad\,\boldsymbol{y} = \tilde{W}.$$

Suppose we now fix a cut-surface. Let $\boldsymbol{x}_0$ be an arbitrarily chosen base point on it. Let $\boldsymbol{x}$ be any other point on the cut-surface. Then, by integrating $(grad\,\boldsymbol{y})^+$ and $(grad\,\boldsymbol{y})^-$ along any curve lying on the cut-surface joining $\boldsymbol{x}_0$ and $\boldsymbol{x}$, it can be observed that

$$[\![\boldsymbol{y}(\boldsymbol{x})]\!] = [\![\boldsymbol{y}(\boldsymbol{x}_0)]\!] + \boldsymbol{\Delta}\,(\boldsymbol{x} - \boldsymbol{x}_0)\,. \tag{5.18}$$

The 'constant vector of translation', $[\![\boldsymbol{y}(\boldsymbol{x}_0)]\!]$, may be evaluated by integrating $\tilde{W}$ on a closed contour that intersects the cut-surface only once, the point of intersection being the base point $\boldsymbol{x}_0$ ($\tilde{W}$ is, in general, discontinuous at the base point). It can be verified that for a fixed cut-surface, $[\![\boldsymbol{y}(\boldsymbol{x})]\!]$ is independent of the choice of the base point used to define it.

The physical result implied by this characterization is as follows: suppose we think of the vector field $\boldsymbol{y}$ as a generally discontinuous deformation of the multiply-connected body, with discontinuity supported on the cut-surface. Then the separation/jump vector $\boldsymbol{y}(\boldsymbol{x})$ for *any* point $\boldsymbol{x}$ of the surface corresponds to a *fixed* affine deformation of the position vector of $\boldsymbol{x}$ relative to the base point $\boldsymbol{x}_0$ (i.e. $\boldsymbol{\Delta}$ independent of $\boldsymbol{x}$), followed by a *fixed* translation.

It is important to note here that, for the given field $\tilde{Y}$ on the multiply-connected domain, while $\boldsymbol{\Delta} = [\![\tilde{W}]\!]$ is independent of the particular cut-surface invoked to define it, the translational part, $[\![\boldsymbol{y}(\boldsymbol{x}_0)]\!]$, of the jump $[\![\boldsymbol{y}]\!]$ on a cut-surface depends on the definition of the cut-surface (both through the dependence on $\boldsymbol{x}_0$ and the impossibility, in general, of defining a continuous $\tilde{W}$ on the original multiply-connected domain), *unless* $\boldsymbol{\Delta} = \boldsymbol{0}$. This is the analog of the known result in classical (disclination-dislocation) defect theory that the Burgers vector of an isolated defect is a well-defined topological object only in the absence of disclinations. In the same spirit, when the (non-trivial) constant tensor $\boldsymbol{\Delta}$ is such that it has a 2-dimensional null-space, then for a specific flat, cut-surface spanning the null-space, it is possible that the jump in $[\![\boldsymbol{y}]\!]$ vanishes. This gives rise to a surface in the (non-simply-connected) body on which the deformation map is continuous but across which the deformation gradient is discontinuous.

Thus, the notion of g.disclinations offers more flexibility in the type of discontinuities that can be represented within continuum theory, as compared to Volterra distortions defining classical disclinations (cf. [Cas04, Nab87]).[8] This is natural since the Volterra distortion question involves a twice-continuously differentiable Right-Cauchy Green field in its formulation (in the context of this subsection, this would amount to enforcing a high degree of smoothness, and therefore continuity, on $\tilde{W}^T \tilde{W}$) so that only the polar decomposition-related rotation field of $\tilde{W}$ can be discontinuous, whereas allowing for an incompatible $\tilde{Y}$ field on a multiply-connected domain, even though irrotational, implies possible discontinuities in the whole field $\tilde{W}$.

---

[8]In the classical disclination-dislocation case, the corresponding question to what we have considered would be to ask for the existence, on a cut-induced simply-connected domain, of a vector field $\boldsymbol{y}$ and the characterization of its jump field across the cut-surface, subject to $(\text{grad}\,\boldsymbol{y})^T \text{grad}\,\boldsymbol{y} = \boldsymbol{C}$ and the Riemann-Christoffel curvature tensor field of (twice continuously differentiable) $\boldsymbol{C}$ (see [Shi73] for definition) vanishing on the original multiply-connected domain. Existence of a global smooth solution can be shown (cf. [Sok51] using the result of [Tho34] and the property of preservation of inner-product of two vector fields under parallel transport in Riemannian geometry). The corresponding result is

$$[\![\boldsymbol{y}(\boldsymbol{x})]\!] = [\![\boldsymbol{y}(\boldsymbol{x}_0)]\!] + [\![\boldsymbol{R}]\!]\boldsymbol{U}\,(\boldsymbol{x} - \boldsymbol{x}_0)\,,$$

where $grad\,\boldsymbol{y} = \boldsymbol{RU}$ on the cut-induced simply-connected domain, and $\boldsymbol{R}$ is a proper-orthogonal, and $\boldsymbol{U} = \sqrt{\boldsymbol{C}}$ is a symmetric, positive-definite, 2nd-order tensor field. $\boldsymbol{U}$ cannot have a jump across any cut-surface and the jump $[\![\boldsymbol{R}]\!]$ takes the same value regardless of the cut-surface invoked to define it, as can be inferred from the results of [Shi73]. By rearranging the independent-of-$\boldsymbol{x}$ term in the above expression, the result can be shown to be identical to that in [Cas04]. Of course, for the purpose of understanding the properties of the Burgers vector of a general defect curve, it is important to observe the dependence of the 'constant' translational term on the cut-surface. An explicit characterization of the jump in $grad\,\boldsymbol{y}$ in terms of the strength of the disclination is given in [DZ11].

5.5 Frame-Indifference and Thermodynamic Guidance on Constitutive Structure

As is known to workers in continuum mechanics, the definition of the mechanical dissipation (5.6) coupled to the mechanical structure of a theory (Sect. 5.4), a commitment to constitutive dependencies of the specific free-energy density, and the consequences of material frame indifference provide an invaluable tool for discovering the correct form of the reversible response functions and driving forces for dissipative mechanisms in a nonlinear theory. This exercise is useful in that constitutive behavior posed in agreement with these restrictions endow the theory with an energy equality that is essential for further progress in developing analytical results regarding well-posedness as well as developing numerical approximations. In exploiting this idea for our model, we first deduce a necessary condition for frame-indifference of the free-energy density function that we refer to as the 'Ericksen identity' for our theory; in this, we essentially follow the treatment of [ACF99] adapted to our context.

