Coupled phase transformations and plasticity as a field theory of deformation incompatibility

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Abstract

The duality between terminating discontinuities of fields and the incompatibilities of their gradients is used to define a coupled dynamics of the discontinuities of the elastic displacement field and its gradient. The theory goes beyond standard translational and rotational Volterra defects (dislocations and disclinations) by introducing and physically grounding the concept of *generalized disclinations* in solids without a fundamental rotational kinematic degree of freedom (e.g. directors). All considered incompatibilities have the geometric meaning of a density of lines carrying appropriate topological charge, and a conservation argument provides for natural physical laws for their dynamics. Thermodynamic guidance provides the driving forces conjugate to the kinematic objects characterizing the defect motions, as well as admissible constitutive relations for stress and couple stress. We show that even though higher-order kinematic objects are involved in the specific free energy, couple stresses may not be required in the mechanical description in particular cases. The resulting models are capable of addressing the evolution of defect microstructures under stress with the intent of understanding dislocation plasticity in the presence of phase transformation and grain boundary dynamics.

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1 Introduction

The dynamic response of solids to mechanical and thermal loading involves material-physics phenomena that are manifested over multiple length and time scales. The material responds to load through atomic level processes involving crystal defects that mediate plasticity, phase transformations and damage. These processes, however, generally occur in materials whose intrinsic microstructure affects bulk properties like strength, ductility, and fracture toughness. Although relevant dimensions and time span for the nucleation of the individual defects can be Å and picoseconds, their collective interaction, evolution and relaxation occur at larger time scales (μs). The objective of the program on which this paper is based is the development of a kinematically rigorous continuum mechanics model to serve as the basis for a simulation framework; the goal is to predict deformation-induced microstructure evolution and its effects on macroscopic properties in materials that undergo coupled plasticity and phase transformation. The kinematic ingredients of the model naturally include structural defects representative of grain boundaries. Such inelastic deformation is complex because of the essentially collective character of the dynamical behavior of structural defects over engineering time and length scales; nevertheless, understanding the underlying dynamics of defects is essential for predicting flow and failure at meso- and macroscopic scales. Due to space limitations, in this paper we outline only the small deformation kinematics and thermodynamics of our model.

This paper may be considered as an extension of the pioneering work of deWit [deW70] on dislocation-disclination statics that was generalized by Fressengeas *et al.* [FTC11] to account for disclination-dislocation dynamics; our work describes the dynamics of a more general class of defects than dislocations and disclinations. It also has broad philosophical similarities with the work of [Kle08]. Here, the whole elastic distortion 'gradient' can be incompatible in order to represent terminating/kinking elastic distortion discontinuities as may arise, e.g., in a martensitic needle or a facet of a phase-transforming inclusion. Through the connection to the kinematics of phase transformations, our work provides an unambiguous physical basis to the notion of generalized disclinations (*g-disclinations*) even in solids without any director degrees of freedom. It is also motivated by that of [AK90] on dynamic phase transformations that allows for full freedom in specifying kinetics of phase front motion, and generalizes it to account for geometric singularities in the surfaces of discontinuity. In this last context, there appear to be connections between our model and the fundamental work of

[SB98], and through that, to the configurational force framework of [Gur00]. However, we believe that the details of generating approximate solutions to our theory based on nonlinear partial differential equations (PDE), while non-trivial, are going to be much simpler[1] than the complications involved in the configurational force setup that, to our knowledge, has not been solved in full 3-d generality as yet. As we understand, these difficulties stem from applying boundary conditions for the field equations on the (solution-dependent) moving boundaries of the cylinders representing the cores of the phase-transformation singularities. A primary future goal of our program is to make contact with the Topological Model put forward by [HP11] in the modeling of displacive phase transformations.

