

INTRODUCTION TO THE THERMOMECHANICS OF CONFIGURATIONAL FORCES

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ABSTRACT. Configurational forces are thermodynamic conjugates to irreversible material body evolutions such as extension of cracks, progress of phase-transition fronts, movement of shock waves, etc. They do correspond to a change of material configuration. Accordingly, their realm is the **material manifold of a body**. Furthermore, they acquire a physical meaning only in so far as they contribute to the global dissipation. Therefore, the present contribution of a pedagogical nature proposes a primer introduction to the thermodynamics of configurational forces. To that purpose, we first introduce a consistent thermomechanics of general deformable continua **on the material manifold** (and not in physical space). This is achieved in a canonical manner by full projection of the balance equation of momentum onto the material manifold and constructing in parallel a formally consistent expression of the energy conservation. Then various configurational forces such as those appearing in inhomogeneous bodies, at the tip of a propagating crack, at the surface of a propagating phase-transition front, or of a shock wave, and those due to local structural rearrangements (plasticity, damage, growth), are examined from the point of view of their dissipated power.

1. INTRODUCTION

Configurational forces ([1]-[6]) are driving forces acting on sets of material points during a change of configuration, i.e., during the irreversible evolution of a material body, such as

- the irreversible progress of a defect (dislocation, crack) in a solid;
- the irreversible progress of a phase into another one during a phase transition (if the phase transition is dissipation-free then the related driving force must vanish);
- the irreversible progress of a shock wave (the very existence of shock waves is related to dissipation);
- the growth of cavities in a material;
- etc.

Such forces of a non-Newtonian nature manifest themselves through the dissipation (the consumption of energy) they cause during this irreversible evolution. They are expressed as forces per unit element of the geometric object (line, surface, volume) to which they apply. They are the thermodynamical conjugates of the velocities of progress of the changes of configuration. Accordingly, their dissipation is generally written as the bi-linear form:

$$\Phi = \mathbf{F} \cdot \overline{\mathbf{V}}$$

where the relationship between \mathbf{F} , the configurational force, and $\overline{\mathbf{V}}$, the velocity of progress of the material point occupied by the object to which the force is applied, is a (generally

unknown) **kinetic law** which is such that the dissipation inequality is **not** violated (second law of thermodynamics). In continuum physics, if we know the solution of the field problem in nondefective parts of the material body, we can evaluate the configurational forces. The kinetic law then provides the progress of the "defect" and we can march in time with this **incremental** view of the problem. However, a microscopic approach may provide the missing kinetic law.

The general methodology to be exploited is as follows: first to express the whole problem on the **material manifold** itself. This gives rise to the notion of **material forces per se** (i.e., forces which are made apparent through a *canonical projection* of the thermomechanical problem onto the material manifold. This leads to the **material mechanics of materials** (M^3) and the theory of material inhomogeneities.

2. CANONICAL THERMOMECHANICS ON THE MATERIAL MANIFOLD (CONSISTENCY BETWEEN MECHANICS AND THERMODYNAMICS)

2.1. Reminder.

We shall use the standard notation of nonlinear continuum mechanics (cf. [7, 1]). Accordingly,

$$\mathbf{x} = \bar{\mathbf{x}}(\mathbf{X}, t)$$

is the time-parametrized motion mapping of material space onto physical Euclidean space; ∇_R and div_R denote the referential (material) nabla and divergence; $d/dt = \partial/\partial t|_X$ or a superimposed dot denotes the material time derivative. We suppose that the following three local balance laws have been deduced from a global statement for sufficiently smooth fields at any regular material point \mathbf{X} in the body. This is the so-called **Piola-Kirchhoff formulation** of the balance of mass, physical (linear) momentum, and energy (no external supply of energy apart from that related to the body force) at any regular material point \mathbf{X} in a continuous body in the presence of a body force \mathbf{f}_0 per unit reference volume:

$$(1) \quad \left. \frac{\partial \rho_0}{\partial t} \right|_{\mathbf{X}} = 0,$$

$$(2) \quad \left. \frac{\partial(\rho_0 \mathbf{v})}{\partial t} \right|_{\mathbf{X}} - div_R \mathbf{T} = \mathbf{f}_0,$$

and

$$(3) \quad \left. \frac{\partial(K + E)}{\partial t} \right|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v} - \mathbf{Q}) = \mathbf{f}_0 \cdot \mathbf{v},$$

where ρ_0 is the mass density in the reference configuration, $\mathbf{v} = \partial \bar{\mathbf{x}}/\partial t|_X$ is the physical velocity, \mathbf{T} is the first Piola-Kirchhoff stress, $K = \rho_0 \mathbf{v}^2/2$ is the kinetic energy, E is the internal energy per unit reference volume, \mathbf{Q} is the material heat flux, and $H = K + E$ is the Hamiltonian per unit reference volume.

At any regular material point \mathbf{X} the *second law of thermodynamics* is written as

$$(4) \quad \left. \frac{\partial S}{\partial t} \right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = (\mathbf{Q}/\theta) + \mathbf{K},$$

where S is the entropy density per unit reference volume, θ is the absolute temperature ($\theta > 0, \inf \theta = 0$), \mathbf{S} is the entropy flux, and the "extra entropy flux" \mathbf{K} vanishes in most cases, but this is not a basic requirement (see various cases hereafter). We note

$$\mathbf{F} = \partial \bar{\mathbf{x}} / \partial \mathbf{X} \Big|_t = \nabla_R \bar{\mathbf{x}}$$

the deformation gradient.