5.5.1 Ericksen Identity for g.disclination Mechanics

We assume a specific free energy density of the form

$$\psi = \psi\left(\boldsymbol{W}, \boldsymbol{S}, \boldsymbol{J}, {}^{\star}\boldsymbol{\Pi}\right). \tag{5.19}$$

All the dependencies above are two-point tensors between the current configuration and the 'intermediate configuration,' i.e. $\{\mathcal{D}_r(\boldsymbol{x}, t) : \boldsymbol{x} \in B(t)\}$, a collection of local configurations with similarly oriented and unstretched atomic configurations in each of them. On superimposing rigid motions on a given motion, each element of this intermediate configuration is naturally assumed to remain invariant. With this understanding, let $\boldsymbol{Q}(s)$ be a proper-orthogonal tensor-valued function of a real parameter p defined by

$$\frac{d\boldsymbol{Q}}{dp}(p) = s\boldsymbol{Q}(p),$$

where s is an arbitrarily fixed skew-symmetric tensor function, and $\boldsymbol{Q}(0) = \boldsymbol{I}$. Thus, $\frac{d\boldsymbol{Q}^T}{dp}(0) = -s$. Also, define $\boldsymbol{A}\, t\, \boldsymbol{B}$ through

$$\left\{\left(A\, t\, B\right)_{jkrl} - A_{jr}B_{kl}\right)\right\}\boldsymbol{e}_j \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_r \otimes \boldsymbol{e}_l = \boldsymbol{0}.$$

Then, frame-indifference of ψ requires that

$$\psi\left(\boldsymbol{W}, \boldsymbol{S}, \boldsymbol{J}, {}^{\star}\boldsymbol{\Pi}\right) = \psi\left(\boldsymbol{W}\boldsymbol{Q}^T, \boldsymbol{S} : \boldsymbol{Q}^T t \boldsymbol{Q}^T, \boldsymbol{J} : \boldsymbol{Q}^T t \boldsymbol{Q}^T, {}^{\star}\boldsymbol{\Pi}\boldsymbol{Q}^T\right) \tag{5.20}$$

for $Q(p)$ generated from any choice of the skew symmetric tensor s. Differentiating (5.20) with respect to p and evaluating at $p = 0$ implies

$$0 = -(\partial_W \psi)_{ij} \, W_{ir} s_{rj} - (\partial_S \psi)_{ijk} \, S_{irs} \left(s_{rj} \delta_{sk} + \delta_{rj} s_{sk} \right)$$
$$- (\partial_J \psi)_{ijk} \, J_{irs} \left(s_{rj} \delta_{sk} + \delta_{rj} s_{sk} \right) - (\partial_{^\star\Pi} \psi)_{ijk} \, {}^\star\Pi_{ijr} s_{rk}$$

where the various partial derivatives of ψ are evaluated at $(W, S, J, {}^\star\Pi)$. This can be rewritten as

$$0 = \big[(\partial_W \psi)_{ij} \, W_{ir} \; + (\partial_S \psi)_{ijk} \, S_{irk} + (\partial_S \psi)_{ikj} \, S_{ikr} \qquad (5.21)$$
$$+ (\partial_J \psi)_{ijk} \, J_{irk} + (\partial_J \psi)_{ikj} \, J_{ikr} + (\partial_{^\star\Pi} \psi)_{ikj} \, {}^\star\Pi_{ikr} \big] \, s_{rj},$$

valid for all skew symmetric s which implies that the term within square brackets has to be a symmetric second-order tensor. *This is a constraint on constitutive structure imposed by Material Frame Indifference.*

5.5.2 The Mechanical Dissipation

Assuming a stored energy density function ψ with arguments as in (5.19), we now re-examine the mechanical dissipation D in (5.6). We first compute the material time derivative of ψ to obtain

$$\dot{\psi} = (\partial_W \psi) : \dot{W} + (\partial_S \psi) \cdot_3 \dot{S} + (\partial_J \psi) \cdot_3 \dot{J} + (\partial_{^\star\Pi} \psi) \cdot_3 {}^\star\dot{\Pi}$$
$$= (\partial_W \psi) : (- WL + \alpha \times V^\alpha)$$
$$+ (\partial_S \psi) \cdot_3 (W^{-1} \{- \dot{W} S^{2T} - W S^{2T} L - \Pi \times V^\Pi \qquad (5.22)$$
$$+ \, grad \, (\, W S^{2T} V^S \,) \}^{2T})$$
$$+ (\partial_J \psi) \cdot_3 \dot{J}$$
$$+ (\partial_{^\star\Pi} \psi) \cdot_3 [- (L : I) {}^\star\Pi + {}^\star\Pi L^T - curl \left(\Pi \times V^\Pi \right)] .$$

In the above, $\cdot_3$ refers to the inner-product of its argument third-order tensors (in indices, a contraction on all three (rectangular Cartesian) indices of its argument tensors). Recalling the dissipation (5.6):

$$\mathsf{D} = \int_{B(t)} \left(T : D + \Lambda : M - \rho \dot{\psi} \right) \, dv,$$

we first collect all terms in (5.22) multiplying $L = D + \Omega$ and $grad \, L$, observing that the coefficient of Ω has to vanish identically for the dissipation to be objective (cf. [AD12]). Noting that

$$\dot{J} = grad \, \dot{W} - (grad \, W) \, L \iff \overline{W_{rw,k}} = \left(\dot{W}_{rw} \right)_{,k} - W_{rw,m} L_{mk},$$

we obtain

$$
\int_{B(t)} [-(\partial_{\boldsymbol{W}}\psi)_{ij}\, W_{ir} L_{rj} \qquad + (\partial_{\boldsymbol{S}}\psi)_{rwk}\, W_{wl}^{-1}\left(W_{lr}L_{rp}S_{rpk} - W_{lp}S_{rpm}L_{mk}\right)
$$
$$
+ (\partial_{\boldsymbol{J}}\psi)_{rwk}\left(-W_{rp,k}L_{pw} - W_{rw,m}L_{mk}\right)
$$
$$
+ (\partial_{\star\boldsymbol{\Pi}}\psi)_{ikj}\left(^{\star}\Pi_{ikr}L_{rj}^{T} - L_{rr}\,{}^{\star}\Pi_{ikj}\right)\,]\,dv
$$
$$
+ \int_{B(t)} (\partial_{\boldsymbol{J}}\psi)_{rwk}\left(-W_{rp}L_{pw,k}\right)\,dv,
$$

