

BASIC ISSUES IN PHASE TRANSITION THEORY AND FRACTURE MECHANICS

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Abstract. A general model of phase transition phenomena in a nonlinear elastic medium undergoing large deformations is developed on the basis of a critical revision of the formal treatment recently contributed by M. Gurtin in discussing the role of configurational forces in the mechanics of materials. The analysis is carried out in the context of a metric approach to material behavior recently developed by the authors, by considering the phase-transition evolution as a propagating shock wave in the material. By reversing Gurtin's interpretation of the relevant balance law, a general expression of the dissipation induced by the evolution of phase-transition interfaces is provided in terms of the jump of Eshelby's stress tensor across the interfaces. This result is a correction of the classical one due to Eshelby. The specialization to fracture mechanics provides the basis for the introduction of James Rice's J -integral for the analysis of non-cohesive and cohesive crack propagation. The analysis of cohesive crack propagation shows that the general expression of the dissipation provides the driving force according to the Barenblatt nonlinear model for the cohesion versus crack-opening constitutive law.

Key words: phase transition, crack propagation, J -integral.

1 Introduction

The mechanical model of a body undergoing phase transition phenomena is based on the analysis of shock waves propagation in the medium since phase-transition fronts evolve according to the kinematical properties of singular surfaces. We present here a theory based on a metric description of material behavior¹⁶. The motion of evolving phase-transition fronts in the material is simulated by the functional dependence of the free energy on a field of piecewise constant parameters, labeling the different material phases in the body, which meets a suitable time evolution law. To get the relevant balance law, we premise a detailed account of the formulation of the virtual work theorem in mechanics with a detailed description of the regularity properties of the fields involved in the analysis. This presentation provides the necessary background to deal with the discontinuous virtual velocity fields involved in the balance law due to the phase-transition shock wave propagation in the material. The equilibrium condition relevant to the phase-transition phenomena is then derived, on the basis of the assumed expression of the free energy density. The transport theorem provides the suitable tool to derive the expression of the singular term in the time-rate of the free energy of the body. The Maxwell jump condition at singular surfaces and Hadamard's condition for shock wave fronts provide the tools for the evaluation of the virtual power expended in the motion of the singular phase-interfaces. In the balance law, the dissipation associated with the propagation of phase transition fronts is expressed in terms of the jump of the flux of Eshelby's stress tensor field across the singular interfaces. The theory is applied to fracture mechanics for the analysis of non-cohesive and cohesive crack propagation. It provides a foundation for the introduction of the J -integral method in fracture mechanics. The invariance property of the J -integral is discussed by providing a general formula for the divergence of Eshelby's stress tensor field.

2 Dynamical equilibrium

2.1 Bodies and deformations

A material body is a set of particles which can be identified with the points $\mathbf{m} \in \mathbb{M}$ of a differentiable submanifold, referred to as the reference placement, embedded in the ambient euclidean space $\{\mathbb{S}, \mathbf{g}\}$ endowed with the standard (constant) metric tensor field $\mathbf{g}(\mathbf{x}) \in BL(\mathbb{T}_{\mathbf{x}}\mathbb{S}, \mathbb{T}_{\mathbf{x}}\mathbb{S}; \mathcal{R})$. We denote by \mathbb{TS} the tangent bundle to the euclidean space, made up of replicae of the tangent space $\mathbb{T}_{\mathbf{x}}\mathbb{S} = \mathcal{R}^3$ at each point $\mathbf{x} \in \mathbb{S}$. In a mechanical theory, experimental tests are assumed to provide metric measurements of the length of the linear material fibers (tangent vectors) at the points of a placement $\varphi(\mathbb{M}) \subset \mathbb{S}$ of the body in the ambient space, described by a diffeomorphic configuration map $\varphi \in C^1(\mathbb{M}; \mathbb{S})$. The results of metric measurements can be interpreted by substituting the standard metric tensor \mathbf{g} in \mathbb{M} with a configuration-induced metric tensor $(\varphi^*\mathbf{g})(\mathbf{m}) \in BL(\mathbb{T}_{\mathbf{m}}\mathbb{M}, \mathbb{T}_{\mathbf{m}}\mathbb{M}; \mathcal{R})$ defined, at any $\mathbf{m} \in \mathbb{M}$, by:

$$(\varphi^*\mathbf{g})(\mathbf{a}, \mathbf{b}) := \mathbf{g}(d_{\mathbf{a}}\varphi, d_{\mathbf{b}}\varphi), \quad \forall \mathbf{a}, \mathbf{b} \in \mathbb{T}_{\mathbf{m}}\mathbb{M}.$$

Here the differential $d\varphi(\mathbf{m}) \in BL(\mathbb{T}_{\mathbf{m}}\mathbb{M}; \mathbb{T}_{\varphi(\mathbf{m})}\mathbb{S})$ of the configuration map at $\mathbf{m} \in \mathbb{M}$ is the linear map which transforms a vector $\mathbf{h} \in \mathbb{T}_{\mathbf{m}}\mathbb{M}$ into the corresponding vector $d\varphi(\mathbf{m})\mathbf{h} \in \mathbb{T}_{\varphi(\mathbf{m})}\mathbb{S}$. In differential geometric terms the tensor field $\varphi^*\mathbf{g}$ is

called the *pull-back* of the metric tensor field \mathbf{g} according to the diffeomorphism $\varphi \in C^1(\mathbb{M}; \mathbb{S})$. The metric tensor induces an algebraic isomorphism between tensors $\mathbf{a} \in BL(\mathbb{T}_m\mathbb{M}, \mathbb{T}_m\mathbb{M}; \mathcal{R})$ and linear operators $\mathbf{A} \in BL(\mathbb{T}_m\mathbb{M}; \mathbb{T}_m\mathbb{M})$ according to the relation $\boldsymbol{\alpha} = \mathbf{g}\mathbf{A}$ defined by the identity

$$\boldsymbol{\alpha}(\mathbf{a}, \mathbf{b}) = \mathbf{g}(\mathbf{A}\mathbf{a}, \mathbf{b}), \quad \forall \mathbf{a}, \mathbf{b} \in \mathbb{T}_m\mathbb{M}.$$

The relation $\varphi^*\mathbf{g} = \mathbf{g}(d\varphi^T d\varphi)$ defines the Piola-Green operator $\mathbf{D}(\varphi) := d\varphi^T d\varphi \in BL(\mathbb{T}_m\mathbb{M}; \mathbb{T}_m\mathbb{M})$. The configuration map $\varphi \in C^1(\mathbb{M}; \mathbb{S})$ changes the volume of the body according to the relation $\varphi^*\boldsymbol{\mu} = \det(d\varphi)\boldsymbol{\mu}$. In the sequel $\langle \bullet, \bullet \rangle$ is the duality pairing between dual fields and $\langle \bullet, \bullet \rangle_{\mathbf{g}}$ is the inner product between linear operators induced by the metric \mathbf{g} .

2.2 Virtual Work

In mechanics the axiom of dynamical equilibrium states that, at any configuration $\varphi \in C^1(\mathbb{M}; \mathbb{S})$ of a body \mathbb{M} , the system of forces acting on it, including inertial force systems and constraint reactions, must perform a null virtual power for any virtual motion of the body which starts as an infinitesimal isometry. A celebrated result stated by Leonhard Euler and extended to riemannian manifolds by Wilhelm Killing around the end of the XIX century, states that infinitesimal isometries are velocity fields characterized by the vanishing of the symmetric part of their spatial derivative. A formal statement of this principle, denoting by V_{RIG} the linear space of infinitesimal isometries from the current placement $\varphi(\mathbb{M})$, is expressed by the variational condition

$$\langle \mathbf{f}, \mathbf{v} \rangle = 0, \quad \forall \mathbf{v} \in V_{\text{RIG}}.$$

Let $\psi_{\tau,t} \in C^1(\varphi(\mathbb{M}); \mathbb{S})$ be a virtual spatial flow of the body \mathbb{M} starting from $\varphi(\mathbb{M})$ at the (pseudo) time t , that is such that

$$(\psi_{t,t} \circ \varphi)(\mathbf{m}) = \varphi(\mathbf{m}), \quad \forall \mathbf{m} \in \mathbb{M}.$$

The initial velocity field $\mathbf{v} \in \mathbb{T}_{\varphi(\mathbb{M})}\mathbb{S}$ of the virtual flow $\psi_{\tau,t}$ is defined by:

$$\mathbf{v} = \dot{\psi} = \left. \frac{d}{d\tau} \right|_{\tau=t} \psi_{\tau,t},$$

and we set $\dot{\varphi} := \mathbf{v} \circ \varphi$. An infinitesimal isometry is characterized by the vanishing of the Lie derivative of the space metric tensor, defined by

$$\mathcal{L}_{\mathbf{v}}\mathbf{g} := (\dot{\psi}^*\mathbf{g}) := \left. \frac{d}{d\tau} \right|_{\tau=t} \psi_{\tau,t}^*\mathbf{g}.$$