Phase field methodology has been used to study phase transformations and plasticity [LLZF09], but the governing dynamical principle there is of finding local minima of energy. In contrast, the dynamics we propose is based on geometrically rigorous conservation laws for line-defect densities carrying appropriate topological charge (much like vortices in fluids and superconductivity) and we have shown, in simple but exact realizations of sub-parts of our model, that the class of equilibria of such conservation laws contains that of phase field models but is strictly larger, while in dynamic behavior it allows defect motion as wave propagation that simply cannot be predicted by phase field models ([AMZ10],[AT11]). Also, generalizing the standard formalism for describing stress (arising from elastic straining) in phase field methodology to the finite deformation setting to incorporate elastic response developed from atomistic considerations appears to be an as yet unsettled matter.

We use more-or-less standard notation. All tensor indices are written with respect to the basis $e_i, i = 1 \text{ to } 3$ of a rectangular Cartesian coordinate system. The symbol e_{ijk} represents the components of the alternating tensor X. Vertical arrays of two or three dots represent contraction of the respective number of 'adjacent' indices on two immediately neighboring symbols (in standard fashion). Also,

$$\left.\begin{array}{rcl} (curl\, A)_{ij \text{ or } ikj} & = & e_{jrs}\partial_r A_{is \text{ or } iks} \\ (div\, A)_{i \text{ or } ik} & = & \partial_r A_{ir \text{ or } ikr} \\ (A \times V)_{ij \text{ or } ikj} & = & e_{jrs} V_s A_{ir \text{ or } ikr} \end{array}\right\} \text{ for } A \text{ a } 2^{nd} \text{ or } 3^{rd} \text{ order tensor}$$

[1] Indeed, Fressengeas et al. [FTC11] have already developed and demonstrated a finite-element implementation of the pure disclination-dislocation dynamics case. An attractive feature is the coherence of the algorithm with that of the pure field dislocation dynamics case first introduced in [RA05].

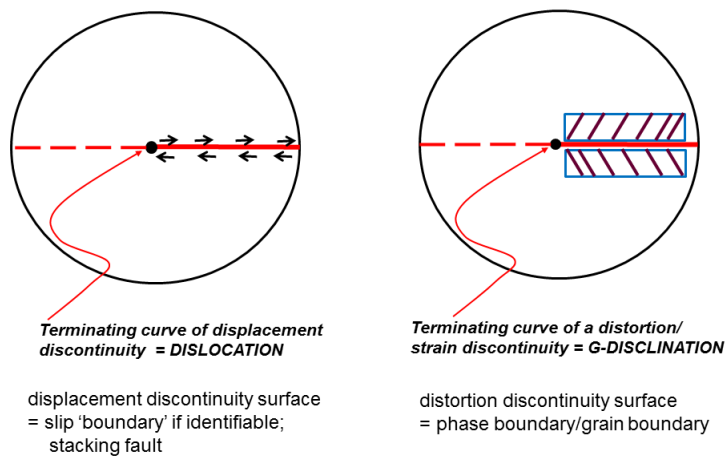

Figure 1: Discontinuity of a discontinuity; cross-section view of straight defect lines terminating displacement/distortion discontinuities.

2 The physical idea

The fundamental theoretical concern is the modeling of the dynamics of the relevant defects that may be viewed as *discontinuities* in the elastic displacement, rotation and distortion fields (slip, grain and phase boundaries, respectively) across surfaces, terminating in line *singularities* (dislocation, standard disclination and *generalized disclination*, respectively) as sketched in Fig. 1. It is well known that when defects are viewed at sufficiently small scales there are no discontinuities and singularities but only appropriately localized smooth fields. Moreover, for the purpose of understanding the nonlinear dynamics of such defects and their collective effects, in particular in the context of nonlinear PDEs, such smooth localized representations of the physical reality of defects are essential from the point of view of mathematical analysis and numerical computation. There is a significant duality between the terminating curves of discontinuities of fields on 2-d surfaces and the *smooth incompatibilities* of the 'gradients' of such fields. The essential idea is that the geometrically defined incompatibilities model defect curves. Each (often closed) curve separates two disjoint pieces of a 2-d sur-