Noting the symmetry of L_{pwk} in the last two indices, we *define*

$$
\left(D_{\boldsymbol{J}}^{sym}\psi\right)_{rwk} := \frac{1}{2}\left[(\partial_{\boldsymbol{J}}\psi)_{rwk} + (\partial_{\boldsymbol{J}}\psi)_{rkw}\right],
$$

and substituting the above in the dissipation (5.6) to collect terms 'linear' in $\boldsymbol{D}$, $\boldsymbol{\Omega}$, and *grad* $\boldsymbol{\Omega}$, we obtain

$$
-\int_{B(t)} -\rho\,[(\partial_{\boldsymbol{W}}\psi)_{ij}\, W_{ir} + (\partial_{\boldsymbol{S}}\psi)_{ijk}\, S_{irk} + (\partial_{\boldsymbol{S}}\psi)_{ikj}\, S_{ikr}
$$
$$
+ (\partial_{\boldsymbol{J}}\psi)_{ijk}\, J_{irk} + (\partial_{\boldsymbol{J}}\psi)_{iwj}\, J_{iwr}
$$
$$
+ (\partial_{\star\boldsymbol{\Pi}}\psi)_{ikj}\,{}^{\star}\Pi_{ikr}]\,\Omega_{rj}\,dv
$$
$$
+ \int_{B(t)} [T_{rj} - \rho\,\{- (\partial_{\boldsymbol{W}}\psi)_{ij}\, W_{ir}
$$
$$
+ (\partial_{\boldsymbol{S}}\psi)_{mrk}\, S_{mjk} - (\partial_{\boldsymbol{S}}\psi)_{mwj}\, S_{mwr}
$$
$$
- (\partial_{\boldsymbol{J}}\psi)_{pjk}\, J_{prk} - (\partial_{\boldsymbol{J}}\psi)_{mwj}\, J_{mwr} \tag{5.23}
$$
$$
+ (\partial_{\star\boldsymbol{\Pi}}\psi)_{ikr}\,{}^{\star}\Pi_{ikj} - (\partial_{\star\boldsymbol{\Pi}}\psi)_{ikm}\,{}^{\star}\Pi_{ikm}\delta_{rj}
$$
$$
+ \left(D_{\boldsymbol{J}}^{sym}\psi\right)_{pjk,k} W_{pr} + \left(D_{\boldsymbol{J}}^{sym}\psi\right)_{pjk} J_{prk}\}]\,D_{rj}\,dv
$$
$$
+ \int_{\partial B(t)} \rho\left(D_{\boldsymbol{J}}^{sym}\psi\right)_{pjk} W_{pr} n_{k}\, D_{rj}\,da
$$
$$
+ \int_{B(t)} [\Lambda_{ik} - e_{imn}\,\rho\,(D_{\boldsymbol{J}}^{sym}\psi)_{rnk}\, W_{rm}]\left(-\frac{1}{2}e_{ipw}\Omega_{pw,k}\right)\,dv.
$$

The remaining terms in the dissipation D are

$$
\begin{aligned}
&- \int_{B(t)} [(\partial_{\boldsymbol{W}}\psi)_{ij}\, e_{jrs}\alpha_{ir} + (\partial_{\boldsymbol{S}}\psi)_{rwk} \left(-e_{pjs} W_{wl}^{-1}\alpha_{lj} S_{rpk}\right) \\
&\qquad\qquad -(\partial_{\boldsymbol{J}}\psi)_{rwk,k}\, e_{wjs}\alpha_{rj}]\, V_s^{\alpha}\, dv \\
&- \int_{B(t)} [(\partial_{\boldsymbol{S}}\psi)_{rwk} \left(-e_{kjs} W_{wl}^{-1}\Pi_{rlj}\right) \\
&\qquad\qquad +(\partial_{\boldsymbol{\Pi}}\psi)_{rwk,m} (\delta_{kp}\delta_{ms} - \delta_{ks}\delta_{mp})\Pi_{rwp}]\, V_s^{\Pi}\, dv \\
&+ \int_{B(t)} (\partial_{\boldsymbol{S}}\psi)_{rwk,k}\, W_{wp} S_{rpj} V_j^{S}\, dv \\
&- \int_{\partial B(t)} (\partial_{\boldsymbol{S}}\psi)_{rwk}\, n_k W_{wp} S_{rpj} V_j^{S}\, da \\
&- \int_{\partial B(t)} (\partial_{\boldsymbol{J}}\psi)_{rwk}\, n_k \alpha_{rj} e_{wjs} V_s^{\alpha}\, da \\
&+ \int_{\partial B(t)} (\partial_{\boldsymbol{\Pi}}\psi)_{rwk}\, n_m (\delta_{kp}\delta_{ms} - \delta_{ks}\delta_{mp})\Pi_{rwp} V_s^{\Pi}\, da.
\end{aligned}
\tag{5.24}
$$

5.5.3 Reversible Response and Dissipative Driving Forces

We deduce ingredients of general constitutive response from the characterization of the dissipation in Sect. 5.5.2.

1. It is a physical requirement that the pointwise dissipation density be invariant under superposed rigid body motions (SRBM) of the body. The 'coefficient' tensor of the spin tensor $\boldsymbol{\Omega}$ in the first integrand of (5.23) transforms as an objective tensor under superposed rigid motions (i.e. $(\cdot) \to \boldsymbol{Q}(\cdot)\boldsymbol{Q}^T$ for all proper orthogonal $\boldsymbol{Q}$), but the spin tensor itself does not (it transforms as $\boldsymbol{\Omega} \to -\boldsymbol{\omega} + \boldsymbol{Q}\boldsymbol{\Omega}\boldsymbol{Q}^T$, where $\boldsymbol{\omega}(t) = \dot{\boldsymbol{Q}}(t)\boldsymbol{Q}^T$). Since an *elastic response* (i.e. $\boldsymbol{V}^{\alpha} = \boldsymbol{V}^S = \boldsymbol{V}^{\Pi} = \boldsymbol{0}$) has to be a special case of our theory and the 2nd, 3rd, and 4th integrals of (5.23) remain invariant under SRBM, the coefficient tensor of $\boldsymbol{\Omega}$ must vanish. This is a stringent requirement validating the nonlinear time-dependent kinematics of the model. Using the Ericksen identity (5.21), it is verified that the requirement is indeed satisfied by our model.

