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Incompatibility-governed elasto-plasticity for continua with dislocations

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In this paper, a novel model for elasto-plastic continua is presented and developed from the ground up. It is based on the interdependence between plasticity, dislocation motion and strain incompatibility. A generalized form of the equilibrium equations is provided, with as additional variables, the strain incompatibility and an internal thermodynamic variable called incompatibility modulus, which drives the plastic behaviour of the continuum. The traditional equations of elasticity are recovered as this modulus tends to infinity, while perfect plasticity corresponds to the vanishing limit. The overall nonlinear scheme is determined by the solution of these equations together with the computation of the topological derivative of the dissipation, in order to comply with the second principle of thermodynamics.

1. Introduction

In classical infinitesimal elasto-plasticity (see standard textbooks, e.g. [1]) the total strain ϵ^{tot} is assumed to satisfy the following two conditions:

- There exists an additive decomposition $\epsilon^{\mathrm{tot}} = \epsilon^{\mathrm{e}} + \epsilon^{\mathrm{p}}$ where the elastic strain satisfies $\epsilon^{\mathrm{e}} = \mathbb{A}^{-1}\sigma$ with $\mathbb{A}$ the elasticity tensor and σ the stress, and where the strain ϵ^{p} is called plastic. Furthermore, the plastic strain is often chosen trace-free.
- The total strain ϵ^{tot} is compatible, that is, there exists a displacement field u such that $\epsilon^{\mathrm{tot}} = \nabla^{\mathrm{S}} u$, with ∇u the gradient of u and $\nabla^{\mathrm{S}} u$ its symmetric part.

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On these bases, the equilibrium relation $-\operatorname{div}\sigma = f$ with appropriate boundary conditions for u together with 'flow rules' for ϵ^{p} (themselves based on the assumption that plasticity takes place at the boundary of a convex set—the so-called elasticity domain—and on postulated dissipation potentials) are jointly solved to find the solution, say $(u, \epsilon^{\mathrm{p}})$. It is not discussed here the fact that this approach has provided enough evidence that such solutions correspond to the observed behaviours of elasto-plastic materials. In this paper, we would like to propose another approach, based on completely different paradigms and mathematical methods. We summarize our point as follows.

- Objectivity is a crucial condition. It is intended field objectivity, that is, the intrinsic character of field measurements for distinct observers but also the independence of this field from any kind of arbitrary prescription: for instance $u, \nabla u$ are not objective in the classical sense, while $\nabla^{\mathrm{S}} u$ still depends on a reference configuration. However, the strain rate d is an intrinsic, objective, unambiguous quantity. It is also intended objectivity of tensor decompositions: is the aforementioned elasto-plastic partition well defined? Is it a physical decomposition (based on experimental evidence) or a mathematical result (based on proofs of existence)?
- Field decomposition must result from a mathematical statement, with clear conditions for existence and uniqueness.
- Elasto-plastic materials are modelled with one governing system of equations (in place of equilibrium + flow rules), of which classical infinitesimal elasticity is a particular case.
- Plastic behaviour is due to the motion of dislocations, which themselves create strain incompatibility (i.e. the fact that ϵ^{p} is not a symmetric gradient) by the famous Kröner's relation $\operatorname{inc}\epsilon^{\mathrm{P}} = -\operatorname{Curl}\kappa$, where κ is the dislocation contortion, directly related to the dislocation density. Therefore, the incompatibility operator inc, defined in such a way that $\operatorname{inc}\epsilon^{\mathrm{tot}} = 0$ represents the classical Saint-Venant compatibility conditions, is a key ingredient of our approach.
- The second principle of thermodynamics must hold, and possibly be at the heart of the model because plasticity is in essence a dissipative phenomenon.

Our model can be briefly described as follows. First, we derive the governing equations by the classical method of virtual powers, together with the Beltrami decomposition of symmetric tensors. We obtain a coupled system of equations which generalizes the classical system of elasticity by involving the strain incompatibility through the fourth-order differential operator $\operatorname{inc}\operatorname{inc}$. A crucial scalar appearing in these equations is the newly defined incompatibility modulus ℓ, whose link with classical Mindlin-like theories of higher-order elasticity is discussed. Moreover, the role of ℓ as an internal variable for plasticity is established. In a second step, we define the associated dissipation of the system. In the last step we compute, in a simplified setting, the topological derivative of the dissipation functional.[1] The resulting quasi-static elasto-plastic model is based on the second principle which allows us to nucleate plastic regions in the otherwise perfectly elastic crystal. This nucleation is based on the creation/motion of dislocations which increases the strain incompatibility while decreasing the modulus ℓ. The incremental formulation in which plastic effects take place in constantly updated regions results in an overall elasto-plastic evolution model which is highly nonlinear (the governing equations are linear in each increment, but the nucleation procedure by topological sensitivity is not).