In a riemannian manifold with Levi-Civita connection ∇ we have that

$$\frac{1}{2}\mathcal{L}_{\mathbf{v}}\mathbf{g} = \mathbf{g}(\text{sym } \nabla \mathbf{v}).$$

In particular this formula holds in the euclidean space $\{\mathbb{S}, \mathbf{g}\}$ with ∇ denoting the ordinary derivative. Since the differential operator $\text{sym } \nabla$ fulfills Korn's inequality, its range is closed and its kernel is finite dimensional if a suitable topology is chosen in the kinematical space^{12,15}. In essence, we need a pre-hilbertian topology which

requires that the kinematic fields \mathbf{v} be square integrable on the current placement $\varphi(\mathbb{M})$ and that the tangent deformation $\mathit{sym} \nabla \mathbf{v}$ be a piecewise square integrable distribution on $\varphi(\mathbb{M})$ on a patchwork $\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))$ of nonoverlapping submanifolds covering $\varphi(\mathbb{M})$. This patchwork may vary from one kinematic field to another one and is dubbed the regularity patchwork of the kinematic field. The pre-Hilbert space endowed with the topology induced by the mean square norm of the kinematic fields and of the regular part of the corresponding tangent deformation is denoted by $\mathcal{V}_{\varphi(\mathbb{M})}$, or simply by \mathcal{V} . The subspace $V_{\text{RIG}} \subset \mathcal{V}$ of rigid kinematic fields is characterized by the property that $\mathit{sym} \nabla \mathbf{v}$ vanishes on every element of the regularity patchwork $\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))$. Force systems acting on the body at the placement $\varphi(\mathbb{M})$ belong to the linear topological dual space \mathcal{V}^* of \mathcal{V} . The kinematic fields $\mathbf{v} \in \mathcal{V}$ which share a common regularity patchwork $\mathcal{T}(\varphi(\mathbb{M}))$ form a linear closed subspace $\mathcal{V}(\mathcal{T}(\varphi(\mathbb{M})))$, or simply $\mathcal{V}_{\mathcal{T}}$, dubbed the \mathcal{T} -conformity kinematic space. By adding homogeneous boundary conditions on $\partial\mathcal{T}(\varphi(\mathbb{M}))$, by means of bounded linear operators, we define a closed subspace $\mathcal{L}(\mathcal{T}(\varphi(\mathbb{M})))$, briefly $\mathcal{L}_{\mathcal{T}}$, dubbed the conformity kinematic space. Hence $\mathcal{L}_{\mathcal{T}} \subset \mathcal{V}_{\mathcal{T}}$ is a Hilbert space for the topology inherited by \mathcal{V} . A load system $\ell \in \mathcal{L}_{\mathcal{T}}^*$ acting on the body placed at $\varphi(\mathbb{M})$, is an element of the Hilbert space $\mathcal{L}_{\mathcal{T}}^*$ topological dual of $\mathcal{L}_{\mathcal{T}}$. If the load $\ell \in \mathcal{L}_{\mathcal{T}}^*$ meets the equilibrium condition

$$\langle \ell, \mathbf{v} \rangle = 0, \quad \forall \mathbf{v} \in \mathcal{L}_{\mathcal{T}} \cap V_{\text{RIG}},$$

the Stefan Banach's closed range theorem¹⁷ ensures then that there exists a (\mathbb{M} -square integrable) field of Lagrange multipliers \mathbf{T} (a Cauchy stress field), whose point-values are \mathbf{g} -symmetric operators $\mathbf{T}(\mathbf{m}) \in BL(\mathbb{T}_{\varphi(\mathbf{m})}\mathbb{S}; \mathbb{T}_{\varphi(\mathbf{m})}\mathbb{S})$ on $\varphi(\mathbb{M})$, fulfilling the virtual work identity

$$\langle \ell, \mathbf{v} \rangle = \int_{\mathcal{T}(\varphi(\mathbb{M}))} \langle \mathbf{T}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \boldsymbol{\mu}, \quad \forall \mathbf{v} \in \mathcal{L}_{\mathcal{T}}.$$

We emphasize that the assumption of \mathbf{g} -symmetry of Cauchy stress fields is a natural choice due to the symmetry of the tangent deformation operator $\mathit{sym} \nabla \mathbf{v}$ and *not* a provable theorem, as claimed in most treatments of continuum mechanics. Simply the choice of non \mathbf{g} -symmetric Cauchy stress fields is not a convenient one, since the ineffective skew-symmetric part of it does not perform virtual work for the symmetric tangent deformation operator. Moreover integration by parts leads to a representation of the force system which includes body couples per unit volume equal to the skew-symmetric part of the stress field¹³. Let the load $\ell \in \mathcal{L}_{\mathcal{T}}^*$ be composed by a body force field $\mathbf{b} \in \mathcal{L}^2(\varphi(\mathbb{M}); V)$ and by a boundary traction field $\mathbf{t} \in \mathcal{L}^2(\partial\mathcal{T}(\varphi(\mathbb{M})); V)$, according to the definition

$$\langle \ell, \mathbf{v} \rangle := \int_{\mathcal{T}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{b}, \mathbf{v}) \boldsymbol{\mu} + \int_{\partial\mathcal{T}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{t}, \mathbf{v}) \boldsymbol{\mu}, \quad \forall \mathbf{v} \in \mathcal{V}.$$

Any stress field \mathbf{T} in equilibrium with ℓ has then a distributional divergence with a ($\varphi(\mathbb{M})$ -square integrable) regular part $\text{div} \mathbf{T} = -\mathbf{b}$ ¹³.

Since the virtual work

$$\int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \langle \mathbf{T}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \boldsymbol{\mu}, \quad \mathbf{v} \in \mathcal{V},$$

is well-defined for any (nonconforming) kinematic field $\mathbf{v} \in \mathcal{V}$, by making recourse to GREEN's formula

$$\int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \langle \mathbf{T}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \boldsymbol{\mu} = \int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{g}(-\operatorname{div} \mathbf{T}, \mathbf{v}) \boldsymbol{\mu} + \int_{\partial \mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{T} \mathbf{n}, \mathbf{v}) \boldsymbol{\mu},$$

where \mathbf{n} is the outward unit normal, we may define the reactive force system $\mathbf{r}(\mathbf{t}, \mathbf{T})$ by the relation

$$\begin{aligned} \langle \mathbf{r}, \mathbf{v} \rangle &:= \int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \langle \mathbf{T}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \boldsymbol{\mu} - \int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{b}, \mathbf{v}) \boldsymbol{\mu} - \int_{\partial \mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{t}, \mathbf{v}) \boldsymbol{\mu} \\ &= \int_{\partial \mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{T} \mathbf{n} - \mathbf{t}, \mathbf{v}) \boldsymbol{\mu}. \end{aligned}$$

From the virtual work identity we infer the well-known characteristic property of linear constraints:

$$\langle \mathbf{r}, \mathbf{v} \rangle = \int_{\partial \mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{g}(\mathbf{T} \mathbf{n} - \mathbf{t}, \mathbf{v}) \boldsymbol{\mu} = 0, \quad \forall \mathbf{v} \in \mathcal{L}_{\mathcal{T}}.$$

2.3 Referential dynamical equilibrium

Recalling the formula $\frac{1}{2} \mathcal{L}_{\mathbf{v}} \mathbf{g} = \mathbf{g}(\mathit{sym} \nabla \mathbf{v})$, the pull-back of the tangent deformation operator from the actual placement $\varphi(\mathbb{M})$ to the reference one \mathbb{M} is provided by

$$\begin{aligned} \varphi^*(\mathbf{g}(\mathit{sym} \nabla \mathbf{v})) &= \varphi^*(\frac{1}{2} \mathcal{L}_{\mathbf{v}} \mathbf{g}) = \frac{1}{2} (\varphi^* \mathbf{g})' = \frac{1}{2} (\mathbf{g}(d\varphi^T d\varphi))' \\ &= \mathbf{g}(\mathit{sym} (d\varphi^T d(\mathbf{v} \circ \varphi))), \end{aligned}$$

being $(d\varphi)'(\mathbf{m}) = d(\mathbf{v} \circ \varphi)(\mathbf{m})$.