2. We would like to define elastic response as being non-dissipative, i.e. $\mathsf{D} = 0$. Sufficient conditions ensuring this are given by the following constitutive choices for $\boldsymbol{\Lambda}^{dev}$, the *deviatoric part* of the couple stress tensor, the *symmetric part* of the Cauchy stress tensor, and a boundary condition:

$$
\Lambda_{jk}^{dev} = e_{jpw}\, \rho\, W_{pr}^T \left(D_{\boldsymbol{J}}^{sym}\psi\right)_{rwk},
\tag{5.25}
$$

$$T_{rj} + T_{jr} = \mathcal{A}_{rj} + \mathcal{A}_{jr}$$

$$\begin{aligned}
\mathcal{A}_{rj} := \rho \{ &- (\partial_{\boldsymbol{W}}\psi)_{ij}\, W_{ir} \\
&+ (\partial_{\boldsymbol{S}}\psi)_{mrk}\, S_{mjk} - (\partial_{\boldsymbol{S}}\psi)_{mwj}\, S_{mwr} \\
&- (\partial_{\boldsymbol{J}}\psi)_{pjk}\, J_{prk} - (\partial_{\boldsymbol{J}}\psi)_{mwj}\, J_{mwr} \\
&+ (\partial_{\star\boldsymbol{\Pi}}\psi)_{ikr}\, {}^{\star}\Pi_{ikj} - (\partial_{\star\boldsymbol{\Pi}}\psi)_{ikm}\, {}^{\star}\Pi_{ikm}\delta_{rj} \\
&+ \left(D_{\boldsymbol{J}}^{sym}\psi\right)_{pjk,k} W_{pr} + \left(D_{\boldsymbol{J}}^{sym}\psi\right)_{pjk} J_{prk}\}
\end{aligned} \tag{5.26}$$

and

$$\left[\mathcal{B}_{pwk} + \mathcal{B}_{wpk}\right] n_k = 0 \;\; \text{on boundary of body}$$

$$\mathcal{B}_{pwk} := \rho\, W_{pr}^{T} \left(D_{\boldsymbol{J}}^{sym}\psi\right)_{rwk}. \tag{5.27}$$

These constitutive choices are meant to be valid for all processes, whether dissipative or not. The following observations are in order:

- The skew-symmetric part of the Cauchy stress, T^{skw}, is constitutively undetermined (cf. [MT62]). Similarly, the hydrostatic part of the couple stress tensor is constitutively undetermined (cf. [UCTF13]), since $e_{ipw}\Omega_{pw,k} = -\left(e_{iwp}v_{p,w}\right)_{,k}$ in (5.23) is deviatoric as the vorticity, being the *curl* of the velocity field, is necessarily divergence-free. Taking the *curl* of the balance of angular momentum (5.15$_3$) and substituting the divergence of T^{skw} in the balance of the linear momentum (5.15$_2$), one derives a higher order equilibrium equation between the symmetric part of the Cauchy stress T^{sym} and the deviatoric couple-stress Λ^{dev}:

$$\rho\dot{\boldsymbol{v}} = \operatorname{div} \boldsymbol{T}^{sym} + \frac{1}{2}curl(\operatorname{div}\boldsymbol{\Lambda}^{dev}) + \rho\boldsymbol{b} + \frac{1}{2}curl\rho\boldsymbol{K} \tag{5.28}$$

  In each specific problem, the fields $\rho, \boldsymbol{x}, \boldsymbol{W}, \boldsymbol{S}$ are obtained by solving (5.15$_{1,4,5,6}$) and (5.28). This amounts to solving all of (5.15), where balance of angular momentum is understood as solved simply by evaluating the skew part of the Cauchy stress from (5.15$_3$).
- The boundary condition (5.27) does not constrain the specification of couple stress related boundary conditions in any way.
- Couple-stresses arise only if the push-forward of the tensor $D_{\boldsymbol{J}}^{sym}\psi$ to the current configuration has a skew-symmetric component. In particular, if $\left(D_{\boldsymbol{J}}^{sym}\right)_{rwk} = 0$, then there are no couple-stresses in the model and, in the absence of body-couples, the stress tensor is symmetric and balance of linear momentum (5.15$_2$), viewed as the basic equation for solving for the position field $\boldsymbol{x}$ or velocity field $\boldsymbol{v}$ is of lower-order (in the sense of partial differential equations) compared to the situation when couple-stresses are present.
- The important physical case of *dislocation mechanics* is one where $\left(D_{\boldsymbol{J}}^{sym}\psi\right)_{rwk} = 0$. Here, the stored-energy function depends upon $\boldsymbol{J} = grad\,\boldsymbol{W}$

only through $\widetilde{\alpha} = -J : X$ and $(\partial_S \psi) = (\partial_{\cdot \Pi} \psi) = \mathbf{0}$. The theory, including dissipative effects, then reduces to the one presented in [Ach04, Ach11].

- In the *compatible, elastic case*, assuming the existence of a stress-free reference configuration from which the deformation is defined with deformation gradient field F, we have $W = F^{-1}$ and the energy function is only a function of $grad\,F^{-1}$, and F^{-1}. In this case, $(\partial_J \psi)_{pjk} = \left(D_J^{sym} \psi \right)_{pjk}$. Defining

$$\psi\left(F^{-1}, grad\,F^{-1} \right) := \tilde{\psi}\left(F\left(F^{-1} \right), Grad\,F\left(F^{-1}, grad\,F^{-1} \right) \right)$$

and using the relations

$$(Grad\,F)_{sP,K} = (grad\,F)_{sP,k}\, F_{kK}$$

$$(grad\,F)_{aB,c} = -F_{aM}\left(grad\,F^{-1} \right)_{Mn,c} F_{nB}$$

along with further manipulation, it can be shown that

$$
\begin{aligned}
\Lambda_{jk} &= e_{jwp}\, \mathcal{H}_{wpk} \\
\mathcal{H}_{wpk} &= \rho F_{wB} \frac{\partial \tilde{\psi}}{\partial F_{pB,K}} F_{kK}
\end{aligned}
\tag{5.29}
$$

and

$$\mathcal{A}_{rj}\big|_{compatible} = \frac{\partial \tilde{\psi}}{\partial F_{rA}} F_{jA} + \frac{\partial \tilde{\psi}}{\partial F_{rB,C}} F_{jB,C} - \mathcal{H}_{jrk,k}. \tag{5.30}$$

The couple-stress and symmetric part of Cauchy stress relations that arise from relations (5.29–5.30) are precisely the ones derived by Toupin [Tou62, TN04], starting from a different (static and variational) premise and invoking the notion of an *hyperstress tensor*, a construct we choose not to utilize. Admittedly, we then need a slightly restricted boundary condition (5.27), but we do not consider this as a major restriction given the difficulty in physical identification of hyperstresses and hypertractions.