2.2. A canonical form of the energy conservation.

By taking the scalar product of eqn. (2) with \mathbf{v} , we traditionally obtain the so-called *theorem of the kinetic energy*:

$$(5) \quad \frac{\partial K}{\partial t} \Big|_{\mathbf{x}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v}) + \mathbf{T} : \dot{\mathbf{F}} - \mathbf{f}_0 \cdot \mathbf{v} = 0.$$

Combining this with the first law of thermodynamics (3) we obtain the so-called *theorem of internal energy*:

$$(6) \quad \frac{\partial E}{\partial t} \Big|_{\mathbf{x}} - \mathbf{T} : \dot{\mathbf{F}} + \nabla_R \cdot \mathbf{Q} = 0.$$

A. In the case where $\mathbf{K} = \mathbf{0}$, introducing the Helmholtz free energy function by $W = E - S\theta$, the second law (4) multiplied by θ yields the celebrated *Clausius-Duhem (C-D) inequality*

$$(7) \quad - \left(\frac{\partial W}{\partial t} + S \frac{\partial \theta}{\partial t} \right) + \mathbf{T} : \dot{\mathbf{F}} - \mathbf{S} \cdot \nabla_R \theta \geq 0.$$

Simultaneously, a most interesting form of the energy equation for subsequent developments reads (with $E := W + S\theta$)

$$(8) \quad \frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \mathbf{Q} = h^{int}, \quad h^{int} := \mathbf{T} : \dot{\mathbf{F}} - \frac{\partial W}{\partial t},$$

where the right-hand side of eqn. (8)₁ is formally an **internal heat source**. In particular, for a typically thermodynamically reversible behavior such as pure nonlinear elasticity (hyperelasticity), where $W = \bar{W}(\mathbf{F})$ depends only on \mathbf{F} , we have from the exploitation of (7),

$$(9) \quad \mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}} \quad \Rightarrow \quad h^{int} = 0.$$

We also note the following other form of the C-D inequality:

$$(10) \quad S\dot{\theta} + \mathbf{S} \cdot \nabla_R \theta \leq h^{int}.$$

B. In the case where $\mathbf{K} \neq \mathbf{0}$, instead of (7) we shall obtain the more general expression

$$(11) \quad - \left(\frac{\partial W}{\partial t} + S \frac{\partial \theta}{\partial t} \right) + \mathbf{T} : \dot{\mathbf{F}} + \nabla_R \cdot (\theta \mathbf{K}) - \mathbf{S} \cdot \nabla_R \theta \geq 0,$$

where \mathbf{S} is still given by the general expression (4)₂ and (11) differs from (7) only by the divergence term. Equations (8) are left unchanged:

$$(12) \quad \frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \mathbf{Q} = h^{int}, \quad h^{int} = \mathbf{T} : \dot{\mathbf{F}} - \frac{\partial W}{\partial t},$$

but eqn. (10) takes on the form

$$(13) \quad S\dot{\theta} + \mathbf{S} \cdot \nabla_R \theta \leq h^{int} + \nabla_R \cdot (\theta \mathbf{K}).$$

2.3. Canonical (material) momentum conservation.

Applying \mathbf{F} to the right of eqn. (2) and noting that (T = transpose)

$$(14) \quad \left(\frac{\partial(\rho_0 \mathbf{v})}{\partial t} \right) \cdot \mathbf{F} = - \frac{\partial \mathbf{P}}{\partial t} \Big|_{\mathbf{X}} - \nabla_R \left(\frac{1}{2} \rho_0 \mathbf{v}^2 \right) + \left(\frac{1}{2} \mathbf{v}^2 \right) \nabla_R \rho_0,$$

and

$$(15) \quad \text{div}_R \mathbf{T} \cdot \mathbf{F} = \text{div}_R (\mathbf{T} \cdot \mathbf{F}) - \mathbf{T} : (\nabla_R \mathbf{F})^T,$$

where we have set

$$(16) \quad \mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{F},$$

the **material momentum**, and introducing plus and minus the material gradient of an (**unspecified**) free energy density $W = \bar{W}(\cdot, \cdot, \cdot, X)$, we then check that eqn. (2) yields the following material balance of momentum

$$(17) \quad \frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{int} + \mathbf{f}^{ext} + \mathbf{f}^{inh},$$

where the material *Eshelby stress* \mathbf{b} , the material *inhomogeneity force* \mathbf{f}^{inh} , the material *external* (or body) force \mathbf{f}^{ext} , and the material *internal force* \mathbf{f}^{int} are defined by

$$(18) \quad \mathbf{b} = -(L_W \mathbf{1}_R + \mathbf{T} \cdot \mathbf{F}), \quad L_W = K - W,$$

$$(19) \quad \mathbf{f}^{inh} := \frac{\partial L_W}{\partial \mathbf{X}} \Big|_{expl} \equiv \frac{\partial L_W}{\partial \mathbf{X}} \Big|_{fixed\ fields} = \left(\frac{1}{2} \mathbf{v}^2 \right) \nabla_R \rho_0 - \frac{\partial \bar{W}}{\partial \mathbf{X}} \Big|_{expl},$$

$$(20) \quad \mathbf{f}^{ext} := -\mathbf{f}_0 \cdot \mathbf{F}, \quad \mathbf{f}^{int} = \mathbf{T} : (\nabla_R \mathbf{F})^T - \nabla_R W|_{impl}.$$

Here the subscript notations *expl* and *impl* mean, respectively, the material gradient keeping the fields fixed (and thus extracting the explicit dependence on \mathbf{X}), and taking the material gradient only through the fields present in the function.

In the present approach, in order to proceed further we need to specify the full functional dependence of W . The general expressions of eqns. (8)₁ and (17)

$$(21) \quad \frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \mathbf{Q} = h^{int}, \quad h^{int} = \mathbf{T} : \dot{\mathbf{F}} - \frac{\partial W}{\partial t},$$

$$(22) \quad \frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{int} + \mathbf{f}^{ext} + \mathbf{f}^{inh},$$

are the most general **canonical equations for momentum and energy** we can write down without a postulate of the full dependency of W . It is remarkable that eqn. (17) reads formally just the same whether the extra entropy vector \mathbf{K} vanishes or does not vanish, so that eqns. (21) and (22) are not only consistent with one another, but they are also independent on whether we remain in the standard thermodynamic framework or we deviate from it by the postulate of existence of an extra entropy flux.