To leave the virtual work invariant, the pull back of the Cauchy stress field must be performed in a contravariant way. To this end we introduce the \mathbf{g} -symmetric Kirchhoff stress $\mathbf{K}(\mathbf{m}) \in BL(\mathbb{T}_{\varphi(\mathbf{m})} \mathbb{S}; \mathbb{T}_{\varphi(\mathbf{m})} \mathbb{S})$ by the formula $\mathbf{K} := \mathbf{J}_{\varphi} \mathbf{T}$, where $\mathbf{J}_{\varphi} = \det(d\varphi)$ is the Jacobian of the configuration map. The Piola-Kirchhoff stress $\mathbf{S}(\mathbf{m}) \in BL(\mathbb{T}_{\mathbf{m}} \mathbb{M}; \mathbb{T}_{\mathbf{m}} \mathbb{M})$ is then defined by imposing the invariance:

$$\langle \mathbf{K}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \circ \varphi = \langle \mathbf{S}, \mathit{sym} (d\varphi^T d(\mathbf{v} \circ \varphi)) \rangle_{\mathbf{g}} = \langle \mathbf{S}, d\varphi^T \mathit{sym} (\nabla \mathbf{v}) d\varphi \rangle_{\mathbf{g}},$$

since, by the chain rule, we have that $d(\mathbf{v} \circ \varphi)(\mathbf{m}) = \nabla \mathbf{v}(\varphi(\mathbf{m})) d\varphi(\mathbf{m})$.

The (\mathbf{g} -symmetric) Piola-Kirchhoff stress is then related to the Kirchhoff stress by the correspondence:

$$\mathbf{K} \circ \varphi = d\varphi \mathbf{S} d\varphi^T \quad \Longleftrightarrow \quad \mathbf{S} = d\varphi^{-1} (\mathbf{K} \circ \varphi) d\varphi^{-T},$$

and the virtual work identity may be written as

$$\begin{aligned}
 \langle \mathbf{f}, \mathbf{v} \rangle &= \int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \langle \mathbf{T}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \boldsymbol{\mu} \\
 &= \int_{\mathcal{T}_{\mathbf{v}}(\varphi(\mathbb{M}))} \mathbf{J}_{\varphi}^{-1} \langle \mathbf{K}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \boldsymbol{\mu} \\
 &= \int_{\mathcal{T}_{(\mathbf{v} \circ \varphi)}(\mathbb{M})} (\langle \mathbf{K}, \mathit{sym} \nabla \mathbf{v} \rangle_{\mathbf{g}} \circ \varphi) \boldsymbol{\mu} \\
 &= \int_{\mathcal{T}_{(\mathbf{v} \circ \varphi)}(\mathbb{M})} \langle \mathbf{S}, \tfrac{1}{2}(d\varphi^T d\varphi) \rangle_{\mathbf{g}} \boldsymbol{\mu} \\
 &= \int_{\mathcal{T}_{(\mathbf{v} \circ \varphi)}(\mathbb{M})} \langle d\varphi \mathbf{S}, (d\varphi) \rangle_{\mathbf{g}} \boldsymbol{\mu}.
 \end{aligned}$$

By assuming that the divergence field $\operatorname{div}(d\varphi \mathbf{S})$ be piecewise square integrable according to a partition $\mathcal{T}_{\operatorname{div}}$, the Green's formula (integration by parts) yields

$$\begin{aligned}
 \langle \mathbf{f}, \mathbf{v} \rangle &= \int_{\mathcal{T}(\mathbb{M})} \langle d\varphi \mathbf{S}, (d\varphi) \rangle_{\mathbf{g}} \boldsymbol{\mu} \\
 &= - \int_{\mathcal{T}(\mathbb{M})} \langle \operatorname{div}(d\varphi \mathbf{S}), \dot{\varphi} \rangle_{\mathbf{g}} \boldsymbol{\mu} + \int_{\partial\mathcal{T}(\mathbb{M})} \langle (d\varphi \mathbf{S}) \mathbf{n}, \dot{\varphi} \rangle_{\mathbf{g}} (\boldsymbol{\mu} \mathbf{n})
 \end{aligned}$$

where $\mathcal{T}(\mathbb{M})$ is a partition finer than both $\mathcal{T}_{\operatorname{div}}$ and $\mathcal{T}_{(\mathbf{v} \circ \varphi)}$, and $\boldsymbol{\mu} \mathbf{n}$ is the area-form induced on $\partial\mathbb{M}$ by the volume-form $\boldsymbol{\mu}$ on \mathbb{M} according to the relation

$$(\boldsymbol{\mu} \mathbf{n})(\mathbf{a}, \mathbf{b}) := \boldsymbol{\mu}(\mathbf{n}, \mathbf{a}, \mathbf{b}), \quad \forall \mathbf{a}, \mathbf{b} \in \mathbb{T}_{\mathbf{m}} \partial\mathbb{M}.$$

The system of referential forces may then be represented by a field of body forces $-\operatorname{div}(d\varphi \mathbf{S})$ and a field of surface tractions $(d\varphi \mathbf{S}) \mathbf{n}$. In terms of the Piola stress field $\mathbf{P} := d\varphi \mathbf{S}$ they may be rewritten as $-\operatorname{div} \mathbf{P}$ and $\mathbf{P} \mathbf{n}$.

2.4 Constitutive behavior

We assume that the constitutive behavior of a single-phase material body¹⁶ is characterized by a natural placement \mathbb{M} , which is a differentiable submanifold of the euclidean space $\{\mathbb{S}, \mathbf{g}\}$, a metric tensor field $\mathbf{g}_{\mathbb{M}} \in BL(\mathbb{T}\mathbb{M}, \mathbb{T}\mathbb{M}; \mathcal{R})$, which describes the *anelastic* deformation of the body and a scalar field $W \in C^1(\mathbb{M}; \mathcal{R})$, which provides the Helmholtz free energy per unit volume in \mathbb{M} . At each material point $\mathbf{m} \in \mathbb{M}$, the free energy density is assumed to be a differentiable function of the configuration-induced metric and of the anelastic metric:

$$W_{\mathbf{m}}(\varphi^* \mathbf{g}, \mathbf{g}_{\mathbb{M}}).$$

Evolutionary processes in which the anelastic metric tensor field $\mathbf{g}_{\mathbb{M}}$ does not change are said to be *purely elastic*.

2.4.1 Phase transition

To describe the evolution of phase transition phenomena in multi-phase material bodies, we consider a partition of the natural placement \mathbb{M} of the body into a finite family $\mathcal{T}(\mathbb{M})$ of non-overlapping submanifolds. Each element of the partition $\mathcal{T}(\mathbb{M})$ is constituted by a single-phase material whose constitutive properties are described by a functional dependence of the free energy density on a scalar field $p \in \mathcal{R}$. Accordingly the free energy density of the multi-phase material is assumed to be functionally dependent on a scalar field $p : \mathbb{M} \mapsto \mathcal{R}$ which is piecewise constant on \mathbb{M} according to the given partition. We then assume for the free energy density the functional dependence

$$W_{\mathbf{m}}(\boldsymbol{\varphi}^* \mathbf{g}, \mathbf{g}_{\mathbb{M}}, p),$$

the separate dependence on \mathbf{m} allowing for each single-phase to be non-homogeneous. The global free energy of the body is then given by

$$\mathbf{E}(\boldsymbol{\varphi}^* \mathbf{g}, \mathbf{g}_{\mathbb{M}}, p) := \int_{\mathbb{M}} W_{\mathbf{m}}(\boldsymbol{\varphi}^* \mathbf{g}, \mathbf{g}_{\mathbb{M}}, p) \boldsymbol{\mu}.$$

The evolution of phase transition is described by a flow $\boldsymbol{\chi}_{\tau,t} \in C^1(\mathbb{M}; \mathbb{M})$ which modifies the reference partition $\mathcal{T}(\mathbb{M})$ into an evolving one $\boldsymbol{\chi}_{\tau,t}(\mathcal{T}(\mathbb{M}))$ at time $\tau \in I$. During the evolution, the time dependent phase-labeling field $p_{\tau} : \mathbb{M} \mapsto \mathcal{R}$ retains its constant value in each element of the partition, at any time:

$$p_{\tau} = p_t \circ \boldsymbol{\chi}_{t,\tau}, \quad \forall \tau \in I.$$

2.4.2 Elastic energy rate due to phase transition evolution

To provide a mathematical formulation of the dissipation phenomena due to phase transition, we consider a virtual motion of the body in the ambient space \mathbb{S} described by a flow $\boldsymbol{\psi}_{\tau,t} \in C^1(\boldsymbol{\varphi}(\mathbb{M}); \mathbb{S})$ starting at the current configuration $\boldsymbol{\varphi} \in C^1(\mathbb{M}; \mathbb{S})$ at time $t \in I$. The time dependence of the free energy density is expressed by

$$W_{\tau} := W((\boldsymbol{\psi}_{\tau,t} \circ \boldsymbol{\varphi})^* \mathbf{g}, \mathbf{g}_{\mathbb{M}_{\tau}}, p_t \circ \boldsymbol{\chi}_{t,\tau}),$$

and the free energy of the body at time $\tau \in I$ is

$$\mathbf{E}_{\tau} := \int_{\mathbb{M}} W_{\tau} \boldsymbol{\mu}.$$

Let us now evaluate the time-rate of the free energy of the body.