3. We refer to dissipative 'driving forces' in this context as the power-conjugate objects to the fields V^{Π}, V^{α}, and V^S in the dissipation D (5.24), since in their absence there can be no mechanical dissipation in the theory (i.e. all power supplied to the body is converted in entirety to stored energy), with the reversible response relations (5.25)–(5.27) in effect. Interestingly, the theory suggests separate driving forces in the bulk and at external boundaries of the body.

- The *bulk* driving forces are given by

$$V_s^\alpha \rightsquigarrow -[(\partial_{\mathbf{W}}\psi)_{ij}\, e_{jrs}\alpha_{ir} + (\partial_{\mathbf{S}}\psi)_{rwk}\left(-e_{pjs}W_{wl}^{-1}\alpha_{lj}S_{rpk}\right)$$
$$- (\partial_{\mathbf{J}}\psi)_{rwk,k}\, e_{wjs}\alpha_{rj}]$$
(5.31)

$$V_s^\Pi \rightsquigarrow -[(\partial_{\mathbf{S}}\psi)_{rwk}\left(-e_{kjs}W_{wl}^{-1}\Pi_{rlj}\right)$$
$$+ ((\partial_{\mathbf{\Pi}}\psi)_{rwp,s} - (\partial_{\mathbf{\Pi}}\psi)_{rws,p})\Pi_{rwp}]$$
(5.32)

$$V_j^S \rightsquigarrow (\partial_{\mathbf{S}}\psi)_{rwk,k}\, W_{wp}S_{rpj}$$
(5.33)

- The *boundary* driving forces at an external boundary point with outward unit normal **n** are given by

$$V_j^S \rightsquigarrow -(\partial_{\mathbf{S}}\psi)_{rwk}\, n_k\, W_{wp}S_{rpj}$$
(5.34)

$$V_s^\alpha \rightsquigarrow -(\partial_{\mathbf{J}}\psi)_{rwk}\, n_k\alpha_{rj}e_{wjs}$$
(5.35)

$$V_s^\Pi \rightsquigarrow ((\partial_{\mathbf{\Pi}}\psi)_{rwp}\, n_s - (\partial_{\mathbf{\Pi}}\psi)_{rws}\, n_p)\,\Pi_{rwp}.$$
(5.36)

When the various defect velocities are chosen to be in the directions of their driving forces, then the mechanical dissipation in the body is guaranteed to satisfy

$$\mathsf{D} \geq 0,$$

i.e. the rate of energy supply in the model is never less than the rate of storage of energy.

5.5.4 A Special Constitutive Dependence

There are many situations when the atoms of the as-received body relieved of applied loads can be re-arranged to form a collection that is stress-free. An example is that of the as-received body consisting of a possibly dislocated perfect single crystal. Let us denote such a stress-free collection of the entire set of atoms in the body as R. When such an atomic structure is available, it is often true that, up to boundary-effects, there are non-trivial homogeneous deformations of the structure that leave it unchanged (modulo rigid body deformations) and this provides an energetic constraint on possible atomic motions of the body. In our modeling, we would like to encapsulate this structural symmetry-related fact as a constitutive energetic constraint.

When defects of incompatibility are disallowed (e.g. compatible phase transformations), then the theory already presented suffices for modeling, employing multiple well-energy functions in the deformation gradient from the perfect crystal reference

with second deformation gradient regularization. In the presence of defects, in particular dislocations, and when the focus is the modeling of individual dislocations, a constitutive modification may be required. There exists a gradient flow-based modeling technique for small deformation analysis called the phase-field method for dislocations [RLBF03, WL10, Den04] that amalgamates the Ginzburg-Landau paradigm with Eshelby's [Esh57] eigenstrain representation of a dislocation loop; for an approach to coupled phase-transformations and dislocations at finite deformations within the same paradigm see [LJ12]. An adaptation of those ideas within our framework of unrestricted material and geometric nonlinearity and conservation-law based defect dynamics requires, for the representation of physical concepts like the unstable stacking fault energy density, a dependence of the stored energy on a measure that reflects deformation of R to the current atomic configuration. This measure cannot be defined solely in terms of the i-elastic 1-distortion W. The following considerations of this section provides some physical justification for the adopted definition (5.37) of this measure.

Let us approximate the spatial region occupied by R by a fixed connected spatial configuration R. We consider any atom in R, say at position X_R, and consider a neighborhood of atoms of it. As the deformation of the body progresses, we imagine tracking the positions of the atoms of this neighborhood around X_R. By approximating the initial and the image neighborhoods by connected domains, one can define a deformation between them. We assume that this deformation is well-approximated by a homogeneous deformation with gradient $F^s(X_R, t)$. We assume that by some well-defined procedure this discrete collection of deformation gradients at each time (one for each atomic position) can be extended to a field on the configuration R,[9] with generic point referred to as X_R. Since R and $B(t)$ are both configurations of the body, we can as well view the motion of the body, say x_R, with R as a reference configuration and with deformation gradient field

$$F_R = Grad_{X_R} x,$$

where the expression on the right hand side refers to the gradient of the position field x on the configuration R.

Through this one-to-one motion referred to R we associate the field

$$W^s(x, t) := F^{s-1}(x, t)$$

---

[9]Note that such a tensor field is not F^p of classical elastoplasticity theory; for instance, its invariance under superposed rigid body motions of the current configuration is entirely different from that of F^p.

with the current configuration $B(t)$ in the natural way and constrain the possible local deformations F^{s} [10] by requiring

$$curl\, W^{\mathsf{s}} = \widetilde{\alpha} \implies curl\,(W - W^{\mathsf{s}}) = \mathbf{0}$$

and choosing the 'free' gradient of a vector field through

$$W = W^{\mathsf{s}} + grad\, x_R^{-1} \implies W^{\mathsf{s}} := W - F_R^{-1}. \tag{5.37}$$

We note that the knowledge of the motion of the body and the evolution of the W field completely determine the evolution of the field W^{s}. In the manner defined, in principle W^{s} is an unambiguously initializable field whenever the atomic configuration in the as-received body is known and a 'perfect' atomic structure R for the body exists.

When a dependence of the energy function on the structural distortion is envisaged, this implies an additional dependence of the stored energy function (5.19) on F_R (and a dependence on the configuration R). This implies corresponding changes in the Ericksen identity, reversible response functions, and the driving forces that may be deduced without difficulty.

We emphasize, however, that it is not clear to us at this point that the constitutive modeling necessarily requires accounting for the structural variable W^{s} (or equivalently the pair W and F_R), despite the viewpoint of the phase-field methodology. In particular, whether a suitable dependence of the stored energy function solely on the element W of the pair suffices for the prediction of observed behavior related to motion of individual dislocations needs to be explored in detail.