face. The field in question is discontinuous by different amounts across the two 2-d pieces, and the advance of the curve represents the spreading of one piece at the expense of the other. The incompatibilities have the rigorous geometric meaning of a density of lines carrying appropriate topological charge, so that a tautological conservation argument provides most of the structural elements of a natural physical law for the dynamics of the field[2]. We exploit this feature to define coupled PDE-dynamics of the discontinuities of the elastic displacement field and its gradient. When restricted to the elastic displacement, a nonlinear theory for the dynamics of dislocation and slip results. When applied to the elastic distortion, the theory provides for the dynamics of *g-disclinations*, going beyond the Volterra construct by including elastic strain discontinuities, and allows dealing with phase and grain boundaries. Unlike the Volterra concept, our continuously distributed approach seamlessly models single defects up to a continuously distributed field in the entire body, as might be encountered in the transition of a solid to a liquid-like state under strong shock loading. These models are capable of addressing phase transformation and dislocation motion-related microstructure evolution under stress. While being based on PDEs in the set of variables involved, they are non-local models in space and time in the standard variables of conventional continuum mechanics, thus providing geometrically rigorous, physics-based, nonlocal generalization of the latter, and leading to well-set models of post-initiation defect mechanics.

3 Motivating kinematical notions

As is well-known, a classical, singular dislocation line in a simply-connected body has a smooth elastic (1-)distortion (strain + rotation) field in the non simply-connected, punctured domain represented by the region excluding its core, even though the elastic displacement field it is considered to arise from has a discontinuity across a (non-unique) 2-d smooth slip surface in the same region. The geometry of any such 2-d surface is arbitrary, except that it terminates along the curve representing the core of the dislocation. Additionally, the important topological fact about such a field is that a line integral of the elastic distortion along any curve encircling the core is non-vanishing and constant over all such curves. This constant represents the strength of the dislocation, *i.e.*, the *Burgers vector*. Thus, as concerns a classical dislocation, it is only its elastic distortion field that one can precisely

[2]This is in contrast to dynamics based on the local "principle of virtual power" whose validity has recently been questioned [Fos11].

discuss, and not the displacement field. The continuously distributed dislocations setting eases this classical description by considering smooth elastic distortion fields on simply connected domains in which they are pointwise irrotational outside the core cylinder (possibly of non-zero volume), and their curl equals the corresponding *Nye dislocation density* tensor fields inside the cylinder. The distribution of the elastic distortion and the dislocation density tensor fields on the body are set up such that the Burgers vector of the dislocation being modeled is obtained on integration of the fields along appropriate surface patches and/or closed curves.

Once understood, this fact enables the definition of a phase boundary, *i.e.*, a 2-d surface of elastic distortion discontinuity (which includes the case of a grain boundary), terminating on a g-disclination curve. In this case, we assume the continuous elastic 2-distortion field (*i.e.*, the incompatible elastic distortion 'gradient' field) to be irrotational outside the g-disclination core, and the g-disclination strength to be the second-order tensor obtained by integrating the 2-distortion field along a closed curve encircling the core. In the pure disclination case, this second-order tensor is a skew-tensor whose axial vector is called the *Frank vector* of the disclination. In the non-singular, continuously distributed setting, one way of setting up the 3rd order, g-disclination density field for a straight g-disclination would be to assign the tensor product of the 2nd order, strength tensor and the core line direction divided by the core cross-sectional area as a constant distribution within the core cylinder and zero outside it. Considered from the dual viewpoint of a discontinuous elastic distortion field with discontinuity terminating at a core singularity, the strength tensor is simply the jump in the elastic distortion across the surface of discontinuity.

It is important to note explicitly that, in the continuously distributed setting, the elastic distortions are no longer gradients but have incompatible parts that may be defined through a Helmholtz decomposition. We would now like to set up a dynamical theory of such dislocation and g-disclination defect curves and (meta)slipped regions, taking into account forces, moments and dissipation.

4 Mechanical structure

Let T be the (generally unsymmetric) stress tensor, Λ the couple stress tensor, X the alternating tensor, u the material displacement vector, v the material velocity vector, D and Ω the symmetric and skew-symmetric parts of the velocity gradient, and $\omega = -(1/2)\ X : \Omega = \mathit{curl}\, v$ the vorticity vector.