In this respect it is important to notice that the time derivative of the free energy density W_{τ} cannot be performed in a classical way since the configuration-induced metric $(\boldsymbol{\psi}_{\tau,t} \circ \boldsymbol{\varphi})^* \mathbf{g}$ and the phase-describing field $p_t \circ \boldsymbol{\chi}_{t,\tau}$ undergo a jump at the points $\mathbf{m} \in \mathbb{M}$ which are crossed by the evolving interfaces at time $\tau \in I$. The corresponding Dirac's impulses at the interfaces may be conveniently evaluated by adopting the following procedure. By additivity, the integral over \mathbb{M} is written as the sum of integrals over the elements \mathcal{P}_{τ} of the partition $\mathcal{T}_{\tau}(\mathbb{M}) = \boldsymbol{\chi}_{\tau,t}(\mathcal{T}(\mathbb{M}))$ at time $\tau \in I$:

$$\mathbf{E}_{\tau} = \int_{\mathcal{T}_{\tau}(\mathbb{M})} W_{\tau} \boldsymbol{\mu} := \sum \int_{\mathcal{P}_{\tau}} W_{\tau} \boldsymbol{\mu}.$$

Then the time derivative is evaluated by making recourse to the transport formula:

$$\partial_{\tau=t} \int_{\mathcal{P}_\tau} W_\tau \boldsymbol{\mu} = \int_{\mathcal{P}} \dot{W} \boldsymbol{\mu} + \int_{\mathcal{P}} \mathcal{L}_{\dot{\boldsymbol{\chi}}}(W \boldsymbol{\mu}).$$

where $\mathcal{L}_{\dot{\boldsymbol{\chi}}}(W \boldsymbol{\mu})$ is the Lie derivative of the free energy volume-form $W \boldsymbol{\mu}$ along the phase-transition describing flow $\boldsymbol{\chi}_{\tau,t} \in C^1(\mathbb{M}; \mathbb{M})$, starting at time $t \in I$ with propagation speed $\dot{\boldsymbol{\chi}} \in C^1(\mathbb{M}; \mathbb{TM})$. By the formula¹⁴ $\mathcal{L}_{\dot{\boldsymbol{\chi}}}(W \boldsymbol{\mu}) = \mathcal{L}_{(W \dot{\boldsymbol{\chi}})} \boldsymbol{\mu} = \operatorname{div}(W \dot{\boldsymbol{\chi}}) \boldsymbol{\mu}$ and the divergence theorem, we get the expression

$$\begin{aligned} \dot{\mathbf{E}} &= \int_{\mathcal{T}(\mathbb{M})} \dot{W} \boldsymbol{\mu} + \int_{\mathcal{T}(\mathbb{M})} \mathcal{L}_{\dot{\boldsymbol{\chi}}}(W \boldsymbol{\mu}) = \int_{\mathcal{T}(\mathbb{M})} \dot{W} \boldsymbol{\mu} + \int_{\mathcal{T}(\mathbb{M})} \mathcal{L}_{(W \dot{\boldsymbol{\chi}})} \boldsymbol{\mu} \\ &= \int_{\mathcal{T}(\mathbb{M})} \dot{W} \boldsymbol{\mu} + \int_{\mathcal{T}(\mathbb{M})} \operatorname{div}(W \dot{\boldsymbol{\chi}}) \boldsymbol{\mu} = \int_{\mathcal{T}(\mathbb{M})} \dot{W} \boldsymbol{\mu} + \int_{\partial \mathcal{T}(\mathbb{M})} W \mathbf{g}(\dot{\boldsymbol{\chi}}, \mathbf{n})(\boldsymbol{\mu} \mathbf{n}), \end{aligned}$$

where $\boldsymbol{\mu} \mathbf{n}$ is the area-form induced on the surfaces $\partial \mathcal{T}(\mathbb{M})$ by the volume form $\boldsymbol{\mu}$ in \mathbb{M} . Since the flow $\boldsymbol{\chi}_{\tau,t} \in C^1(\mathbb{M}; \mathbb{M})$ leaves the boundary $\partial \mathbb{M}$ invariant, we have that $\mathbf{g}(\dot{\boldsymbol{\chi}}, \mathbf{n}) = 0$ on $\partial \mathbb{M}$.

Then, defining the jump $[[W]] = W^+ - W^-$ across the phase-transition interfaces and setting $\mathbf{n} = \mathbf{n}^-$, the outward normal to $\partial \mathcal{P}^-$, we get the final result:

$$\dot{\mathbf{E}} = \int_{\mathcal{T}(\mathbb{M})} \dot{W} \boldsymbol{\mu} - \int_{\mathcal{I}} [[W]] v_{\boldsymbol{\chi}}(\boldsymbol{\mu} \mathbf{n}),$$

where \mathcal{I} is the set of phase-transition interfaces traveling with normal speed $v_{\boldsymbol{\chi}} = \mathbf{g}(\dot{\boldsymbol{\chi}}, \mathbf{n})$. Since the normal speed points towards the \mathcal{P}^+ phase, the impulsive term, provided by the integral over the interfaces, measures the rate of decrease of the free energy due to the motion of phase-transition fronts.

2.5 Dissipation due to phase transition

Phase-transition phenomena are characterized by the continuity of the configuration map with a possible finite jump of its differential across the transition fronts. These singular surfaces are shock-waves and their propagation requires a dissipation of energy.

2.5.1 Kinematics of shock waves

To deal with discontinuity surfaces traveling in the material body, it is compelling to consider the general case in which the configuration map $\boldsymbol{\varphi} \in C^0(\mathbb{M}; \mathbb{S}) \cap C^1(\mathcal{T}(\mathbb{M}); \mathbb{S})$ is continuous on \mathbb{M} and continuously differentiable in each element of the partition $\mathcal{T}(\mathbb{M})$ whose interfaces may travel in the material according to a flow $\boldsymbol{\chi}_{\tau,t} \in C^1(\mathbb{M}; \mathbb{M})$. By continuity, the derivatives of $\boldsymbol{\varphi}$ along tangent directions on each side of the interfaces \mathcal{I} of $\mathcal{T}(\mathbb{M})$ are equal:

$$d_{\mathbf{t}} \boldsymbol{\varphi}^+(\mathbf{m}) = d_{\mathbf{t}} \boldsymbol{\varphi}^-(\mathbf{m}), \quad \forall \mathbf{t} \in \mathbb{T}_{\mathbf{m}} \mathcal{I}.$$

It follows that the differential $d\boldsymbol{\varphi}(\mathbf{m}) \in BL(\mathbb{T}_{\mathbf{m}} \mathbb{M}; \mathbb{T}_{\boldsymbol{\varphi}(\mathbf{m})} \mathbb{S})$ must meet at the interfaces the *Maxwell jump condition*:

$$[[d\boldsymbol{\varphi}]] = [[d\boldsymbol{\varphi}]] \mathbf{n} \otimes \mathbf{n}.$$

Then, across a shock wave front, the configuration map is continuous and its differential may undergo a finite jump. The spatial speed $(\varphi \circ \chi)'$ of the points traveling on the shock wave, propagating in the material with speed $\dot{\chi} \in C^1(\mathbb{M}; \mathbb{T}\mathbb{M})$, may be evaluated, by the Leibniz rule, on each side of the shock wave to get:

$$(\varphi \circ \chi)' = \dot{\varphi} + d_{\dot{\chi}}\varphi = \mathbf{v} \circ \varphi + d_{\dot{\chi}}\varphi.$$

Since the l.h.s. is continuous across the interface, the following jump condition must be met:

$$[[\mathbf{v}]] \circ \varphi + [[d\varphi]] \dot{\chi} = 0.$$

From the Maxwell jump condition we then get the *Hadamard condition* for shock waves:

$$[[\mathbf{v}]] \circ \varphi + v_{\dot{\chi}} [[d\varphi]] \mathbf{n} = 0.$$

This condition tells us that the velocity field will undergo, across the shock wave front, a finite jump equal to the opposite of the finite jump of the normal derivative of the configuration map times the normal speed of propagation of the shock wave. As shown below, the Hadamard condition plays a basic role in the evaluation of the dissipation induced by evolving phase transition interfaces.