Remark on jump relations: Just like for other equations in continuum mechanics, we could also write the jump relations associated with (21)₁ and (22) at a singular surface by using elements of the theory of hyperbolic systems or a more naive method such as the pill-box method. But since the "conservation laws" (21)₁ and (22) already exhibit source terms in the bulk (i.e., they are not conservation laws in a strict mathematical sense), the **associated jump relations** will also contain surface source terms. The latter, a priori unknown but responsible for the dissipation at the singularity, have to be computed with the help of the standard jump relations associated with eqns. (1)-(3).

2.4. Examples.

Example 1: Inhomogeneous thermoelasticity of conductors (no body force)

In this case of explicit material inhomogeneity, we a priori have the following functional dependencies: *Inertial inhomogeneity*:

$$(23) \quad \rho_0 = \bar{\rho}_0(\mathbf{X}),$$

and *thermomechanical inhomogeneities*:

$$(24) \quad W = \bar{W}(\mathbf{F}, \theta, \mathbf{X}).$$

With $\mathbf{K} = \mathbf{0}$ from the start, a standard procedure yields the **constitutive equations**:

$$(25) \quad \mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}.$$

We directly obtain that

$$(26) \quad \mathbf{f}^{int} = \mathbf{f}^{th},$$

$$(27) \quad h^{int} = h^{th} := S\dot{\theta},$$

where

$$(28) \quad \mathbf{f}^{th} := S\nabla_R \theta,$$

is the **material thermal force** [8, 9]. Accordingly, the canonical system of balance of momentum and energy reads:

$$(29) \quad \frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{inh} + \mathbf{f}^{th}, \quad \frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \mathbf{Q} = h^{th},$$

and is obviously non-Hamiltonian due to the explicit appearance of thermal effect in the right-hand sides of eqns. (29). Kalpakides and Maugin [10], basing on a different thermodynamics of continua, have succeeded to construct a Hamiltonian system of momentum and energy, but this to the price of a high degree of artificiality.

Example 2. (a sufficiently complex example): Homogeneous *dissipative* solid material described by means of a diffusive internal variable.

Here material inhomogeneities and external force are discarded for the sake of simplicity. For the general thermodynamics with internal variables we refer the reader to Maugin and Muschik [11]. Let α the internal variable of state whose tensorial nature is not specified. This may relate to damage, or anelasticity of some sort with a possible diffusion of the said

variable so that its material gradient must be taken into account (e.g., in strain-gradient plasticity). Then W is specified as the general sufficiently regular function

$$(30) \quad W = \overline{W}(\mathbf{F}, \theta, \alpha, \nabla_R \alpha).$$

A. First we assume that \mathbf{K} vanishes. The *equations of state* (in a sense, mere definition of the partial derivatives of the free energy) are given by *Gibbs' equation* as

$$(31) \quad \mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad A := -\frac{\partial \overline{W}}{\partial \alpha}, \quad \mathbf{B} := -\frac{\partial \overline{W}}{\partial \nabla_R \alpha}.$$

Accordingly, we find that the "internal" material force and heat source each split in two terms according to

$$(32) \quad \mathbf{f}^{int} = \mathbf{f}^{th} + \mathbf{f}^{intr}, \quad h^{int} = h^{th} + h^{intr},$$

where the *thermal sources* have already been defined and the "*intrinsic*" sources are given by

$$(33) \quad \mathbf{f}^{intr} := A(\nabla_R \alpha)^T + \mathbf{B} \cdot \nabla_R(\nabla_R \alpha)^T, \quad h^{intr} := A\dot{\alpha} + \mathbf{B} \cdot (\nabla_R \dot{\alpha})^T,$$

so that we have the following consistent (obviously non-Hamiltonian) system of canonical balance laws:

$$(34) \quad \frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{th} + \mathbf{f}^{intr}, \quad \frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \mathbf{Q} = h^{th} + h^{intr},$$

while the dissipation reads

$$(35) \quad \Phi = h^{intr} - \mathbf{S} \cdot \nabla_R \theta \geq 0, \quad \mathbf{K} \equiv \mathbf{0}.$$

Here the thermodynamical forces A and \mathbf{B} are purely dissipative by virtue of the "internal" character of the state variable α .

Remark: This approach with $\mathbf{K} \equiv \mathbf{0}$ favors the **continuum mechanics (Coleman-Noll) standard viewpoint** by accepting the classical relationship between heat and entropy flux, and assuming that α and its material gradient are essentially independent (see [12]).

B. A more **field-theoretic viewpoint** is to envisage the set of eqns. (11) through (13) as holding true and selecting the non-zero \mathbf{K} such that the total divergence term obtained in (11) in its exploitation with (30)-(31), be identically zero, i.e.,

$$(36) \quad \mathbf{K} = -\theta^{-1} \mathbf{B} \dot{\alpha}.$$

This follows the scheme originally developed by Maugin [13] for materials with *diffusive* dissipative processes described by means of internal variables of state.