5.6 'Small Deformation' Model

In this section we present a model where many of the geometric nonlinearities that appear in the theory presented in Sect. 5.5 are ignored. This may be considered as an extension of the theory of *linear elasticity* to account for the dynamics of phase boundaries, g.disclinations, and dislocations. A main assumption is that the all equations are posed on a fixed, known, configuration that enters 'parametrically' in the solution to the equations. Such a model has been described in [AF12]. In what we present here, there is a difference in the reversible responses from those proposed in [AF12], even though the latter also ensure that the dissipation vanishes in the model for elastic processes. The choices made here render our model consistent with Toupin's [Tou62] model of higher-order elasticity in the completely compatible case.

---

[10]This may also be viewed as a constraint on the atomic re-arrangement leading to the choice of the particular R.

The eigenwall field in the small deformation case is denoted by $\hat{S}$. All g.disclination density measures are denoted by $\hat{\Pi}$. The elastic 1-distortion is approximated by $I - U^e$ where U^e is a 'small' elastic distortion measure and we further introduce a *plastic distortion* field by the definition

$$U^e := grad\,u - U^p,$$

where u is the displacement field of the body from the given distinguished reference configuration. The strain tensor is defined as $\varepsilon := (grad\,u)_{sym}$. The elastic 2-distortion is defined as $G^e := grad\,U^e + \hat{S}$, with the g.disclination density as curl $G^e = curl\,\hat{S} = \hat{\Pi}$. The dislocation density is defined as $\hat{\alpha} := -G^e : X = curl\,U^e - \hat{S} : X$.

The governing equations are

$$
\begin{aligned}
\rho\ddot{u} &= div\,T + \hat{b} \\
0 &= \mathbf{div}\,\Lambda - X : T + \hat{K} \\
\dot{U}^p &= \hat{\alpha} \times \hat{V}^\alpha \\
\dot{\hat{S}} &= -\Pi \times \hat{V}^\Pi + grad\left(\hat{S}\hat{V}^S\right) \\
\dot{\hat{\Pi}} &= -curl\left(\hat{\Pi} \times \hat{V}^\Pi\right).
\end{aligned}
\tag{5.38}
$$

Here $\hat{V}^S$ is the eigenwall velocity, $\hat{V}^\alpha$ the dislocation velocity, $\hat{V}^\Pi$ the disclination velocity, and $\hat{b}$ and $\hat{K}$ are body force and couple densities per unit volume. We also define $\hat{J} := grad\,U^e$.

The stored energy density response (per unit volume of the reference) is assumed to have the following dependencies:

$$\psi = \psi\left(U^e, \hat{S}, \hat{\Pi}, \hat{J}\right),$$

and a necessary condition for the invariance of the energy under superposed infinitesimal rigid deformations is

$$(\partial_{U^e}\psi) : s = 0 \ \text{ for all skew tensors } s,$$

which implies that $(\partial_{U^e}\psi)$ has to be a symmetric tensor, thus constraining the functional form of ψ.

On defining $\left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{ijk} := \frac{1}{2}\left[\left(\partial_{\hat{\boldsymbol{J}}}\psi\right)_{ijk} + \left(\partial_{\hat{\boldsymbol{J}}}\psi\right)_{ikj}\right]$, the dissipation can be characterized as:

$$
\begin{aligned}
\mathsf{D} = & \int_B T_{ij}\dot{\varepsilon}_{ij}\,dv - \frac{1}{2}\int_B \Lambda_{ij}e_{irs}\Omega_{rs,j}\,dv - \int_B \dot{\psi}\,dv \\
= & \int_B \left[T_{ij} - (\partial_{\boldsymbol{U}^e}\psi)_{ij} + \left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{ijk,k}\right] D_{ij}\,dv \\
& + \int_B \left[-\frac{1}{2}e_{irs}\Lambda_{ij} - \left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{rsj}\right]\Omega_{rs,j}\,dv \\
& + \int_B \left[e_{sjr}\left\{(\partial_{\boldsymbol{U}^e}\psi)_{ij} - \left(\partial_{\hat{\boldsymbol{J}}}\psi\right)_{ijk,k}\right\}\right]\hat{\alpha}_{ir}\hat{V}_s^{\alpha}\,dv \\
& + \int_B \left(\partial_{\hat{\boldsymbol{S}}}\psi\right)_{ijk,k}\hat{S}_{ijr}\hat{V}_r^{S}\,dv \\
& + \int_B \left[e_{snr}\left\{(\partial_{\hat{\boldsymbol{S}}}\psi)_{ijn} + e_{nmk}\left(\partial_{\hat{\boldsymbol{\Pi}}}\psi\right)_{ijk,m}\right\}\right]\hat{\Pi}_{ijr}\hat{V}_s^{\Pi}\,dv \\
& - \int_{\partial B}\left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{ijk}n_k\dot{\varepsilon}_{ij}\,da \\
& + \int_{\partial B} e_{sjr}\left(\partial_{\hat{\boldsymbol{J}}}\psi\right)_{ijk}n_k\hat{\alpha}_{ir}\hat{V}_s^{\alpha}\,da \\
& - \int_{\partial B}\left(\partial_{\hat{\boldsymbol{S}}}\psi\right)_{ijk}n_k\hat{S}_{ijr}\hat{V}_r^{S}\,da \\
& + \int_{\partial B}\left(\partial_{\hat{\boldsymbol{\Pi}}}\psi\right)_{ijk}[\delta_{kr}\delta_{ms} - \delta_{ks}\delta_{mr}]n_m\hat{\Pi}_{ijr}\hat{V}_s^{\Pi}\,da.
\end{aligned}
\tag{5.39}
$$

5.6.1 Reversible Response and Driving Forces in the Small Deformation Model

Motivated by the characterization (5.39), we propose the following constitutive guidelines that ensure non-negative dissipation in general and vanishing dissipation in the elastic case:

$$
\begin{aligned}
T_{ij} + T_{ji} &= \hat{\mathcal{A}}_{ij} + \hat{\mathcal{A}}_{ji} \\
\hat{\mathcal{A}}_{ij} &:= (\partial_{\boldsymbol{U}^e}\psi)_{ij} - \left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{ijk,k} \\
\Lambda_{ij}^{dev} &= -e_{irs}\left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{rsj} \\
\left[\left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{ijk} + \left(D_{\hat{\boldsymbol{J}}}^{sym}\psi\right)_{jik}\right]n_k\Big|_{boundary} &= 0
\end{aligned}
$$

$$\hat{V}_s^\alpha\big|_{bulk} \rightsquigarrow e_{sjr}\left\{(\partial_{U^e}\psi)_{ij} - \left(\partial_{\hat{\jmath}}\psi\right)_{ijk,k}\right\}\hat{\alpha}_{ir}$$