2.5.2 Evolution problem

The equilibrium of the body at the current configuration is expressed by the virtual work condition, which, in the reference placement, is written as

$$\langle \mathbf{f}, \mathbf{v} \rangle = \int_{\mathcal{T}(\mathbf{v} \circ \varphi)(\mathbb{M})} \langle \mathbf{S}, \mathbf{D}(\varphi)' \rangle_{\mathbf{g}} \mu, \quad \forall \mathbf{v} \in \mathcal{V}$$

where $\mathbf{v} = \dot{\psi} \in \mathcal{V}$ is the initial speed along the virtual trajectory described by the flow $\psi_{\tau,t} \in C^1(\varphi(\mathbb{M}); \mathbb{S})$ and $\mathbf{D}(\varphi)' := \partial_{\tau=t}(\mathbf{D}(\psi_{\tau,t} \circ \varphi))$.

Let us now assume that the virtual speed $\mathbf{v} \in \mathcal{V}$ be compatible with the normal speed of the phase-transition interfaces traveling according to the flow $\chi_{\tau,t} \in C^1(\mathbb{M}; \mathbb{M})$. This means that the phase-describing partition $\mathcal{T}(\mathbb{M})$ is a regularity patchwork for the virtual speed $\mathbf{v} \in C^1(\mathcal{T}(\mathbb{M}); \mathbb{S})$ and that it fulfils the Hadamard condition for shock waves:

$$[[\mathbf{v}]] \circ \varphi + v_{\dot{\chi}} [[d\varphi]] \mathbf{n} = 0,$$

at the interfaces \mathcal{I} of the partition $\mathcal{T}(\mathbb{M})$. Let us express the free energy in terms of operators $W(\mathbf{D}(\varphi), \Delta, p)$, with $\mathbf{g}\Delta = \mathbf{g}_{\mathbb{M}}$. The equilibrium condition is then obtained by imposing the constitutive requirement $\mathbf{S} = d_1 W$ and setting $\mathbf{S}_{\mathbb{M}} := -d_2 W$. The time derivative in each element \mathcal{P} of $\mathcal{T}(\mathbb{M})$ is given by

$$\begin{aligned} (W(\mathbf{D}(\varphi), \Delta, p))' &:= \partial_{\tau=t}(W(\mathbf{D}(\psi_{\tau,t} \circ \varphi), \Delta_{\tau}, p_{\tau})) \\ &= \langle d_1 W, \mathbf{D}(\varphi)' \rangle_{\mathbf{g}} + \langle d_2 W, \dot{\Delta} \rangle_{\mathbf{g}} \\ &= \langle \mathbf{S}, \mathbf{D}(\varphi)' \rangle_{\mathbf{g}} - \langle \mathbf{S}_{\mathbb{M}}, \dot{\Delta} \rangle_{\mathbf{g}}, \end{aligned}$$

since $\dot{p} = 0$ due to the constancy of p_{τ} in each \mathcal{P}_{τ} at any time $\tau \in I$.

The equilibrium condition may then be written as

$$\begin{aligned}\langle \mathbf{f}, \mathbf{v} \rangle &= \int_{\mathcal{T}(\mathbb{M})} \langle \mathbf{S}, \mathbf{D}(\boldsymbol{\varphi}) \rangle_{\mathbf{g}} \boldsymbol{\mu} \\ &= \int_{\mathcal{T}(\mathbb{M})} \dot{W} \boldsymbol{\mu} + \int_{\mathbb{M}} \langle \mathbf{S}_{\mathbb{M}}, \dot{\boldsymbol{\Delta}} \rangle_{\mathbf{g}} \boldsymbol{\mu} \\ &= \dot{\mathbf{E}} + \int_{\mathcal{I}} [[W]] v_{\chi}(\boldsymbol{\mu}\mathbf{n}) + \int_{\mathbb{M}} \langle \mathbf{S}_{\mathbb{M}}, \dot{\boldsymbol{\Delta}} \rangle_{\mathbf{g}} \boldsymbol{\mu}.\end{aligned}$$

The virtual work of the force system acting on the body can be split into the sum of two contributions. The former is the virtual work performed by the loading $\ell \in \mathcal{L}_{\mathcal{T}}^*$ in correspondence of the virtual velocity $\mathbf{v} \circ \boldsymbol{\varphi} \in C^1(\mathcal{T}(\mathbb{M}); \mathbb{S})$. The latter is the virtual work performed by the reactive forces \mathbf{r} acting on the faces of each phase-transition interface due to the finite jump of the virtual velocity across the phase-transition interfaces:

$$\langle \mathbf{f}, \mathbf{v} \rangle = \langle \ell, \mathbf{v} \rangle + \langle \mathbf{r}, \mathbf{v} \rangle.$$

The boundary equilibrium condition at the interfaces implies that $[[\mathbf{P}\mathbf{n}]] = 0$, and hence the reactive term is given by

$$\langle \mathbf{r}, \mathbf{v} \rangle = - \int_{\mathcal{I}} [[\langle \mathbf{P}\mathbf{n}, \mathbf{v} \circ \boldsymbol{\varphi} \rangle]]_{\mathbf{g}}(\boldsymbol{\mu}\mathbf{n}) = - \int_{\mathcal{I}} \langle \mathbf{P}\mathbf{n}, [[\mathbf{v}]] \circ \boldsymbol{\varphi} \rangle_{\mathbf{g}}(\boldsymbol{\mu}\mathbf{n}).$$

The minus sign above is due to the usual notation $[[\mathbf{v}]] = \mathbf{v}^+ - \mathbf{v}^-$ with $\mathbf{n} = \mathbf{n}^-$ the outward normal to $\partial\mathcal{P}^-$. The equilibrium condition may then be written as

$$\langle \ell, \mathbf{v} \rangle = \dot{\mathbf{E}} + \int_{\mathcal{I}} [[W]] v_{\chi}(\boldsymbol{\mu}\mathbf{n}) + \int_{\mathcal{I}} \langle \mathbf{P}\mathbf{n}, [[\mathbf{v}]] \circ \boldsymbol{\varphi} \rangle_{\mathbf{g}}(\boldsymbol{\mu}\mathbf{n}) + \int_{\mathbb{M}} \langle \mathbf{S}_{\mathbb{M}}, \dot{\boldsymbol{\Delta}} \rangle_{\mathbf{g}} \boldsymbol{\mu}.$$

Imposing the fulfilment of Hadamard's condition for shock waves at the interfaces \mathcal{I} of phase-transition:

$$[[\mathbf{v}]] \circ \boldsymbol{\varphi} + v_{\chi} [[d\boldsymbol{\varphi}]] \mathbf{n} = 0.$$

we get the following formula for the virtual power balance law:

$$\langle \ell, \mathbf{v} \rangle = \dot{\mathbf{E}} + \int_{\mathcal{I}} ([[W]] - \mathbf{g}(\mathbf{P}\mathbf{n}, [[d\boldsymbol{\varphi}]] \mathbf{n})) v_{\chi}(\boldsymbol{\mu}\mathbf{n}) + \int_{\mathbb{M}} \langle \mathbf{S}_{\mathbb{M}}, \dot{\boldsymbol{\Delta}} \rangle_{\mathbf{g}} \boldsymbol{\mu},$$

to hold for all spatial speed $\mathbf{v} \in C^1(\mathcal{T}(\mathbb{M}); \mathbb{S})$ and for all phase-transition speed $\dot{\boldsymbol{\chi}} \in C^1(\mathbb{M}; \mathbb{T}\mathbb{M})$ fulfilling Hadamard's condition.

Now, observing that $W = \mathbf{g}(W\mathbf{n}, \mathbf{n})$, we introduce the Eshelby's tensor:

$$\mathbf{Y} := W\mathbf{I} - d\boldsymbol{\varphi}^T \mathbf{P} = W\mathbf{I} - d\boldsymbol{\varphi}^T d\boldsymbol{\varphi} \mathbf{S},$$

and write the virtual power balance law as

$$\langle \ell, \mathbf{v} \rangle = \dot{\mathbf{E}} + \int_{\mathcal{I}} \mathbf{g}([[Y]]\mathbf{n}, \mathbf{n}) v_{\chi}(\boldsymbol{\mu}\mathbf{n}) + \int_{\mathbb{M}} \langle \mathbf{S}_{\mathbb{M}}, \dot{\boldsymbol{\Delta}} \rangle_{\mathbf{g}} \boldsymbol{\mu}.$$