Then it is readily shown that the canonical equation of momentum and energy read:

$$(37) \quad \frac{d\mathbf{P}}{dt} - \text{div}_R \tilde{\mathbf{b}} = \mathbf{f}^{th} + \tilde{\mathbf{f}}^{intr}, \quad \frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \tilde{\mathbf{Q}} = h^{th} + \tilde{h}^{intr},$$

and

$$(38) \quad \Phi = \tilde{h}^{intr} - \tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0, \quad \tilde{h}^{intr} := \tilde{A} \dot{\alpha}$$

where we have introduced the new definitions

$$(39) \quad \tilde{A} \equiv -\frac{\delta \overline{W}}{\delta \alpha} := -\left(\frac{\partial \overline{W}}{\partial \alpha} - \nabla_R \cdot \frac{\partial \overline{W}}{\partial (\nabla_R \alpha)} \right) = A - \nabla_R \cdot \mathbf{B}, \quad \tilde{\mathbf{S}} = \theta^{-1} \tilde{\mathbf{Q}}, \quad \tilde{\mathbf{Q}} = \mathbf{Q} - \mathbf{B} \dot{\alpha}$$

and

$$(40) \quad \tilde{\mathbf{b}} = -(L\mathbf{1}_R + \mathbf{T} \cdot \mathbf{F} - \mathbf{B} \cdot (\nabla_R \alpha)^T), \quad \tilde{\mathbf{f}} := \tilde{A} \nabla_R \alpha.$$

In this formulation the Eshelby stress complies with its role of grasping all effects presenting gradients since the material gradient of α plays a role parallel to that of the deformation gradient \mathbf{F} .

As an illustration one could consider the case of **finite-strain elastoplasticity** (cf. [14]), where we would select only the elastic deformation "gradient" \mathbf{F}^e instead of the full gradient $\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p$ as observable variable of state, and then the set of internal variables α can be made of the plastic deformation "gradient" \mathbf{F}^p and a set β of hardening variables, yielding a sufficiently general framework.

3. THE CASE OF A PROGRESSING CRACK

First we remind the reader of what we called the **analytical mechanics of brittle fracture** (the material itself is homogeneous and not dissipative, but possibly anisotropic, cf. [15]). The medium is purely elastic with constitutive equations

$$(41) \quad W = \overline{W}(\mathbf{F}), \quad \mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}.$$

3.1. Outside singularity sets. (i.e., at all *regular* material points \mathbf{X} in \mathcal{B}) we have locally the following reduced forms of the equations of momentum and energy (**strict** conservation laws):

$$(42) \quad \left. \frac{\partial \mathbf{p}}{\partial t} \right|_{\mathbf{X}} - \text{div}_R \mathbf{T} = \mathbf{0}, \quad \frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{0}, \quad \left. \frac{\partial H}{\partial t} \right|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v}) = 0.$$

On account of the assumed *smoothness* of all fields (in particular, \mathbf{F}), each of these can be integrated over an extended *regular* material region \mathcal{B} , where the Green's divergence and Reynolds' transport theorems can be used without specific precaution. We have commutation rules for space integration and time differentiation since (\mathbf{X}, t) is a good set of independent space-time parameters from that viewpoint. We obtain thus the following *global conservation laws*:

$$(43) \quad \frac{d}{dt} \int_{\mathcal{B}} \mathbf{p} dV = \int_{\partial \mathcal{B}} \mathbf{N} \cdot \mathbf{T} dA,$$

$$(44) \quad \frac{d}{dt} \int_{\mathcal{B}} \mathbf{P} dV = \int_{\partial \mathcal{B}} \mathbf{N} \cdot \mathbf{b} dA,$$

$$(45) \quad \frac{d}{dt} \int_{\mathcal{B}} H dV = \int_{\partial \mathcal{B}} \mathbf{N} \cdot \mathbf{T} \cdot \mathbf{v} dA.$$

3.2. Case of singular fields.

Now if the fields \mathbf{v} and \mathbf{T} , which are time and space derivatives of the basic field (motion), present a certain order of **singularity over some subset** of M^3 , quantities like \mathbf{P} , H , and \mathbf{b} which are at least quadratic in these fields, will even be *more* singular.

Thus, if the stress \mathbf{T} is *not* a good indicator of the presence of field singularities (see [2] Sec.5), \mathbf{b} may be a good indicator of this. This is exactly what happens in brittle fracture

where the integration of (42)₂ and (42)₃ over a subset of M^3 containing a field singularity, captures this singularity by making **additional nonvanishing terms**, characteristic of the singularity, appear in global equations of the type of (44) and (45). These terms are, respectively, the **material driving force (configurational force)** acting on the singularity and the so-called **energy-release rate** associated with the energy consumed in the irreversible progress of the defect.

3.3. The case of a steadily progressing notch.

Following Rice [16], a sharp-ended straight through crack C is viewed as the uniform limit of a family of end-rounded notches. The flat faces of the notch and the rounded cylindrical end are assumed free of traction. We consider the body \mathcal{B} of limiting surface $\partial\mathcal{B}$ excluding the notch, and the notch's end Γ_δ which is assumed to propagate inside the body with uniform material velocity $\bar{\mathbf{V}}$ parallel to the flat faces and to the axis \mathbf{E}_1 . This region is regular but geometrically evolving in time (configurational change) due to the extension of the notch. While integrating the local equations over material space (over \mathcal{B}) we simply have to use **generalized Green's** (divergence) and **Reynolds'** (transport) theorems. These yield (see Figures in [15])

$$(46) \quad \frac{d}{dt} \int_{\mathcal{B}} \mathbf{P} dV + F^{notch}(\delta) = \int_{\partial\mathcal{B}} \mathbf{N} \cdot \mathbf{b} dA,$$

$$(47) \quad \frac{d}{dt} \int_{\mathcal{B}} H dV + G^{notch}(\delta) = \int_{\partial\mathcal{B}} \mathbf{N} \cdot \mathbf{T} \cdot \mathbf{v} dA.$$

where we have defined a *material force* $F^{notch}(\delta)$ and an *energy-release rate* $G^{notch}(\delta)$ by

$$(48) \quad F^{notch}(\delta) = \mathbf{E}_1 \int_{\Gamma_\delta} (\mathbf{P}_1(\bar{\mathbf{V}} \cdot \mathbf{N}) - LN_1) dA,$$

$$(49) \quad G^{notch}(\delta) = \int_{\Gamma_\delta} H(\bar{\mathbf{V}} \cdot \mathbf{N}) dA,$$