Let U^e be the elastic 1-distortion tensor and G^e the elastic 2-distortion tensor (in gradient elasticity these would be $grad\, u$ and $gradgrad\, u$, respectively). We define

$$G^e - grad\, U^e =: P^s \tag{1}$$

$$-G^e : X =: \alpha^s \tag{2}$$

$$curl\, G^e = curl\, P^s = \Pi^s, \tag{3}$$

where α^s is the dislocation density (2nd-order) tensor and Π^s is the g-disclination density (3rd-order) tensor. Both the dislocation density and the g-disclination density tensors are 'vector(tensor)-valued axial vector' fields representing third (fourth) order tensor fields that are skew in their last two indices. Thus, they form densities that can be integrated over area elements. Physically, such fields represent densities of lines carrying appropriate tensorial attributes.

It is helpful for physical interpretation to invoke a Stokes-Helmholtz-like orthogonal decomposition of the field P^s into compatible and incompatible parts:

$$\left.\begin{array}{rcl} P^s & = & P^{s\perp} + grad\, Z^s \\ div\, P^{s\perp} & = & 0 \\ \text{with } P^{s\perp} n & = & 0 \text{ on boundary of the body } B. \end{array}\right\} \tag{4}$$

It is clear from (3) and (4) that when $\Pi^s = 0$ then $P^{s\perp} = 0$. Thus, referring back to our physical picture of a single terminating elastic distortion discontinuity, the expression

$$G^e = P^{s\perp} + grad\, U^e + grad\, Z^s \tag{5}$$

implies that a smooth representation of elastic distortion discontinuities across surfaces that do not terminate or have discontinuities in their tangent plane orientation field is embodied in the *compatible* part of G^e, characterized by $grad\, U^e + grad\, Z^s$. Thus, the compatible part of G^e characterizes smoothed phase/grain boundaries without kinks or corners. $P^{s\perp}$, on the other hand, characterizes phase/grain boundaries with kinks or corners. Also, recognizing $curl\, U^e = -grad\, U^e : X$ as representative of *slip* dislocations arising from slip discontinuities, the expression

$$\alpha^s = -G^e : X = -P^{s\perp} : X - grad\, U^e : X - grad\, Z^s : X$$

implies that $-grad\, Z^s : X$ is representative of pure *transformation* dislocations, while $-P^{s\perp} : X$ is representative of *g-disclination-induced transformation* dislocations. Thus, it becomes clear why an infinite grain boundary/incoherent phase boundary can often be represented by slip dislocations.

In addition, (5) also makes clear what parts of the structure of a general grain/phase boundary cannot be represented by slip dislocations.

We now assume that the dislocation and the g-disclination densities representing line-like objects have velocity fields, V^α and V^π, associated with them. In situations when these fields represent individual defects through non-singular localization in core cylinders, the corresponding local value of the velocity field represents the velocity of the movement of the core cylinders. Furthermore, because these defect fields are line densities, conservation laws for their evolution are an immediate consequence [Ach11]. The local form of the conservation law for Π^s is given by

$$\dot{\Pi}^s = -curl\ (\Pi^s \times V^\pi)\,. \tag{6}$$

As for the evolution of the line density field $curl\, U^e$, we note from (5) that

$$\dot{\alpha}^s + \dot{P}^s : X = curl\, \dot{U}^e \tag{7}$$

which we set equal to $-curl\,(\alpha^s \times V^\alpha)$ from the kinematics of flux of lines moving into an area patch through its bounding curve[3] to obtain

$$\dot{\alpha}^s = -curl\ (\alpha^s \times V^\alpha) - \dot{P}^s : X, \tag{8}$$

which implies

$$div\, \dot{\alpha}^s = \dot{\Pi}^s : I.$$

Physically, this means that in contrast to the pure dislocation case, dislocation lines can terminate within the body on phase/grain boundaries, but the locations at which they do so necessarily involve a variation in the strength of the elastic distortion discontinuity along the phase/grain boundary.