Then from the properties

$$\begin{aligned} \mathbf{g}(\mathbf{n}, \mathbf{t}) = 0 &\implies \mathbf{g}([[W]] \mathbf{n}, \mathbf{t}) = [[W]] \mathbf{g}(\mathbf{n}, \mathbf{t}) = 0, \\ \mathbf{g}(\mathbf{n}, \mathbf{t}) = 0 &\implies \mathbf{g}([[d\boldsymbol{\varphi}^T]] \mathbf{P}\mathbf{n}, \mathbf{t}) = \mathbf{g}(\mathbf{P}\mathbf{n}, [[d\boldsymbol{\varphi}]] \mathbf{t}) \\ &= \mathbf{g}(\mathbf{P}\mathbf{n}, [[d\boldsymbol{\varphi}]] (\mathbf{n} \otimes \mathbf{n}) \mathbf{t}) = \mathbf{g}(\mathbf{P}\mathbf{n}, [[d\boldsymbol{\varphi}]] \mathbf{n}) \mathbf{g}(\mathbf{n}, \mathbf{t}) = 0, \end{aligned}$$

the latter being a consequence of Maxwell jump condition, we infer that

$$\mathbf{g}(\mathbf{n}, \mathbf{t}) = 0 \implies \mathbf{g}([[Y]] \mathbf{n}, \mathbf{t}) = 0,$$

that is, the flux of the jump of Eshelby's tensor at an interface is directed along the normal to the interface. Hence, being $v_{\boldsymbol{\chi}} = \mathbf{g}(\boldsymbol{\chi}, \mathbf{n})$, we infer the equality

$$\mathbf{g}([[Y]] \mathbf{n}, \mathbf{n}) v_{\boldsymbol{\chi}} = \mathbf{g}([[Y]] \mathbf{n}, \dot{\boldsymbol{\chi}}),$$

and the virtual power balance law may be rewritten as

$$\langle \ell, \mathbf{v} \rangle = \dot{\mathbf{E}} + \int_{\mathcal{I}} \mathbf{g}([[Y]] \mathbf{n}, \dot{\boldsymbol{\chi}}) (\boldsymbol{\mu} \mathbf{n}) + \int_{\mathbb{M}} \langle \mathbf{S}_{\mathbb{M}}, \dot{\boldsymbol{\Delta}} \rangle_{\mathbf{g}} \boldsymbol{\mu}.$$

This result may be phrased by stating that the (virtual) power performed by the applied load is equal to the (virtual) increase in free energy plus the (virtual) dissipation due to the evolution of phase transition and to the anelastic deformation rate. In the actual motion, we get a mechanical statement of the principle of conservation of the power expended.

Remark

Eshelby's tensor $\mathbf{Y} = W\mathbf{I} - d\boldsymbol{\varphi}^T d\boldsymbol{\varphi} \mathbf{S}$ is not \mathbf{g} -symmetric, but symmetry holds with respect to the metric $(d\boldsymbol{\varphi}^T \mathbf{g})(\mathbf{m}) \in BL(\mathbb{T}_{\mathbf{m}}\mathbb{M}, \mathbb{T}_{\mathbf{m}}\mathbb{M}; \mathcal{R})$ defined at $\mathbf{m} \in \mathbb{M}$ by

$$(d\boldsymbol{\varphi}^T \mathbf{g})(\mathbf{a}, \mathbf{b}) := \mathbf{g}(d\boldsymbol{\varphi}^{-T} \mathbf{a}, d\boldsymbol{\varphi}^{-T} \mathbf{b}), \quad \forall \mathbf{a}, \mathbf{b} \in \mathbb{T}_{\mathbf{m}}(\mathbb{M}).$$

This property is a direct consequence of the \mathbf{g} -symmetry of the Piola-Kirchhoff stress tensor \mathbf{S} since

$$(d\boldsymbol{\varphi}^T \mathbf{g})(d\boldsymbol{\varphi}^T d\boldsymbol{\varphi} \mathbf{S} \mathbf{a}, \mathbf{b}) = \mathbf{g}(d\boldsymbol{\varphi}^{-T} d\boldsymbol{\varphi}^T d\boldsymbol{\varphi} \mathbf{S} \mathbf{a}, d\boldsymbol{\varphi}^{-T} \mathbf{b}) = \mathbf{g}(\mathbf{S} \mathbf{a}, \mathbf{b}).$$

Eshelby's tensor is then symmetrizable and enjoys all the useful properties of a symmetric operator: it has a spectral representation with real eigenvalues since there exists in $\mathbb{T}_{\mathbf{m}}\mathbb{M}$ a principal basis of mutually orthogonal eigenvectors according to the metric $(d\boldsymbol{\varphi}^T \mathbf{g})(\mathbf{m})$. Setting $\mathbf{C} = d\boldsymbol{\varphi}^T d\boldsymbol{\varphi}$ the symmetry of Eshelby's tensor can be written as $\mathbf{Y}\mathbf{C} = \mathbf{C}\mathbf{Y}^T$, a result quoted by Epstein and Maugin².

Remark

The previous expression of the virtual power balance law is based on the analysis developed by Morton Gurtin, in discussing the role of what he calls configurational forces (formula 1-6)⁶. Gurtin's formula is derived under the assumption of fixed

kinematic boundary conditions, and vanishing body forces and anelastic deformation rate so that $\langle \ell, \mathbf{v} \rangle = 0$ and $\dot{\mathbf{\Delta}} = 0$. In our notations, his formula reads

$$-\dot{\mathbf{E}} = - \int_{\mathcal{T}(\mathbb{M})} \langle \mathbf{S}, \mathbf{D}(\varphi) \rangle_{\mathbf{g}} \boldsymbol{\mu} + \int_{\mathcal{I}} [[W]] \mathbf{g}(\dot{\boldsymbol{\chi}}, \mathbf{n}) (\boldsymbol{\mu}\mathbf{n}),$$

to hold for all $\mathbf{v} \in C^1(\mathcal{T}(\mathbb{M}); \mathbb{S})$ and $\dot{\boldsymbol{\chi}} \in C^1(\mathbb{M}; \mathbb{T}\mathbb{M})$ fulfilling Hadamard's condition for shock waves on \mathcal{I} . This is equivalent to

$$-\dot{\mathbf{E}} = \int_{\mathcal{I}} \mathbf{g}([[Y]]\mathbf{n}, \dot{\boldsymbol{\chi}}) (\boldsymbol{\mu}\mathbf{n}) = \int_{\mathcal{I}} \mathbf{g}([[Y]]\mathbf{n}, \mathbf{n}) v_{\boldsymbol{\chi}} (\boldsymbol{\mu}\mathbf{n}).$$

He then assumes that $\dot{\mathbf{E}} = 0$ for all $v_{\boldsymbol{\chi}}$ concluding that $\mathbf{g}([[Y]]\mathbf{n}, \mathbf{n}) = 0$, a condition which he claims to be often referred to as the *Maxwell relation* (but it has in fact no connection with the Maxwell jump condition illustrated above). From the property $\mathbf{g}([[Y]]\mathbf{n}, \mathbf{t}) = 0$ for all \mathbf{t} such that $\mathbf{g}(\mathbf{n}, \mathbf{t}) = 0$, he then concludes that $[[Y]]\mathbf{n} = 0$ at phase-transition interfaces. We must confess to be unable to find a physical motivation for Gurtin's assumption that $\dot{\mathbf{E}} = 0$ for all $v_{\boldsymbol{\chi}}$. As a consequence, his conclusion that $\mathbf{g}([[Y]]\mathbf{n}, \mathbf{n}) = 0$ and $[[Y]]\mathbf{n} = 0$ cannot be agreed on, since it implies that the evolution of the phase-transition interfaces requires no power to be expended, despite of experimental evidences in solid state physics and fracture mechanics. Reasoning in the opposite direction, we are led to conclude that the singular term

$$\int_{\mathcal{I}} \mathbf{g}([[Y]]\mathbf{n}, \dot{\boldsymbol{\chi}}) (\boldsymbol{\mu}\mathbf{n}), \quad \dot{\boldsymbol{\chi}} \in C^1(\mathbb{M}; \mathbb{T}\mathbb{M}),$$

provides the (virtual) power dissipated in the motion of the evolving phase-transition interfaces.

2.6 Divergence of Eshelby's stress tensor

We provide hereafter the expression of the divergence of Eshelby's tensor in each phase of the multi-phase material, since the vanishing of the divergence is at the basis of the invariance property of the J -integral in fracture mechanics.