2. Preliminary results

(a) Notations and conventions

Let Ω be a bounded domain of $\mathbb{R}^d$, $d = 2, 3$, with smooth boundary $\partial\Omega$. By smooth we mean C^∞, but this assumption could be considerably weakened. Let $\mathbb{M}^3$ denote the space

[1]The detailed computations are published online in a specific document.

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of square 3-matrices, and $\mathbb{S}^3$ of symmetric 3-matrices. The superscripts t and S are used to denote the transpose and the symmetric part, respectively, of a matrix. Divergence, curl, incompatibility and cross-product with second-rank tensors are defined componentwise as follows with the summation convention on repeated indices: $(\operatorname{div} E)_i := \partial_j E_{ij}$, $(\operatorname{Curl} T)_{ij} := (\nabla \times T)_{ij} = \varepsilon_{jkm}\partial_k T_{im}$, $(\operatorname{inc} E)_{ij} := (\operatorname{Curl}(\operatorname{Curl} E)^{\mathrm{t}})_{ij} = \varepsilon_{ikm}\varepsilon_{jln}\partial_k\partial_l E_{mn}$, $(N \times T)_{ij} := -(T \times N)_{ij} = \varepsilon_{jkm} N_k T_{im}$. Here, E and T are second-rank tensors, N is a vector, and ε is the Levi-Civita third-rank tensor.

(b) Function spaces used and preliminary results

Define

$$\left.\begin{aligned} \mathcal{H}(\Omega) &:= \{E \in H^2(\Omega, \mathbb{S}^3),\ \operatorname{div} E = 0\} \\ \text{and}\qquad \mathcal{H}_0(\Omega) &:= \{E \in \mathcal{H}(\Omega):\ E = (\partial_{\mathrm{N}} E \times N)^{\mathrm{t}} \times N = 0 \text{ on } \partial\Omega\} \end{aligned}\right\}. \tag{2.1}$$

These spaces are naturally endowed with the Hilbertian structure of $H^2(\Omega, \mathbb{S}^3)$. Note that $(\partial_{\mathrm{N}} E \times N)^{\mathrm{t}} \times N = 0$ exactly mean that the tangential components of $\partial_{\mathrm{N}} E$ vanish. Furthermore, it is proved in [2] (see also [3]) that the following holds on $\partial\Omega$:

$$E = (\partial_{\mathrm{N}} E \times N)^{\mathrm{t}} \times N = 0 \quad \Rightarrow \quad \operatorname{Curl}^{\mathrm{t}} E \times N = 0 \quad \Rightarrow \quad \operatorname{inc} EN = 0. \tag{2.2}$$

Tensor $\operatorname{Curl}^{\mathrm{t}} E$ is called the Frank tensor (see [4–6]).

(c) Some important theorems

Theorem 2.1 (Coercivity [2]). *Let Ω be a bounded and connected domain with C^1-boundary. There exists a constant $C > 0$ s.t. for each $E \in \mathcal{H}_0(\Omega)$, $\|E\|_{H^2(\Omega)} \le C\|\operatorname{inc} E\|_{L^2(\Omega)}$.*

The following result is given for the sake of generality in $L^p(\Omega)$ with $1 < p < \infty$ but should here be considered for $p = 2$.

Theorem 2.2 (Beltrami decomposition [7]). *Assume that Ω is simply connected. Let $p \in (1, +\infty)$ be a real number and let $d \in L^p(\Omega, \mathbb{S}^3)$. Then, for any $v_0 \in W^{1/p,p}(\partial\Omega)$, there exists a unique $v \in W^{1,p}(\Omega, \mathbb{R}^3)$ with $v = v_0$ on $\partial\Omega$ and a unique $F \in L^p(\Omega, \mathbb{S}^3)$ with $\operatorname{Curl} F \in L^p(\Omega, \mathbb{R}^{3\times 3})$, $\operatorname{inc} F \in L^p(\Omega, \mathbb{S}^3)$, $\operatorname{div} F = 0$ and $FN = 0$ on $\partial\Omega$ such that*