The statements (3) and (6) imply

$$\dot{P}^s = -\Pi^s \times V^\pi + grad\, K^s, \tag{9}$$

where K^s is a strain rate (2nd-order tensor) and $grad\, K^s$ is a compatible contribution to the elastic 2-distortion rate associated with the transverse motion of (physically identifiable) phase/grain boundaries. K^s requires specification based on geometric and constitutive considerations.

We now introduce the definition

$$U^p := grad\, u - U^e. \tag{10}$$

[3] an equally plausible expression would be to set $-curl\,(curl\, U^e \times V^\alpha)$, but the one we choose appears to have a definite advantage for the modeling of disclination and dislocation free phase transformations.

Then, (7,8,10) imply

$$\dot{U}^p = \alpha^s \times V^\alpha, \tag{11}$$

where, unlike the 2-distortion case, we do not include the free gradient (representing an inelastic strain rate) that arises in deducing (11) due to the assumption that slip-boundaries are often not physically identifiable. Even when they are, as in the case of stacking faults, their evolution typically consists of expansion or shrinkage in the slip plane governed by the motion of their bounding dislocation curve(s), so that no generation of independent inelastic strain rate may be assigned to this evolution.

Summarizing, one minimal representation of the field equations of the model consist of equations (1,2,3,9,11) along with

$$div\, T = 0 \tag{12}$$

$$div\, \Lambda - X : T = 0 \tag{13}$$

representing balance of linear momentum and angular momentum, ignoring body forces and couples and inertia terms (without loss of essential generality for the present purpose). The last two equations serve to determine the displacement field, when appended with constitutive equations for the stress and couple stress tensors. In addition, constitutive equations are also required for the dislocation and g-disclination velocities as well as the potential K^s for the compatible part of the elastic 2-distortion rate, G^e.

5 Constitutive guidance from thermodynamics

Following [MT62], we consider the following statement to characterize the work of external agents on the body:

$$\int_{\partial\mathcal{B}} (Tn)\cdot v\ dv + \int_{\partial\mathcal{B}} (\Lambda n)\cdot \omega\ dv,$$

where $\mathcal{B}$ is the body, $\partial\mathcal{B}$ its boundary and n the outward unit normal to the boundary. Denoting by ψ the free energy per unit volume field on the body, we define the (mechanical) dissipation to be

$$\begin{aligned} \mathsf{D} &= \int_{\partial\mathcal{B}} (Tn)\cdot v\ dv + \int_{\partial\mathcal{B}} (\Lambda n)\cdot \omega\ dv - \int_{\mathcal{B}} \dot{\psi}\ dv \\ &= \int_{\mathcal{B}} T_{sym} : D\ dv - \frac{1}{2}\int_{\mathcal{B}} \Lambda : grad\,(X:\Omega)\ dv - \int_{\mathcal{B}} \dot{\psi}\ dv. \end{aligned} \tag{14}$$

We now consider three possible constitutive dependencies for ψ and show that even though 'higher-order' kinematic objects are involved in the specific

free energy, in two of these cases no couple stress is required, at least based on thermodynamic considerations. We also derive the driving forces for the dissipative mechanisms of dislocation motion (characterized by V^{α}), g-disclination motion (characterized by V^{π}) and phase/grain boundary motion (characterized by K^s, up to further future geometric refinement to go from a strain-rate to a phase-front velocity).

By substituting these constitutive hypotheses into (14) we identify the dissipative power-conjugates to the defect motion variables as driving forces. We also identify constitutive equations for the stress and couple stress tensors by requiring that $\mathsf{D} = 0$ for all possible motions of the body in the absence of the dissipative mechanisms.