Since in each material phase the property p is constant, we may assume the following reduced functional dependence for the free energy density:

$$W(\mathbf{D}(\varphi)(\mathbf{m}), \mathbf{\Delta}(\mathbf{m}), \mathbf{m}).$$

Evaluating the spatial derivative in a direction $\mathbf{h} \in \mathbb{T}_{\mathbf{m}}\mathbb{M}$, by the Leibniz rule we have that

$$\mathbf{g}(dW, \mathbf{h}) = \langle d_1W, d_{\mathbf{h}}\mathbf{D}(\varphi) \rangle_{\mathbf{g}} + \langle d_2W, d_{\mathbf{h}}\mathbf{\Delta} \rangle_{\mathbf{g}} + \mathbf{g}(d_3W, \mathbf{h}),$$

where dW is the total gradient and d_iW , $i = 1, 2, 3$ are the partial gradients. By the formula $dW = \text{div}(W\mathbf{I})$ we may write

$$\mathbf{g}(d_3W, \mathbf{h}) + \langle d_2W, d_{\mathbf{h}}\mathbf{\Delta} \rangle_{\mathbf{g}} = \mathbf{g}(\text{div}(W\mathbf{I}), \mathbf{h}) - \langle d_1W, d_{\mathbf{h}}\mathbf{D}(\varphi) \rangle_{\mathbf{g}},$$

which is the formula prodromic to the classical Eshelby's one. Now in terms of the Piola tensor field \mathbf{P} we have that

$$\langle d_1 W, d_{\mathbf{h}} \mathbf{D}(\varphi) \rangle_{\mathbf{g}} = \langle \mathbf{S}, d_{\mathbf{h}} \mathbf{D}(\varphi) \rangle_{\mathbf{g}} = \langle \mathbf{P}, d_{\mathbf{h}} d\varphi \rangle_{\mathbf{g}}.$$

Accordingly, the formula above becomes

$$\mathbf{g}(d_3 W, \mathbf{h}) - \langle \mathbf{S}_{\mathbb{M}}, d_{\mathbf{h}} \Delta \rangle_{\mathbf{g}} = \mathbf{g}(\operatorname{div}(W\mathbf{I}), \mathbf{h}) - \langle \mathbf{P}, d_{\mathbf{h}} d\varphi \rangle_{\mathbf{g}}.$$

Hence, recalling that the divergence of a field $\mathbf{A} \in C^1(\mathbb{M}; BL(\mathbb{T}\mathbb{M}; \mathbb{T}\mathbb{M}))$ is the vector field $\operatorname{div} \mathbf{A} \in C^0(\mathbb{M}; \mathbb{T}\mathbb{M})$ defined by

$$\mathbf{g}(\operatorname{div} \mathbf{A}, \mathbf{v}) := \operatorname{div}(\mathbf{A}^T \mathbf{v}) - \langle \mathbf{A}, d\mathbf{v} \rangle_{\mathbf{g}}, \quad \forall \mathbf{v} \in C^1(\mathbb{M}; \mathbb{T}\mathbb{M}),$$

observing that $d_{\mathbf{h}} d\varphi = d(d_{\mathbf{h}} \varphi)$ and setting $\mathbf{A} = \mathbf{P}$ and $\mathbf{v} = d_{\mathbf{h}} \varphi$, we get

$$\langle \mathbf{P}, d_{\mathbf{h}} d\varphi \rangle_{\mathbf{g}} = \langle \mathbf{P}, d d_{\mathbf{h}} \varphi \rangle_{\mathbf{g}} = \operatorname{div}(\mathbf{P}^T d_{\mathbf{h}} \varphi) - \mathbf{g}(\operatorname{div} \mathbf{P}, d_{\mathbf{h}} \varphi).$$

The differential equilibrium condition, under a body force field \mathbf{b} , and the divergence formula again, with $\mathbf{A} = d\varphi^T \mathbf{P}$ and $\mathbf{v} = \mathbf{h}$, imply that

$$\operatorname{div} \mathbf{P} = -\mathbf{b}, \quad \operatorname{div}(\mathbf{P}^T d_{\mathbf{h}} \varphi) = \operatorname{div}((\mathbf{P}^T d\varphi)\mathbf{h}) = \mathbf{g}(\operatorname{div}(d\varphi^T \mathbf{P}), \mathbf{h}).$$

It follows that

$$\mathbf{g}(d_3 W, \mathbf{h}) - \langle \mathbf{S}_{\mathbb{M}}, d_{\mathbf{h}} \Delta \rangle_{\mathbf{g}} = \mathbf{g}(\operatorname{div}(W\mathbf{I} - d\varphi^T \mathbf{P}), \mathbf{h}) - \mathbf{g}(\mathbf{b}, d_{\mathbf{h}} \varphi),$$

and, in terms of the Eshelby's tensor $\mathbf{Y} := W\mathbf{I} - d\varphi^T \mathbf{P}$, we may write

$$\begin{aligned} \mathbf{g}(\operatorname{div} \mathbf{Y}, \mathbf{h}) &= \mathbf{g}(dW, \mathbf{h}) - \langle \mathbf{S}, d_{\mathbf{h}} \mathbf{D}(\varphi) \rangle_{\mathbf{g}} + \mathbf{g}(\mathbf{b}, d_{\mathbf{h}} \varphi) \\ &= \mathbf{g}(d_3 W, \mathbf{h}) - \langle \mathbf{S}_{\mathbb{M}}, d_{\mathbf{h}} \Delta \rangle_{\mathbf{g}} + \mathbf{g}(\mathbf{b}, d_{\mathbf{h}} \varphi). \end{aligned}$$

In an homogeneous elastic phase, under homogeneous anelastic metric and no body forces, we have that $\operatorname{div} \mathbf{Y} = 0$.

3 Small displacement formulation

Many engineering applications can be dealt with by a geometrically linearized formulation. To specialize the previous theory to this important class of problems, it is convenient to re-formulate the analysis in terms of the displacement field $\mathbf{u} \in C^0(\mathbb{M}; \mathbb{T}\mathbb{S}) \cap C^1(\mathcal{T}(\mathbb{M}); \mathbb{T}\mathbb{S})$ defined by $\mathbf{u}(\mathbf{m}) := \varphi(\mathbf{m}) - \mathbf{m}$, so that $d\mathbf{u} = d\varphi - \mathbf{I}$ in $\mathcal{T}(\mathbb{M})$. For the jump across the phase-transition interfaces \mathcal{I} we have the equality $[[d\mathbf{u}]] = [[d\varphi]]$ and hence the Eshelby's stress tensor can be equivalently defined in terms of displacement field as

$$\mathbf{Y}_{\mathbf{u}} := W\mathbf{I} - d\mathbf{u}^T \mathbf{P} = W\mathbf{I} - d\varphi^T \mathbf{P} + \mathbf{P} = \mathbf{Y} + \mathbf{P},$$

with $[[\mathbf{Y}_{\mathbf{u}}]]\mathbf{n} = [[\mathbf{Y}]]\mathbf{n}$ since $[[\mathbf{P}\mathbf{n}]] = 0$.

In the geometrically linearized theory, the reference and the actual placements of the body are taken to be coincident so that the Piola stress \mathbf{P} and the Cauchy stress \mathbf{T} may be identified. Accordingly the Eshelby stress tensor takes the form

$$\mathbf{Y}_{\mathbf{u}} = W\mathbf{I} - d\mathbf{u}^T \mathbf{T},$$

and its divergence is given by

$$\mathbf{g}(\operatorname{div} \mathbf{Y}_{\mathbf{u}}, \mathbf{h}) = \mathbf{g}(d_3 W, \mathbf{h}) - \langle \mathbf{S}_{\mathbb{M}}, d_{\mathbf{h}} \Delta \rangle_{\mathbf{g}} + \mathbf{g}(\mathbf{b}, d_{\mathbf{h}} \mathbf{u}).$$

3.1 Crack propagation

The evaluation of what in fracture mechanics is commonly dubbed the *driving force* on traveling cracks can be based on a suitable specialization of the general expression of the dissipation contributed above. To this end, we consider the motion of a crack traveling in the material. Assuming that the crack-tip moves with a translational speed $\dot{\boldsymbol{\chi}}(\mathbf{m}) = \dot{\chi} \mathbf{d}$ directed along its axis (labeled by the unit vector \mathbf{d}), and writing the dissipation as $F \dot{\chi}$, the driving force F is given by the relation

$$F = \int_{\mathcal{I}} \mathbf{g}([\mathbf{Y}]\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}) = \int_{\mathcal{I}} \mathbf{g}([W]\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}) - \int_{\mathcal{I}} \mathbf{g}(\mathbf{P}\mathbf{n}, [d_{\mathbf{d}}\boldsymbol{\varphi}]) (\boldsymbol{\mu}\mathbf{n}),$$

where \mathbf{n} is the outward normal oriented from the crack towards the surrounding material. The result embodied in this formula is in contrast to the usual statement according to which the driving force on a translating defect is provided by the projection along the travel direction of the outward flux of Eshelby's stress tensor thru the boundary of a control volume surrounding the defect^{3,4,5,9}.