Assuming the **convergence** of the family of notches indexed δ towards the sharp crack and that the limit of the solutions of the corresponding sequence of elasticity problems converges towards the solution for the sharp crack and the first term in each of (46) and (47) converges to zero in this limit (this follows from the singularity of elasticity solutions), we obtain for the driving force on the crack and the corresponding energy-release rate the following illuminating formulas:

$$(50) \quad F^{crack} = - \lim_{\delta \rightarrow 0} \mathbf{E}_1 \int_{\Gamma_\delta} (LN_1 - \mathbf{P}_1(\bar{\mathbf{V}} \cdot \mathbf{N})) dA,$$

and

$$(51) \quad G^{crack} = \lim_{\delta \rightarrow 0} \int_{\Gamma_\delta} H(\bar{\mathbf{V}} \cdot \mathbf{N}) dA.$$

This is the **analytical theory of brittle fracture**, because the two relevant equations involve the **Lagrangian** and **Hamiltonian** densities L and H , respectively. We note that the **tip of the crack here acts as an energy sink**.

But we can equally well integrate over the regular material region of volume extension G of external (cylindrical) boundary Γ equipped with unit outward normal \mathbf{N} and the notch as indicated in the Figure in [15], and moving inward with uniform material velocity $\bar{\mathbf{V}}$. Combining then the resulting expression with (48) and (49), we obtain more classical (but less elegant) formulas for the quantities (50) and (51):

$$(52) \quad F_1^{crack} = \int_{\Gamma} ((\mathbf{N} \cdot \mathbf{b})_1 + \mathbf{P}_1(\bar{\mathbf{V}} \cdot \mathbf{N})) dA - \frac{\partial}{\partial t} \int_G \mathbf{P}_1 dV,$$

$$(53) \quad G^{crack} = \int_{\Gamma} (H(\bar{\mathbf{V}} \cdot \mathbf{N}) + \mathbf{N} \cdot \mathbf{T} \cdot \mathbf{v}) dA - \frac{\partial}{\partial t} \int_G H dV.$$

It is readily checked that eqn. (52) reduces to the celebrated path-independent J -integral of brittle fracture in quasi-statics and small strains

$$(54) \quad F_1^{crack} = J = \int_{\Gamma} \left(W N_1 - \mathbf{t} \cdot \frac{\partial \mathbf{u}}{\partial X_1} \right) dL,$$

per unit thickness of the body, where \mathbf{t} is the traction at Γ , and \mathbf{u} is the elastic displacement. More remarkably, a relationship can be established between (51) and (50) in the **fully dynamical and finite-strain** case. Let P a point of Γ_{δ} for the notch δ and \mathbf{r} the vectorial position of any point with respect to P . We can write $\chi(\mathbf{X}, t) = \chi(\mathbf{X}_p + \mathbf{r}, t)$, and through differentiation ([17])

$$(55) \quad \mathbf{v} = -\mathbf{F} \cdot \bar{\mathbf{V}} + \frac{\partial \bar{\chi}}{\partial t}, \quad \bar{\mathbf{V}} := \frac{\partial \mathbf{X}_p}{\partial t}.$$

On multiplication by \mathbf{F}^{-1} to the left of (55)₁ we get

$$(56) \quad \mathbf{V} = \bar{\mathbf{V}} - \mathbf{F}^{-1} \cdot \frac{\partial \bar{\chi}}{\partial t}, \quad \bar{\mathbf{V}} \parallel \mathbf{E}_1.$$

Let all the points of Γ_{δ} be in **uniform motion**, then we can reasonably assume that the deformation is the same at all points of Γ_{δ} and set $\partial \bar{\chi} / \partial t = \mathbf{0}$. Since the only nonzero component of $\bar{\mathbf{V}}$ is along \mathbf{E}_1 , multiplying the one-component of (48) by $\bar{\mathbf{V}}_1$, and accounting for the simplified form of (56) and the identity $\mathbf{V} \cdot \mathbf{C} \cdot \mathbf{V} = \mathbf{v}^2$, we obtain for the notch

$$(57) \quad G^{notch}(\delta) = \bar{\mathbf{V}}_1 F^{notch}(\delta).$$

Accordingly, for a uniform motion of the points of the notch, we find that the power expended by the material force driving the notch coincides with the energy released during the notch progress of a unit length inside the body. Relation (57) is meaningful only if $\bar{\mathbf{V}}$ is a function of \mathbf{X} . This shows the intimate relationship between the notion of material configurational force with that of rigid-body ("en bloc") motion. In the limit case of the straight crack, we obtain

$$(58) \quad G^{crack} = \bar{\mathbf{V}}_1 F_1^{crack}.$$

This is the **dissipation rate** due to the crack extension. It is in the classical bilinear form favored in irreversible thermodynamics. It is thus ready for the construction of crack-extension criteria for this.