5.1 $\psi = \hat{\psi}\left(U^e, P^s, \Pi^s\right)$ implies no couple stress

The considered constitutive class is one that contains elastic 2-distortion contributions in the specific free energy arising only from disclination and phase/grain boundary-induced fields, but none from the gradient of the elastic 1-distortion. We require that

$$\hat{\psi}\left(U^e, P^s, \Pi^s\right) = \hat{\psi}\left(U^e + W, P^s, \Pi^s\right) \ \forall\ W \text{ skew},$$

which implies that $\partial_{U^e}\psi$ has to be symmetric (and more). Also,

$$\dot{\psi} = \left(\partial_{U^e}\hat{\psi}\right)_{sym} : grad\, v - \left(\partial_{U^e}\hat{\psi}\right)_{sym} : \dot{U}^p + \partial_{P^s}\hat{\psi} : \dot{P}^s + \partial_{\Pi^s}\hat{\psi} : \dot{\Pi}^s$$

which, along with (11,9,6) and (14) implies,

$$\begin{aligned}
\mathsf{D} \ = \ & \int_{\mathcal{B}} \left[T_{sym} - \left(\partial_{U^e}\hat{\psi}\right)_{sym}\right] : D \ dv \\
& -\frac{1}{2}\int_{\mathcal{B}} \Lambda : grad\left(X : \Omega\right) \ dv \\
& +\int_{\mathcal{B}} \left[X \left(\partial_{U^e}\hat{\psi}\right)_{sym} \alpha^s\right] \cdot V^{\alpha} \ dv \\
& +\int_{\mathcal{B}} \left[X \left\{\left(\partial_{P^s}\hat{\psi} + curl\, \partial_{\Pi^s}\hat{\psi}\right)_{ijl} \ \Pi^s_{ijk} e_l \otimes e_k\right\}\right] \cdot V^{\pi} \ dv \\
& +\int_{\mathcal{B}} div\left(\partial_{P^s}\hat{\psi}\right) : K^s \ dv \\
& -\int_{\partial\mathcal{B}} \left(K^s : \partial_{P^s}\hat{\psi}\right) n \ da + \int_{\partial\mathcal{B}} \left(\Pi^s \times V^{\pi}\right) \vdots \left(\partial_{\Pi^s}\hat{\psi} \times n\right) \ da.
\end{aligned} \tag{15}$$

Thus we conclude that

$$T = \left(\partial_{U^e}\hat{\psi}\right)_{sym} \tag{16}$$

$$\Lambda = 0 \tag{17}$$

$$X\left(T^T \alpha^s\right) \hookrightarrow V^\alpha \text{ in bulk} \tag{18}$$

$$X\left\{\left(\partial_{P^s}\hat{\psi} + curl\,\partial_{\Pi^s}\hat{\psi}\right)_{ijl} \Pi^s_{ijk} e_l \otimes e_k\right\} \hookrightarrow V^\pi \tag{19}$$

$$K^s \hookrightarrow div\left(\partial_{P^s}\hat{\psi}\right) \text{ in bulk,} \tag{20}$$

form a consistent set of constitutive guidelines that satisfies balance of angular momentum identically. Here $\hookrightarrow$ is used as shorthand for "is the driving force for." In addition, the last line of (15) may be interpreted as providing driving forces for K^s and V^π on the boundary of the body.

The driving 'force' in (18) is the analog of the Peach-Koehler force of classical dislocation theory; it has physical units of $force/volume$, to be interpreted as the force acting on unit volume of the dislocation core cylinders. The driving force in (19) is the corresponding thermodynamic force on unit volume along the length of a g-disclination cylinder; this is a new construct whose analog for the pure disclination case arises in [FTC11]. Finally, (20) shows the driving force for the inelastic strain-gradient rate produced due to the motion of phase/grain boundaries.

5.2 $\psi = \hat{\psi}(U^e, P^s, \Pi^s, curl\,U^e)$ implies no couple stress

Define $\tilde{\alpha} = curl\,U^e$. Then, an additional term to the dissipation (15) is

$$-\int_{\mathcal{B}} \partial_{\tilde{\alpha}}\hat{\psi} : \dot{\tilde{\alpha}}\ dv = \int_{\mathcal{B}} \partial_{\tilde{\alpha}}\hat{\psi} : curl\left(\alpha^s \times V^\alpha\right)\ dv.$$

The results (16,17,19) remain unchanged and (18) changes to

$$X\left(T + curl\,\partial_{\tilde{\alpha}}\hat{\psi}\right)^T \alpha^s \hookrightarrow V^\alpha \text{ in bulk,}$$

with an additional boundary term in the dissipation (15) given by

$$-\int_{\partial\mathcal{B}} \partial_{\tilde{\alpha}}\hat{\psi} : \left[(\alpha^s \times V^\alpha) \times n\right]\ da.$$

It is interesting to note that the presence of a special combination of $grad\,U^e$, *i.e.*, the part only related to slip dislocation content, allows a theory without couple stress and a symmetric stress tensor on thermodynamic grounds. A special case of the constitutive class considered here was treated, with similar results, in [Ach10].