$$d = \nabla^{\mathrm{S}} v + \operatorname{inc} F. \tag{2.3}$$

We call $\nabla^{\mathrm{S}} v$ the compatible part and $\operatorname{inc} F$ the (solenoidal) incompatible part of the Beltrami decomposition. Of course, prescribing v on a portion of $\partial\Omega$ only is sufficient for the existence of the decomposition. In fact, for our purpose, uniqueness will not be needed because the decomposition will only serve as a convenient mathematical tool to project our model equations onto orthogonal subspaces. The fields $\nabla^{\mathrm{S}} v$ and $\operatorname{inc} F$ will be said non-objective. It is however important to note that the relation $\operatorname{inc} d = 0 \Rightarrow d = \nabla^{\mathrm{S}} v$ for some $v \in W^{1,p}(\Omega, \mathbb{R}^3)$ (see [7]).

Theorem 2.3 (Divergence-free lifting [2]). *Let $\mathbb{E} \in H^{3/2}(\partial\Omega, \mathbb{S}^3)$ with $\int_{\partial\Omega} \mathbb{E} N \,\mathrm{d}S(x) = 0$, and $\mathbb{G} \in H^{1/2}(\partial\Omega, \mathbb{S}^3)$. There exists $E \in \mathcal{H}(\Omega)$ such that*

$$E = \mathbb{E} \quad \text{on } \partial\Omega,$$

$$(\partial_{\mathrm{N}} E)_{\mathrm{T}} = \mathbb{G}_{\mathrm{T}} \quad \text{on } \partial\Omega,$$

in the sense of traces, where subscript T stands for the restriction to the tangential components.

Lemma 2.4 (Green formula for the incompatibility [2]). *Suppose that* $T \in \mathcal{C}^2(\bar{\Omega}, \mathbb{S}^3)$ *and* $\eta \in H^2(\Omega, \mathbb{S}^3)$*. Then*

$$\int_\Omega T \cdot \operatorname{inc} \eta \, \mathrm{d}x = \int_\Omega \operatorname{inc} T \cdot \eta \, \mathrm{d}x + \int_{\partial\Omega} \mathcal{T}_1(T) \cdot \eta \, \mathrm{d}S(x) + \int_{\partial\Omega} \mathcal{T}_0(T) \cdot \partial_\mathrm{N} \eta \, \mathrm{d}S(x) \tag{2.4}$$

with the trace operators defined as

$$\mathcal{T}_0(T) := (T \times N)^\mathrm{t} \times N \tag{2.5}$$

and

$$\mathcal{T}_1(T) := (\operatorname{Curl}(T \times N)^\mathrm{t})^\mathrm{S} + ((\partial_\mathrm{N} + k) T \times N)^\mathrm{t} \times N + (\operatorname{Curl}^\mathrm{t} T \times N)^\mathrm{S}, \tag{2.6}$$

where k is twice the mean curvature on $\partial\Omega$*.*

Remark 2.5. Alternative expressions for $\mathcal{T}_1(T)$ are given in [2]. In particular,

$$\mathcal{T}_1(T) = -\sum_R k^R (T \times \tau^R)^\mathrm{t} \times \tau^R + ((-\partial_\mathrm{N} + k) T \times N)^\mathrm{t} \times N - 2 \left(\sum_R (\partial_R T \times N)^\mathrm{t} \times \tau^R \right)^\mathrm{S}, \tag{2.7}$$

where (τ_A, τ_B) form an orthonormal basis of the tangent plane to $\partial\Omega$ oriented along the principal directions of curvature and ∂_R stands for the derivative along τ_R.

Remark 2.6. It is not hard to see that every $E \in \mathcal{H}_0(\Omega)$ satisfies $\operatorname{div}(\operatorname{Curl} E)^\mathrm{t} = 0$ in Ω and $\partial_\mathrm{N} E = 0$ on $\partial\Omega$. Moreover, $\int_\Omega \operatorname{inc} E \cdot F \, \mathrm{d}x = \int_\Omega E \cdot \operatorname{inc} F \, \mathrm{d}x$, for every $E, F \in \mathcal{H}_0(\Omega)$.