3.4. Case of smoothly materially inhomogeneous elastic materials.

In this case eqn. (52) is replaced by

$$(59) \quad F_1^{crack} = \int_{\Gamma} ((\mathbf{N} \cdot \mathbf{b})_1 + \mathbf{P}_1(\bar{\mathbf{V}} \cdot \mathbf{N})) dA - \left(\frac{\partial}{\partial t} \int_G \mathbf{P}_1 dV - \int_G f_1^{inh} dV \right)$$

More generalizations: In the case of a homogeneous but thermoelastic body, this equation is replaced by one that contains a thermal source:

$$(60) \quad F_1^{crack} = \int_{\Gamma} ((\mathbf{N} \cdot \mathbf{b})_1 + \mathbf{P}_1(\bar{\mathbf{V}} \cdot \mathbf{N})) dA + \int_G (\mathbf{f}^{th})_1 dV - \frac{\partial}{\partial t} \int_G \mathbf{P}_1 dV,$$

and, accordingly,

$$(61) \quad G^{crack} = \int_{\Gamma} (H(\bar{\mathbf{V}} \cdot \mathbf{N}) + \mathbf{N} \cdot (\mathbf{T} \cdot \mathbf{v} - \mathbf{Q})) dA - \frac{\partial}{\partial t} \int_G H dV.$$

We recognize in the last expression minus the change in *potential energy* (*dynamic thermoelastic, homogeneous case*), that is, the *dissipation rate* in the progress of the notch inside the material body. Accordingly, there must be a relationship between the latter quantity and the *power expended* irreversibly by the *material force* of component F_1^{crack} . Because of the universal form of the expressions for F^{crack} and G^{crack} , just the same as before it is shown that

$$(62) \quad \bar{\mathbf{V}}_1 F_1^{crack} = G^{crack} \geq 0,$$

where the inequality sign indicates the thermodynamical irreversibility of the crack growth phenomenon. This corresponds to the presence of a hot heat source at the crack tip, an effect that can be observed by means of **infrared thermography**.

4. THE CASE OF A DISSIPATIVE PHASE TRANSITION FRONT (driving force on a singular surface Σ)

The presence of a discontinuity surface (transition front) Σ breaks the material symmetry of the material body as a whole and manifests a *material inhomogeneity*. Consequently, the critical equation for the description of the phenomenon is not only that relating to dissipation, but also the equation associated with the **lack of conservation of material momentum across Σ** , i.e., the associated *jump relation* that is generated by a change of "particle" on the material manifold: the driving force acting on the transition front will, therefore, be a "**material force**".

4.1. Jump relations.

Notation: Let $[A] = A^+ - A^-$, the jump of a discontinuous field A across Σ , the unit normal \mathbf{N} to Σ being oriented from the "minus" to the "plus" side. Let $\bar{\mathbf{V}}$ the material velocity of a geometrical point of Σ .

The phase transition fronts considered are **homothermal** (no jump in temperature; the two phases coexist at the same temperature) and **coherent** (they present no defects such as dislocations). Consequently, we have the following continuity conditions:

$$(63) \quad [\theta] = 0 \quad \text{and} \quad [\mathbf{V}] = \mathbf{0} \quad \text{at} \quad \Sigma.$$

Jump relations associated with strict conservation laws in the bulk, are formulated according to the theory of **weak solutions of hyperbolic systems**. That is, we merely replace the operators $\partial/\partial t|_{\mathbf{X}}$ and ∇_R by the jump operators $-(\bar{\mathbf{V}} \cdot \mathbf{N})[\dots]$ and $\mathbf{N} \cdot [\dots]$, respectively.

Thus the jump equations associated with the bulk equations (1), (2) and (3) - in the absence of body force - that are then strict conservation laws, read

$$(64) \quad \bar{V}_N[\rho_0] = 0,$$

$$(65) \quad \bar{V}_N[\mathbf{p}] + \mathbf{N} \cdot [\mathbf{T}] = 0,$$

$$(66) \quad \bar{V}_N[H] + \mathbf{N} \cdot [\mathbf{T}\mathbf{v} - \mathbf{Q}] = 0,$$

where $\bar{V}_N = \bar{\mathbf{V}} \cdot \mathbf{N}$ is the normal speed of the points of Σ .

The same pragmatic rule can be applied to the bulk equations (21) and (22) - that are *not* strict conservation laws - if we formally add *unknown* source terms, i.e., we *a priori* write the following two jump equations:

$$(67) \quad \bar{V}_N[S] - \mathbf{N} \cdot [\mathbf{Q}/\theta] = \sigma_\Sigma,$$

$$(68) \quad \bar{V}_N[\mathbf{P}] + \mathbf{N} \cdot [\mathbf{b}] + \mathbf{f}_\Sigma = 0.$$

The second law of thermodynamics at Σ reads

$$(69) \quad \sigma_\Sigma \geq 0.$$

Problem: it consists in finding the expressions of σ_Σ and \mathbf{f}_Σ that are *consistent*. We know the formal expression of both \mathbf{P} and \mathbf{b} . The only manipulation we can do on eqn. (68) is to compute the power expended by \mathbf{f}_Σ in the irreversible motion of Σ . To that purpose, we compute

$$(70) \quad p_\Sigma = \bar{\mathbf{V}} \cdot \mathbf{f}_\Sigma$$

on account of the remaining jump equations (64) through (66). The result of these manipulations is

$$(71) \quad p_\Sigma = f_\Sigma \bar{V}_N = \theta_\Sigma \sigma_\Sigma \geq 0$$

together with the fact that

$$(72) \quad q_\Sigma = p_\Sigma = \theta_\Sigma \sigma_\Sigma \geq 0$$

is a **hot heat source** localized at Σ . In these equations θ_Σ is the temperature at Σ , f_Σ is the scalar driving force for which we need a *kinetic equation*, and we have at Σ the following *balance of "material" forces*

$$(73) \quad f_\Sigma + Hugop_T = 0, \quad Hugop_T := [W - \langle \mathbf{N} \cdot \mathbf{T} \rangle \cdot \mathbf{F} \cdot \mathbf{N}]$$

the symbolism $\langle \dots \rangle$ indicating the mean value at Σ . The **surface "balance" equation** (73)₁ is written down just to emphasize the different roles of $Hugop_T$ - a field quantity that is known once we know the field solution by any means on both sides of Σ - and the driving force f_Σ that is the **thermodynamic conjugate** of the normal speed \bar{V}_N . The expression of \bar{V}_N in terms of f_Σ is the **kinetic law** for normal progress of which examples basing on a more microscopic approach can be found in Truskinovsky [18]. In the absence of microscopic justification, one simply applies the thermodynamical constraint (71) to formulate *a priori* an admissible kinetic law.