5.3 $\psi = \hat{\psi}(U^e, P^s, \Pi^s, grad\, U^e)$ implies model with couple stress

We use the notation $grad\, U^e =: \nabla U^e$ and observe that a functional dependence of the specific free energy on the whole elastic 2-distortion, *i.e.*, $\psi = \tilde{\psi}(U^e, G^e, \Pi^s)$ is a special case of the constitutive class being considered for which

$$\partial_{\nabla U^e}\hat{\psi}\,(U^e, P^s, \Pi^s, \nabla U^e) = \partial_{G^e}\tilde{\psi}\,(U^e, G^e, \Pi^s).$$

In this case, the additional terms in the dissipation (15) are

$$-\int_{\mathcal{B}} \partial_{\nabla U^e}\hat{\psi} \,\vdots\, grad grad\, v\ dv + \int_{\mathcal{B}} \partial_{\nabla U^e}\hat{\psi} \,\vdots\, grad\,(\alpha^s \times V^\alpha)\ dv.$$

Noting that

$$\Lambda : grad\,(X\Omega) = -e_{mni}\Lambda_{ij} v_{m,nj},$$

(17) is replaced by the relation

$$e_{mni}\Lambda_{ij} + e_{mji}\Lambda_{in} = -\left[\left(\partial_{\nabla U^e}\hat{\psi}\right)_{mnj} + \left(\partial_{\nabla U^e}\hat{\psi}\right)_{mjn}\right],$$

(18) is replaced by

$$X\left(T - div\, \partial_{\nabla U^e}\hat{\psi}\right)^T \alpha^s \hookrightarrow V^\alpha \text{ in bulk},$$

with an additional boundary term in the dissipation (15) given by

$$\int_{\partial\mathcal{B}} \left[(\alpha^s \times V^\alpha) : \partial_{\nabla U^e}\hat{\psi}\right] n\ da.$$

Thermodynamical considerations leave the following parts of the stress and couple stress tensors,

$$T_{ij} - T_{ji}$$

$$e_{mni}\Lambda_{ij} - e_{mji}\Lambda_{in},$$

constitutively unspecified. Balance of linear momentum (12) and angular momentum (13) along with boundary conditions serve as two constraints for their determination.

6 Concluding remarks

A 'small-deformation' theory of coupled plasticity and phase transformation accounting for the dynamics of generalized defects, *i.e.*, dislocations and g-disclinations, has been proposed. When the elastic strain-gradient is

compatible, the present theory reduces to that of [FTC11], which involves only dislocations and pure disclinations.

A fundamental premise of our work is that it is not necessary, neither efficient, to resolve atomic level vibrations to model defect dynamics leading to inelasticity at meso- and macroscopic scales. Our PDE-based modeling paradigm is to account for the defects in atomic configurations in (material-specific) nonlinear elastic media, focusing on the dynamics of distributions of defects in such configurations, rather than the dynamics of the atoms themselves. This requires minimal, but essential, input on the mobility of single defects and nonlinear (and non-monotone) elastic behavior from MD/Quantum mechanics. Such transfer of information has the potential for computational efficiency because one does not have to resolve atomic vibrations anymore. Our general philosophy is motivated by the great success of the Peierls model in elucidating basic dislocation physics, and is a generalization of that approach to deal with unrestricted geometric nonlinearity, full-fledged non-monotone bulk elasticity and inertia. Moreover, the most noteworthy merit of such a PDE-based approach is that it suggests rational and natural ways for developing coarse-grained meso/macroscale models of averaged defect densities interacting with stress and leading to inelastic flow and failure, a subject of great current interest.

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