(d) Some identities in the local basis

Let us consider a local orthonormal basis (τ^A, τ^B, N) on $\partial\Omega$ (for details on such bases and their extension in Ω, cf. [2]). For a general symmetric tensor T, one has in this basis

$$T = \begin{pmatrix} T_{AA} & T_{AB} & T_{AN} \\ T_{BA} & T_{BB} & T_{BN} \\ T_{NA} & T_{NB} & T_{NN} \end{pmatrix}, \quad T \times N = \begin{pmatrix} T_{AB} & -T_{AA} & 0 \\ T_{BB} & -T_{BA} & 0 \\ T_{NB} & -T_{NA} & 0 \end{pmatrix},$$

$$(T \times \tau^A)^\mathrm{t} \times \tau^A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & T_{NN} & -T_{BN} \\ 0 & -T_{NB} & T_{BB} \end{pmatrix}, \quad (T \times \tau^B)^\mathrm{t} \times \tau^B = \begin{pmatrix} T_{NN} & 0 & -T_{AN} \\ 0 & 0 & 0 \\ -T_{NA} & 0 & T_{AA} \end{pmatrix}, \tag{2.8}$$

and

$$(T \times N)^\mathrm{t} \times \tau^A = \begin{pmatrix} 0 & T_{NB} & -T_{BB} \\ 0 & -T_{NA} & T_{BA} \\ 0 & 0 & 0 \end{pmatrix}, \quad (T \times N)^\mathrm{t} \times \tau^B = \begin{pmatrix} -T_{NB} & 0 & T_{AB} \\ T_{NA} & 0 & -T_{AA} \\ 0 & 0 & 0 \end{pmatrix}. \tag{2.9}$$

3. Construction of the model equations for a continuum with dislocations

(a) À-la-d'Alembert method of virtual powers

In this work, the method of virtual power will be considered to produce balance equations for continua with microstructure. In general, this method is used together with the principle of objectivity, in order to select admissible virtual velocity fields. The great advantage of this approach is that it implies no restriction to thermodynamical reversible processes. It is also not specified *a priori* whether the matter is solid or liquid, nor if the solid is elastic or plastic. By virtue of this procedure, which will be briefly recalled, a model is constructed for our purposes in a rational manner, as soon as a set $\mathscr{V} = \mathscr{V}_0 \times \cdots \times \mathscr{V}_\mathrm{N}$ is chosen to represent certain virtual rate fields, as for instance a velocity field, or an elementary displacement taking place during a time interval δt. Let us emphasize that these virtual rate fields need not be a displacement or a velocity, but in general it is the rate of some well-defined kinematical descriptor (not necessarily objective, or frame-invariant, see below). This space of virtual fields is selected together with a chosen number of linear and continuous functionals defined on the Hilbert spaces $\mathscr{V}_i$. In the following, we consider a family of virtual fields $v = (v^0, \ldots, v^N) \in \mathscr{V}_0 \times \cdots \times \mathscr{V}_\mathrm{N}$.

(i) Virtual external power

A first family of linear functionals represents the virtual power of external bulk and contact forces. The virtual power of these external forces writes as (with summation convention on i),

$$\mathscr{P}_{(e)}(v, \Omega) = \langle \Phi^i, v^i \rangle,$$

where $\langle \cdot, \cdot \rangle$ stands for the duality pairing in $\mathscr{V}_i$. Hence, the given (data) field $\Phi^i \in \mathscr{V}_i$ may represent any quantity which is work-conjugate to v^i.

(ii) Virtual intrinsic power

Another family of linear and continuous maps are considered, defining the virtual intrinsic power, that is the power exerted by matter on itself. It is written as

$$\mathscr{P}_{(i)}(v, \Omega) = \langle \Lambda^i, v^i \rangle.$$

The functional structure, i.e. the chosen scalar product, will determine whether v^i alone, or also some of its derivatives will be taken into account in the model equations. Depending on the nature of the generalized velocity v^i, its conjugate field Λ^i may represent either classical or configurational forces [8], as at the present stage we do not distinguish between intrinsic efforts resulting from smooth deformations and those due to microstructural changes.

(iii) General conservation law

D'Alembert principle in the absence of inertia is then stated as

$$\mathscr{P}_{(i)}(v, \Omega) = \mathscr{P}_{(e)}(v, \Omega), \tag{3.1}$$

for all $v \in \mathscr{V}$ satisfying some kinematic assumptions. The latter ones amount to choosing a subspace of $\mathscr{V}$, thus they could have been directly incorporated in $\mathscr{V}$. However, it is generally useful to define the intrinsic power on a larger space, because it is associated with the matter itself and not to a particular configuration, as explained thereafter. Upon incorporating in $\mathscr{V}$ fields accounting for heat transfer, D'Alembert principle expresses the first principle of thermodynamics.