$$\hat{V}_r^S\big|_{bulk} \rightsquigarrow (\partial_{\hat{S}}\psi)_{ijk,k}\,\hat{S}_{ijr}$$

$$\hat{V}_s^\Pi\big|_{bulk} \rightsquigarrow e_{snr}\left\{(\partial_{\hat{S}}\psi)_{ijn} + e_{nmk}\left(\partial_{\hat{\Pi}}\psi\right)_{ijk,m}\right\}\hat{\Pi}_{ijr}$$

$$\hat{V}_s^\alpha\big|_{boundary} \rightsquigarrow e_{sjr}\left(\partial_{\hat{\jmath}}\psi\right)_{ijk}n_k\,\hat{\alpha}_{ir} \qquad (5.40)$$

$$\hat{V}_r^S\big|_{boundary} \rightsquigarrow -(\partial_{\hat{S}}\psi)_{ijk}\,n_k\,\hat{S}_{ijr}$$

$$\hat{V}_s^\Pi\big|_{boundary} \rightsquigarrow \left[(\partial_{\hat{\Pi}}\psi)_{ijr}\,n_s - (\partial_{\hat{\Pi}}\psi)_{ijs}\,n_r\right]\hat{\Pi}_{ijr}.$$

As before, a dependence of the energy on F^S in the nonlinear case translates to an extra dependence of the stored energy on

$$U^p = grad\,u - U^e = I - U^e - (I - grad\,u) \approx W - F_R^{-1} = W^S$$

in the small deformation case, with corresponding changes in the reversible response and driving forces.

5.7 Contact with the Differential Geometric Point of View

For the purpose of this section it is assumed that we operate on a simply-connected subset of the current configuration B. Arbitrary (3-d) curvilinear coordinate systems for the set will be invoked as needed, with the generic point denoted as (ξ^1, ξ^2, ξ^3). Lower-case Greek letters will be used to denote indices for such coordinates. The natural basis of the coordinate system on the configuration B will be denoted as the list of vectors

$$e_\alpha = \frac{\partial x}{\partial \xi^\alpha}\ \ \alpha = 1, 2, 3,$$

with dual basis $\left(e^\beta = grad\,\xi^\beta,\ \beta = 1, 2, 3\right)$. We will assume all fields to be as smooth as required; in particular, equality of second partial derivatives will be assumed throughout.

Beyond the physical motivation provided for it in Sect. 5.4.3 as a line density carrying a tensorial attribute, the disclination density field $\Pi = curl\,Y$ alternatively characterizes whether a solution $\tilde{W}$ (2nd-order tensor field) exists to the equation

$$grad\,\tilde{W} = Y, \qquad (5.41)$$

with existence guaranteed when $\Pi = curl\,Y = curl\,S = 0$ which, in a rectangular Cartesian coordinate system, amounts to

$$S_{ijk,l} - S_{ijl,k} = e_{rlk}e_{rqp}S_{ijp,q} = e_{rlk}\,(curl\,S)_{ijr} = 0. \qquad (5.42)$$

This is a physically meaningful question in continuum mechanics with a simple answer. Moreover, when such a solution exists, the existence of a triad $\tilde{d}_\alpha$, $\alpha = 1, 2, 3$ of vectors corresponding to each choice of a coordinate system for B is also guaranteed by the definition

$$\tilde{d}_\alpha := \tilde{W} e_\alpha.$$

This question of the existence of a triad of vectors related to arbitrary coordinate systems for B and the integrability of Y can also be posed in a differential geometric context, albeit far more complicated.

We first consider the i-elastic 1-distortion W that is assumed to be an *invertible* 2nd-order tensor field by definition. Defining

$$\bar{d}_\alpha = W e_\alpha$$

and noting that $\bar{d}_\alpha$, $\alpha = 1, 2, 3$ is necessarily a basis field, there exists an array $\bar{\Gamma}^\mu_{\alpha\beta}$ satisfying

$$\bar{d}_{\alpha,\beta} = \bar{\Gamma}^\mu_{\alpha\beta} \bar{d}_\mu. \tag{5.43}$$

Let the dual basis of $(\bar{d}_\alpha, \alpha = 1, 2, 3)$ be $\left(\bar{d}^\alpha = W^{-T} e^\alpha, \alpha = 1, 2, 3 \right)$. Then

$$\bar{\Gamma}^\rho_{\alpha\beta} = e^\rho \cdot W^{-1} \left(\left[\{ grad\, W \} e_\beta \right] e_\alpha + W e_{\alpha,\beta} \right).$$

We observe that even though (5.43) is an overconstrained system of 9 vector equations for 3 vector fields, solutions exist due to the invertibility of W, and the following 'integrability' condition arising from $\bar{d}_{\alpha,\beta\gamma} = \bar{d}_{\alpha,\gamma\beta}$, holds:

$$\bar{\Gamma}^\mu_{\alpha\beta,\gamma} - \bar{\Gamma}^\mu_{\alpha\gamma,\beta} + \bar{\Gamma}^\rho_{\alpha\beta} \bar{\Gamma}^\mu_{\rho\gamma} - \bar{\Gamma}^\rho_{\alpha\beta} \bar{\Gamma}^\mu_{\rho\gamma} = 0. \tag{5.44}$$

Guided by the integrability/existence question suggested by (5.43) we now turn the argument around and ask for conditions of existence of a vector field triad (d_α) *given* the connection symbols Γ defined by

$$\Gamma^\rho_{\alpha\beta} := \bar{\Gamma}^\rho_{\alpha\beta} + S^\rho_{.\alpha\beta}$$
$$S^\rho_{.\alpha\beta} := e^\rho \cdot W^{-1} \left(\{ S e_\beta \} e_\alpha \right).$$

Thus, we ask the question of existence of smooth solutions to

$$d_{\alpha,\beta} = \Gamma^\mu_{\alpha\beta} d_\mu. \tag{5.45}$$

Based on a theorem of Thomas [Tho34], it can be shown that a 9-parameter family of (global) solutions on simply-connected domains may be constructed when the following condition on the array Γ holds:

$$R^\mu_{.\alpha\beta\gamma}(\Gamma) := \Gamma^\mu_{\alpha\beta,\gamma} - \Gamma^\mu_{\alpha\gamma,\beta} + \Gamma^\rho_{\alpha\beta} \Gamma^\mu_{\rho\gamma} - \Gamma^\rho_{\alpha\beta} \Gamma^\mu_{\rho\gamma} = 0. \tag{5.46}$$