Remarks

(i) **Nondissipative phase transitions:** What must be remarked concerning the above construct is that the normal "material force" Hug_{PT} is practically never zero since it must satisfy the inequality (71). However, one may *artificially* impose a **vanishing** Hug_{PT} for a progressing front (non zero \bar{V}_N). This means a *nondissipative* phase transition although we relate through Σ the phases which are in nonadiabatic evolution ($\mathbf{Q} \neq \mathbf{0}$). This is a **singular situation** for which one shows in one dimension that the transition then obeys *Maxwell's rule of equal areas* (cf. [19]). For a fluid, this condition in fact materializes in the continuity of the **chemical potential**. The relationship of chemical potential and the Eshelby stress (sometimes called chemical potential tensor) was noticed by Grinfeld [20].

(ii) However, there is something more in the above results: it is that **no** quasi-static hypothesis was used, although it is exactly *shown* that no kinetic energy can enter the final expression (73). This agrees with the perspicacious view of Gibbs and Duhem who indeed foresaw that only the free enthalpy must govern the local matter rearrangement represented by a phase transition. Thus only the quasi-static part of the Eshelby stress finally contributes to the Hugoniot-Gibbs functional Hug_{PT} - in agreement with their vision.

(iii) The above result can be generalized to more complex material bodies such as electromagnetic ones (e.g., in Fomethé and Maugin [21]) or polar thermoelasticity [22], as also thermo-anelastic materials. Furthermore, there is fundamentally nothing changed in the above-given argument in the presence of anelastic behaviors described by means of internal variables of state (cf. [23]).

5. THE CASE OF THERMOMECHANICAL SHOCK WAVES

In this case we do not satisfy the condition (63)₁. But we can keep the dependence on internal variables and therefore treat the general case of thermo-anelasticity, since the presence of α (without gradients) does not formally alter the presentation. The jump relations (64) through (66) constitute the general point of departure. However, if we kept the idea of a transition zone of small but finite thickness from one side of Σ to the other, then the source quantities in eqns. (67) and (68) would be known in terms of **excess quantities** computed throughout the thickness of the transition zone. That is, without loss in generality in the absence of surface tension along Σ , imagine that this zone is locally a flat strip orthogonal to the coordinate axis X_1 and the problem is independent of the other two (transverse) coordinates X_2 and X_3 . Then, assuming the transition zone of thickness δ we could write eqns. (67) and (68) as follows:

$$(74) \quad \bar{V}_N[S] - \mathbf{N} \cdot [\mathbf{Q}/\theta] = \int_{-\delta/2}^{+\delta/2} (\sigma^{th} + \sigma^{intr}) dX_1 \geq 0,$$

and

$$(75) \quad \bar{V}_N[\mathbf{P}] + \mathbf{N} \cdot [\mathbf{b}] = - \int_{-\delta/2}^{+\delta/2} (\mathbf{f}^{th} + \mathbf{f}^{intr}) dX_1,$$

where the jump now means the difference between the values a little bit before and beyond the ends of the interval δ , i.e., outside the transition zone.

This, which can be conceived as a *zoom* on the front, shows the remarkable role played by **thermal and intrinsic entropy sources** in the condition of entropy growth at Σ and the parallel role of the material forces \mathbf{f}^{th} and \mathbf{f}^{intr} in writing the jump of the balance of pseudomomentum at Σ . Equations such as (74) are suggested by Mandel ([24], pp. 268-9) and considered by some authors [25, 26], but eqn. (75) is quite recent [19, 22]. It is the consistency between the source terms in eqns. (74)-(75) which provides the connection between entropy growth at Σ and the power expended by the material driving forces, even in the general theory of shock waves where the notion of driving force was heretofore ignored.

General thermomechanical formulation:

We shall consider the purely jump-like description (64)-(66), bearing (74)-(75) in mind as some "microscopic" justification. We then define the following scalar and vectorial quantities at Σ (such quantities are meaningful in themselves only if they are invariant across Σ . Otherwise, they become mathematically meaningful only once an operator such as [...] or $\langle \dots \rangle$, attached to Σ , is applied to them):

$$(76) \quad m := \rho_0 \bar{V}_N,$$

$$(77) \quad T_\Sigma := m\mathbf{v} + \mathbf{N} \cdot \mathbf{T},$$

$$(78) \quad mQ_\Sigma := m\bar{H} + \mathbf{N} \cdot (\mathbf{T} \cdot \mathbf{v} - \mathbf{Q}),$$

$$(79) \quad B_\Sigma := m\bar{\mathbf{P}} + \mathbf{N} \cdot \mathbf{b},$$

$$(80) \quad mN := m\bar{S} + (\mathbf{N} \cdot \mathbf{Q}/\theta),$$

where, apart from \bar{V}_N , quantities with overbars are per unit mass in the reference configuration (e.g., $\bar{S} = S/\rho_0$). On account of definitions (76)-(80) the jump relations (64) through (66) now read

$$(81) \quad [m] = 0, \quad [T_\Sigma] = \mathbf{0}, \quad m[Q_\Sigma] = 0,$$

and

$$(82) \quad m[N] = \sigma_\Sigma \geq 0, \quad [B_\Sigma] + \mathbf{f}_\Sigma = \mathbf{0}.$$

This is merely a rewriting, but it allows us to perform some simple manipulations and to express some remarkable results in an attractive manner. Define

$$(83) \quad \bar{L}^{th} = L^{th}/\rho_0 = \tilde{L}^{th}(\mathbf{F}, \mathbf{v}, \theta, \alpha).$$