(iv) Objectivity

The virtual intrinsic power determines the internal forces, that is, the forces exerted by the matter on itself. The general velocities that work against these forces are said to be objective, i.e. they are independent of the observer and the kinematic assumptions. Independence of the observer means that these quantities obey the standard rules for the transformation of scalars, vectors, tensors through a roto-translation of the frame with arbitrary speed. It is for example well known that the field 'velocity' is not objective, nor is its gradient, whereas its symmetric part is at least frame-independent [9]. However, our concern is that it is not always possible to define a velocity field in an intrinsic manner. Indeed, the traditional approach of continuum mechanics relies on the definition of a smooth bijective transformation between two configurations of the same material, whereby the velocity is obtained through its time derivative when one of these configurations is chosen as reference. But in the presence of crystal defects like dislocations such a construction is no longer possible [10]. At the microscopic scale, one could think of using a transformation to describe the motion of atoms, but this would be insufficient to describe changes in the crystal arrangement, which nevertheless produce work. For instance, atomic bonds can move while atoms remain fixed. For us the velocity field is only the name given to one element of the Beltrami decomposition [7] of a symmetric tensors d, i.e. $d = \nabla^{\mathrm{S}} v + \operatorname{inc} F$, which is a mere mathematical decomposition of d whose uniqueness relies on the kinematical assumption $v = v_0$ on $\partial\Omega$. Of course a change of frame, which amounts to changing $v_0(x)$ into $v_0(x) + a + \omega \times x$, with (a, ω) the speeds of translation and rotation of the new frame with respect to the former one, does not change either $\nabla^{\mathrm{S}} v$ or $\operatorname{inc} F$ as only $v(x)$ is changed into $v(x) + a + \omega \times x$. But a more

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general change of the boundary condition (like changing v_0) would change the decomposition. We emphasize that neither $\nabla^S v$ nor $\mathrm{inc}\, F$ alone are objective in our generalized sense, simply because they follow from a decomposition which is non-unique. As already mentioned, uniqueness would indeed require to fix boundary conditions for v and F in the Beltrami decomposition, which is by definition dependent on external kinematical constraints.

(b) Model objective tensors: strain and strain rate

In our model, we consider the deformation rate d as the principal objective field. Recall it is a symmetric tensor whose components at point x can be defined in the following manner. Identify three fibres at x, denoted by a_1, a_2, a_3, which at time t are oriented along the axes of a Cartesian coordinate system and of unit lengths. The deformation rate at x is defined as ([11])

$$d_{ij}(t) = \frac{1}{2}\left(\frac{\partial}{\partial t}(a_i \cdot a_j)\right)_t. \tag{3.2}$$

It is easily checked that this definition corresponds to the classical interpretation of the strain rate in linearized or finite elasticity: the diagonal components of d represent unit rates of extension in the coordinate directions, whereas the off-diagonal terms of the rate of deformation tensor represent shear rates, i.e. the rate of change of the right angle between line elements aligned with the coordinate directions. In the presence of dislocations, the above definition can still be used at the microscopic scale, and permits the definition of its macroscopic counterpart by local averaging. We point out that choosing the strain rate as primary unknown is also the main idea of the so-called intrinsic approach of elasticity. However, this approach still hinges on compatibility relations [12].

Now, the Beltrami decomposition yields the vector v and the symmetric and solenoidal tensor F such that

$$d(t) = \nabla^S v(t) + \mathrm{inc}\, F(t). \tag{3.3}$$

For a compatible deformation one has $\mathrm{inc}\, d = \mathrm{inc}\, F = 0$ hence v is determined up to rigid motions [7]. Thus, one recovers the classical picture: for any compatible deformation rate, there exists a unique (up to rigid-body motions) velocity field such that $d = \nabla^S v$, and this symmetric gradient is objective in the classical sense. For smooth fields and fixing boundary conditions, this amounts to the Mitchell–Cesaro path integral formulae [7]. However, in the incompatible case, as for instance in the presence of dislocations, the incompatible strain rate $\mathrm{inc}\, F$ is non-vanishing due to the volumic source $\mathrm{inc}\, d$, and hence, the velocity field appears in conjunction with the symmetric and solenoidal tensor F, which we call the incompatibility tensor field.

Having fixed an initial time $t_0 = 0$, the time integral of the objective tensor d, called the strain or deformation tensor reads

$$\epsilon(t) = \int_0^t d(s)\,\mathrm{d}s = \nabla^S u + \mathrm{inc}\, E, \tag{3.4}$$

where by Beltrami decomposition one has $v = \dot{u}$ and $F = \dot{E}$.