3.1.1 J-integral for non-cohesive cracks

Let us consider the motion of a non-cohesive crack traveling in the material. Since there is no material inside the crack, we may assume that there $W^- = 0$ so that $[W] = W^+$. Moreover the interface between the non-cohesive crack and the surrounding material is traction-free, that is $\mathbf{P}\mathbf{n} = 0$ on \mathcal{I} . Then $[\mathbf{Y}]\mathbf{n} = \mathbf{Y}^+\mathbf{n} = W^+\mathbf{n}$ and the driving force takes the expression

$$F = \int_{\mathcal{I}} \mathbf{g}(\mathbf{Y}^+\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}) = \int_{\mathcal{I}} \mathbf{g}(W^+\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}),$$

where the interface \mathcal{I} is a closed surface surroundings the crack nose, that is the terminal crack zone where $\mathbf{g}(\mathbf{n}, \mathbf{d})$ is non-vanishing. Following James Rice¹⁰ we consider a surface Σ whose union with the crack-nose boundary forms a closed surface bounding a domain $C(\Sigma)$. The J -integral associated with the surface Σ is then defined as:

$$J(\Sigma) := \int_{\Sigma} \mathbf{g}(\mathbf{Y}\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}),$$

so that $J(\Sigma) = F$ when $\Sigma = \mathcal{I}$, due to the assumption that $\mathbf{T}\mathbf{n} = 0$ on \mathcal{I} . By the divergence theorem and the formula for $\text{div } \mathbf{Y}$ derived in section 2.6, we get the following general invariance property:

$$\begin{aligned} F &= J(\Sigma) - \int_{C(\Sigma)} \mathbf{g}(\text{div } \mathbf{Y}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}) \\ &= J(\Sigma) - \int_{C(\Sigma)} \mathbf{g}(d_3W, \mathbf{d}) \boldsymbol{\mu} + \int_{C(\Sigma)} \langle \mathbf{S}_{\mathbb{M}}, d_{\mathbf{d}}\boldsymbol{\Delta} \rangle_{\mathbf{g}} \boldsymbol{\mu} - \int_{C(\Sigma)} \mathbf{g}(\mathbf{b}, d_{\mathbf{d}}\boldsymbol{\varphi}) \boldsymbol{\mu}. \end{aligned}$$

Special instances of this formula are quoted in the recent literature^{7,8} concerning the J -integral. In an homogeneous phase, under homogeneous anelastic metric and no body forces, the divergence of Eshelby's tensor field vanishes, i.e. $\text{div } \mathbf{Y} = 0$, and the driving force F is equal to the J -integral evaluated on any surface Σ . In plane

problems of fracture mechanics, the invariance property $J(\Sigma) = F$ is commonly referred to as the path independence of the J -integral.

Remark

In the literature on fracture mechanics¹¹, in the wake of Griffith's treatment, crack propagation criteria are discussed in terms of an augmented total potential energy of the body which includes a so-called separation energy due to newly created crack faces. This is a nice example of a wrong way to a right result. Not completely right to be honest, since it is correct only if a geometrically linearized modelization is applicable. Indeed, in the nonlinear geometrical range, a total potential energy exists only under conservative loadings and such a requirement is completely extraneous to the physics of the problem at hand. Fortunately what really enters in the analysis is the (pseudo)-time derivative of the augmented total potential energy and this amounts in evaluating a virtual dissipation rate.

3.1.2 Cohesive cracks

Cohesive cracks are characterized by a process zone, extending ahead the crack-tip, in which cohesive ties oppose the opening of the crack, till the separation of the crack faces reaches a characteristic value that breaks the cohesive bonds. In the Barenblatt model for brittle fracture¹ a nonlinear relation is assumed between the cohesive restraining action and the separation between the crack faces. The bond-reactions are variable with the opening, first increasing from the pointed nose of the process zone until a maximum is reached, and then decreasing to zero, in correspondence of a threshold value of the opening, where breaking of the bonds occurs, at the crack tip. To provide the expression of the driving force F acting on cohesive cracks, propagating with a translational speed $\dot{\chi}(\mathbf{m}) = \dot{\chi} \mathbf{d}$, we rely again upon the general expression of the driving force:

$$F = \int_{\mathcal{I}} \mathbf{g}([\mathbf{Y}]\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}),$$

where the interface \mathcal{I} is the closed contour of the process zone. Following Rice¹⁰, we make the simplifying assumption that, due to the slit-shape of the crack, it is $\mathbf{g}(\mathbf{n}, \mathbf{d}) = 0$ along the crack faces. Since the flux-jump $[\mathbf{Y}]\mathbf{n}$ of Eshelby's tensor is directed along the normal \mathbf{n} at the interface, the contribution of the crack faces to the driving force vanishes. Then the integral can be extended only to the portion \mathcal{B} of the interface which cuts the crack in correspondence of the end of the process zone, where breaking of the bonds occurs. Along \mathcal{B} we have that $\mathbf{g}(\mathbf{n}, \mathbf{d}) = -1$, $\mathbf{P}\mathbf{n} = 0$ and $W^+ = 0$. Hence $\mathbf{Y}^+ = 0$ and the driving force is given by

$$F = \int_{\mathcal{B}} \mathbf{g}(-\mathbf{Y}^-\mathbf{n}, \mathbf{d}) (\boldsymbol{\mu}\mathbf{n}) = \int_{\mathcal{B}} W^- (\boldsymbol{\mu}\mathbf{n}).$$

The energy W^- is the one accumulated in the cohesive bonds per unit volume in correspondence of the breaking surface \mathcal{B} . Its integral over the surface \mathcal{B} is equal to the area of the Barenblatt diagram for the cohesive bond and its product by the propagation speed provides the energy release rate due to the bond breaking.

The driving force F is equal to the J -integral evaluated on any surface Σ which includes the crack-nose and such that $\Sigma \cup \mathcal{B}$ is a closed surface. Indeed, assuming that $\operatorname{div} \mathbf{Y}^- = 0$ inside the process-zone, by the divergence theorem we get

$$\int_{\mathcal{I}} \mathbf{g}(\mathbf{Y}^- \mathbf{n}, \mathbf{d}) (\boldsymbol{\mu} \mathbf{n}) = 0.$$

Moreover W^+ and $\mathbf{P} \mathbf{n}$ vanish on \mathcal{B} , so that $\mathbf{Y}^+ \mathbf{n} = 0$ on \mathcal{B} . Being $\mathbf{g}(\mathbf{n}, \mathbf{d}) = 0$ on $\mathcal{I} \setminus \mathcal{B}$, we also have that

$$\int_{\mathcal{I} \setminus \mathcal{B}} \mathbf{g}(W^+ \mathbf{n}, \mathbf{d}) (\boldsymbol{\mu} \mathbf{n}) = 0.$$

If we assume that $\operatorname{div} \mathbf{Y}^+ = 0$ in the material surrounding the process-zone, the driving force acting on cohesive cracks can be written as

$$\begin{aligned} F &= \int_{\mathcal{I}} \mathbf{g}(\mathbf{Y}^+ \mathbf{n}, \mathbf{d}) (\boldsymbol{\mu} \mathbf{n}) = \int_{\mathcal{I} \setminus \mathcal{B}} \mathbf{g}(\mathbf{Y}^+ \mathbf{n}, \mathbf{d}) (\boldsymbol{\mu} \mathbf{n}) \\ &= - \int_{\mathcal{I} \setminus \mathcal{B}} \mathbf{g}(\mathbf{P} \mathbf{n}, d\boldsymbol{\varphi}^+ \mathbf{d}) (\boldsymbol{\mu} \mathbf{n}) = \int_{\Sigma} \mathbf{g}(\mathbf{Y}^+ \mathbf{n}, \mathbf{d}) (\boldsymbol{\mu} \mathbf{n}) = J(\Sigma). \end{aligned}$$

This result is in accordance with the conclusions obtained by Rice¹⁰ on the basis of an *a priori* definition of the J -integral.

3.2 Conclusions

The approach for the description of phase-transition phenomena, in which propagating fronts are considered as shock waves traveling in the material, is based on the kinematical analysis proposed by Gurtin⁶.

However Gurtin's original point of view was strongly influenced by the attempt to prove that configurational forces are basic concepts of continuum physics. The intention of endowing Eshelby's stress with properties similar to Piola's stress, led him to make the assumption that no free energy release rate is associated with the evolution of phase transition fronts (see Gurtin⁶, chapter 1, section b, page 4).

By removing this assumption, we have shown that the balance law, derived from the virtual work principle of mechanics under a suitable definition of the free energy density for multi-phase materials, provides the basic expression of the dissipation associated with the evolution of phase-transition fronts. The theory has been then applied to analyze crack propagation phenomena in fracture mechanics and to show that the J -integral, introduced *a priori* by Rice¹⁰, stems out as a special expression of the dissipation formula for phase-transition fronts traveling in the material. The evaluation of the driving forces relevant to cohesive and non-cohesive crack propagations has been discussed in a mechanical context, under the usual assumptions concerning crack geometry.

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