Then it is proved that the entropy source at Σ is given by (cf. [27])

$$(84) \quad \sigma_\Sigma = m [\bar{L}^{th}/\theta] + mQ_\Sigma [\theta^{-1}] - T_\Sigma [\mathbf{v}/\theta] \geq 0.$$

Guided by this, introduce the following **generating or Massieu function** M at Σ by

$$(85) \quad M := \theta^{-1} \left(m(Q_\Sigma + \bar{L}^{th}) - T_\Sigma \cdot \mathbf{v} \right).$$

Then we can prove the following two results ([27])

$$(86) \quad \sigma_\Sigma = [M] \geq 0,$$

and

$$(87) \quad p_\Sigma = \bar{\mathbf{V}} \cdot \mathbf{f}_\Sigma = [\theta M].$$

That is, the **generating function** M - a notion already used in hydrodynamics and magnetohydrodynamics by P. Germain [28] - provides *both* the entropy source and the power of the driving force at Σ , although we do not know yet the explicit form of the latter. From (86) and (87) there follows the following general relationship between p_Σ , σ_Σ , and the jump in temperature for a general shock wave relating two regions where adiabaticity is *not* supposed:

$$(88) \quad p_\Sigma = \sigma_\Sigma \langle \theta \rangle + \langle M - (mQ_\Sigma/\theta) \rangle [\theta].$$

It is clear from the above results (86)-(87) that in the case of a phase-transition front across which temperature is constant we immediately have the result (71) since:

$$(89) \quad p_\Sigma = \theta_\Sigma [M] = \theta_\Sigma \sigma_\Sigma \geq 0.$$

Otherwise, we have at hand a *consistent theory of shock waves* because, contrary to the simple theory in which the shock relates two regions in adiabatic situations, we here relate two regions in which dissipation of both thermal and intrinsic origins is taken into account so that we have a justification for the existence of σ_Σ of which the non-negativity is not imposed out of the blue. What about the celebrated **Hugoniot equation of classical shock-wave theory** (in which there are neither heat flux nor variables α present)? This is normally obtained by expanding the following identity on account of other (classical) jump relations:

$$(90) \quad [T_\Sigma] \cdot \langle \mathbf{v} \rangle \equiv 0,$$

resulting in

$$(91) \quad \text{Hugo}_{SW} := [E(\mathbf{F}, S, \alpha) - \langle \mathbf{N} \cdot \mathbf{T} \rangle \cdot \mathbf{F} \cdot \mathbf{N}] \equiv 0 \quad \text{at } \Sigma,$$

where it is the **internal energy** E that is involved.

This is the difference with the Hugoniot-Gibbs functional (73) of phase-transition fronts where it is the *free energy* that is involved. But in our formalism Hugo_{SW} is a material driving force (more precisely, the double normal component of the jump of a material tensor) and the identity (90) clearly exhibits the inconsistency of classical shock-wave theory in which the driving force is set equal to zero (providing the Hugoniot equation) for a still propagating shock wave while the power expended by the driving force should be strictly related to the entropy growth, itself *not* supposed to be zero in general. Whether it is free or internal energy that is involved in the definition of the Eshelby stress depends on the problem at hand, i.e., as shown by the transition front and shock wave problem, whether the thermodynamic conditions that prevail correspond to isothermal or adiabatic evolutions (cf. [29]).

6. THE CASE OF DISSIPATIVE DISTRIBUTED MATERIAL REARRANGEMENTS

In 1990 Epstein and Maugin [30] have shown in the case of elasticity that if material inhomogeneity is represented by a local change \mathbf{K} of material reference configuration, then

the static Eshelby stress tensor is given by the following aesthetically pleasant definition

$$(92) \quad \mathbf{b} := -\frac{\partial \widetilde{W}}{\partial \mathbf{K}} \mathbf{K}^T = W \mathbf{1}_R - \mathbf{T} \cdot \mathbf{F},$$

where

$$(93) \quad W = \overline{W}(\mathbf{F}, \mathbf{X}), \quad \mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}},$$

and the volume energy density \widetilde{W} is such that

$$(94) \quad \overline{W}(\mathbf{F}, \mathbf{X}) = J_K^{-1} \widetilde{W}(\mathbf{F} \cdot \mathbf{K}(\mathbf{X})).$$

Accordingly, the local material inhomogeneity force is given by (cf. eqn. (19))

$$(95) \quad \mathbf{f}^{inh} = -\left. \frac{\partial \overline{W}}{\partial \mathbf{X}} \right|_{expl} = -div_R \mathbf{b}.$$

The material transformation \mathbf{K} may be referred to as a *local structural rearrangement*. Such transformations are typical of such thermodynamically irreversible effects as *plasticity*, but also of many effects (thermoelasticity in conductors, viscoplasticity in crystals, bulk phase-transition, uniform magnetization, damage, volumetric growth) that may be considered as *pseudo-plastic* or *pseudo-inhomogeneity* effects (cf. [31]) in the sense that they manifest their existence on the material manifold (i.e., in the balance of material momentum) as additional material forces (\mathbf{f}^{th} and \mathbf{f}^{intr} in eqn. (34) are examples of such manifestations). In a general way, *internal stresses* are associated with such effects. Now consider a *continuous distribution* of pseudo-plastic effects represented by the local structural rearrangement. Considering a self-equilibrated infinitesimal element of matter at \mathbf{X} of volume dV_0 , one easily shows on the basis of eqn. (95), that the elementary power expended by the pseudo-inhomogeneity force \mathbf{f}^{inh} is none other than (*tr* = *trace*)

$$(96) \quad (dV_0)^{-1} \mathbf{f}^{inh} \cdot \mathbf{V} \approx tr(\mathbf{b} \cdot (\nabla_R \mathbf{V})^T).$$

This is the *elementary dissipated power* related to the considered pseudo-inhomogeneity effect. The result (96) applies in particular to finite-strain elastoplasticity [32] and the material theory of volumetric growth [33].

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