The condition corresponds to the mixed components of the curvature tensor of the connection Γ vanishing and results in $\boldsymbol{d}_{\alpha,\beta\gamma} = \boldsymbol{d}_{\alpha,\gamma\beta}$ for the $(\boldsymbol{d}_\alpha)$ triad that can be constructed. We note that

$$R^\alpha_{.\mu\beta\gamma}(\Gamma) = R^\alpha_{.\mu\beta\gamma}(\bar{\Gamma}) + R^\alpha_{.\mu\beta\gamma}(S) + \bar{\Gamma}^\alpha_{\nu\gamma}S^\nu_{.\mu\beta} + \bar{\Gamma}^\nu_{\mu\beta}S^\alpha_{.\nu\gamma} - \bar{\Gamma}^\alpha_{\nu\beta}S^\nu_{.\mu\gamma} - \bar{\Gamma}^\nu_{\mu\gamma}S^\alpha_{.\nu\beta}$$

with $R^\alpha_{.\mu\beta\gamma}(\bar{\Gamma}) = 0$ from (5.44). Furthermore, the typical differential geometric treatment [Kon55, Bil60, KL92, CMB06] imposes the condition of a metric differential geometry, i.e. the covariant derivative of the metric tensor (here $\boldsymbol{W}^T\boldsymbol{W}$) with respect to the connection Γ is required to vanish. There is no need in our development to impose any such requirement.

The difference in complexity of the continuum mechanical and differential geometric integrability conditions (5.42) and (5.46), even when both are expressed in rectangular Cartesian coordinates, is striking. It arises because of the nature of the existence questions asked in the two cases. The differential geometric question (5.45) involves the unknown vector field on the right hand side while the continuum mechanical question (5.41), physically self-contained and sufficiently general for the purpose at hand, is essentially the question from elementary vector analysis of when a potential exists for a *completely prescribed* vector field.

Finally, we note that both in the traditional metric differential geometric treatment of defects [Kon55, Bil60, KL92, CMB06] and our continuum mechanical treatment at finite strains, it is not straightforward, if possible at all, to separate out the effects of strictly rotation-gradient and strain-gradient related incompatibilities/non-integrabilities. Fortunately from our point of view, this is not physically required either (for specifying, e.g., the defect content of a terminating elastic distortion discontinuity from observations).

5.8 Concluding Remarks

A new theoretical approach for studying the coupled dynamics of phase transformations and plasticity in solids has been presented. It extends nonlinear elasticity by considering new continuum fields arising from defects in compatibility of deformation. The generalized eigendeformation based kinematics allows a natural framework for posing *kinetic* balance/conservation laws for defect densities and consequent dissipation, an avenue not available through simply higher-gradient, 'capillary'/surface energy regularizations of compatible theory. Such a feature is in the direction of theoretical requirements suggested by results of sharp-interface models from nonlinear elasticity in the case of phase transformations [AK06]. In addition, finite-total-energy, non-singular, defect-like fields can be described (that may also be expected to be possible with higher-gradient regularizations), and their evolution can be followed without the cumbersome tracking of complicated, evolving, multiply-connected geometries. This feature has obvious beneficial implications for practical

numerical implementations where the developed model introduces interesting combinations of elliptic and hyperbolic (when material inertia is included) systems with degenerate parabolic equations for numerical discretization. The elliptic component includes $div - curl$ systems, novel in the context of their use in solid mechanics. Significant components of such problems have been dealt with computationally in our prior work e.g. [RA05, VBAF06, FTC11, TCF13a], and detailed considerations for the present model will be the subject of future work.

The generalized eigendeformation fields have striking similarities with gauge fields of high-energy particle physics, but do not arise from considerations of gauge invariance of an underlying Hamiltonian. Instead, they arise from the physical requirement of modeling finite total energies in bodies that contain commonly observed 1 and 2-dimensional defects, and from a desire to be able to model their observed motion and interactions.

In formulating a continuum mechanical model of solid-solid phase transformation behavior based squarely on the kinematics of deformation incompatibility, our work differs from that of [FG94] and those of [Kha83, Roi78]. In the context of dislocation plasticity alone, for the same reason it differs from the strain-gradient plasticity work of [Aif84, FH01, GHNH99]. There is an extended body of work in strain-gradient plasticity that accounts for the dislocation density in some form [Ste96, Gur02, FS03, EBG04, LS06, KT08, Gud04, FW09] but none have been shown to build up from a treatment of the statics and dynamics of individual dislocations as in our case [Ach01, Ach03, VBAF06, DAZM, ZCA13, TCF13a].

Finally, we mention a widely used, and quite successful, framework for grain-boundary network evolution [Mul56, KLT06, EES09]. This involves postulating a grain boundary energy density based on misorientation and the normal vector to the boundary and evolving the network based on a gradient flow of this energy (taking account of the natural boundary condition that arises at triple lines). Given that a grain boundary is after all a sharp transition layer in lattice orientation and the latter is a part of the elastic distortion of a lattice that stretches and bends to transmit stresses and moments, it is reasonable to ask why such modeling succeeds with the complete neglect of any notions of stress or elastic deformation and what the model's relation might be to a theory where stresses and elastic strains are not constrained to vanish. The Mullins model does not allow asking such questions. With localized concentrations of the eigenwall field representing the geometry of grain boundaries (including their normals), g.disclinations representing triple (or higher) lines, dependence of the energy on the eigenwall field and the i-elastic 1-distortion representing effects of misorientation, and the eigenwall velocity representing the grain boundary velocity, our model provides a natural framework, accounting for compatibility conditions akin to Herring's relation at triple lines, for the response of grain boundaries to applied stress [TCF13a, FTUC12]. Moreover, it allows asking the question of whether stress-free initializations can remain (almost) stress-free on evolution. Interestingly, it appears that it may be possible to even have an exact analog of the stress-free/negligible stress model by allowing for general evolution of the eigenwall field S, and constraining the dislocation density field α to ensure that $\widetilde{\alpha} = -curl\, W$ always belongs to the space of *curls* of (proper-orthogonal tensor) rotation

fields. We leave such interesting physical questions for further study along with the analysis of 'simple' ansatz-based, exact reduced models of phase boundary evolution coupled to dislocation plasticity within our setting that have been formulated.

Ericksen [Eri98, Eri08] raises interesting and important questions about the (in)adequacy of modeling crystal defects with nonlinear elasticity, the interrelationships between the mechanics of twinning and dislocations, and the conceptual (un)importance of involving a reference configuration in the mechanics of crystalline solids, among others. It is our hope that we have made a first step in answering such questions with the theory presented in this paper.

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