(c) Generalized rate fields for continua with dislocations

(i) The virtual intrinsic power

Following the approach recalled above, the first step in the description of internal efforts is the definition of spaces of objective fields. Our point of view is that the prototype of such fields is the strain rate d, which we henceforth denote by $\hat{d}$ to emphasize that it is a virtual (or test) field. We choose $\mathscr{V}^0 := L^2(\Omega, \mathbb{S}^3)$ as single space of virtual objective fields. Therefore, by the Riesz representation theorem, the intrinsic power generated by the virtual strain rate $\hat{d}$ takes the form

$$\mathscr{P}_{(i)}(\hat{d}, \Omega) = \int_\Omega \Sigma \cdot \hat{d}\,\mathrm{d}x,$$

with $\Sigma \in L^2(\Omega, \mathbb{S}^3)$. In classical models, a constitutive law of form $\Sigma = \mathbb{A}\epsilon$ is chosen; however, it does not take into account the material distortion which we consider as crucial in the modelling of continua with dislocations.

Here, we assume that there exists a partition of Ω as $\Omega = \Omega_1 \sqcup \cdots \sqcup \Omega_n$ with mutually disjoint subsets Ω_i, such that, in each Ω_i, the material is homogeneous and linear in the sense that the intrinsic power generated by the virtual strain $\hat{d} \in \mathcal{C}_0^\infty(\Omega_i, \mathbb{S}^3)$ is the classical Mindlin model [13]

$$\mathscr{P}_{(i)}(\hat{d}, \Omega_i) = \int_{\Omega_i} (\mathbb{A}_i\epsilon \cdot \hat{d} + \mathbb{B}_i\nabla\epsilon \cdot \nabla\hat{d})\,\mathrm{d}x,$$

where $\mathbb{A}_i$ and $\mathbb{B}_i$ are constant second- and third-rank tensors, respectively. In the literature [10,13], $\sigma_i := \mathbb{A}_i\epsilon$ and $\tau_i := \mathbb{B}_i\nabla\epsilon$ are referred to as the stress and the hyperstress tensors in Ω_i, respectively. Recall that all subsequent gradients of $\hat{d}$ are also objective tensors. By the Green formula, one has

$$\mathscr{P}_{(i)}(\hat{d}, \Omega_i) = \int_{\Omega_i} (\sigma_i - \operatorname{div} \tau_i) \cdot \hat{d}\,\mathrm{d}x.$$

Supposing that $\sigma_i - \operatorname{div} \tau_i \in L^2(\Omega, \mathbb{M}^3)$, the above expression extends by continuity to any $\hat{d} \in L^2(\Omega_i, \mathbb{S}^3)$. Hence, we have for an arbitrary strain $\hat{d} \in L^2(\Omega, \mathbb{S}^3)$

$$\mathscr{P}_{(i)}(\hat{d}, \Omega) = \sum_{i=1}^n \mathscr{P}_{(i)}(\hat{d}, \Omega_i) = \sum_{i=1}^n \int_{\Omega_i} (\sigma_i - \operatorname{div} \tau_i) \cdot \hat{d}\,\mathrm{d}x.$$

(ii) The virtual external power

By Beltrami decomposition, $\hat{d}$ can be decomposed in a compatible part and an incompatible part, and the general approach (see [9]) allows the use of these non-objective test fields to describe external actions. However, we believe that exerting surface or volume efforts that work against these fields independently is not very natural as the two fields are combined at every point. Therefore, we suppose that the external power is a linear functional of $\hat{d}$, that is,

$$\mathscr{P}_{(e)}(\hat{d}, \Omega) = \int_\Omega \mathbb{K} \cdot \hat{d}\,\mathrm{d}x,$$

for some given tensor field $\mathbb{K} \in L^2(\Omega, \mathbb{S}^3)$. We emphasize that $\mathbb{K}$ is given by mere functional duality at this stage.

Observe that, considering the decomposition $\hat{d} = \nabla^S\hat{v} + \operatorname{inc}\hat{F}$ and assuming sufficient regularity, integrating by parts using lemma 2.4 yields

$$\mathscr{P}_{(e)}(\hat{d}, \Omega) = \int_\Omega (-\operatorname{div}\mathbb{K} \cdot \hat{v} + \operatorname{inc}\mathbb{K} \cdot \hat{F})\,\mathrm{d}x + \int_{\partial\Omega} (\mathbb{K}N \cdot \hat{v} + \mathcal{T}_0(\mathbb{K}) \cdot \partial_N\hat{F} + \mathcal{T}_1(\mathbb{K}) \cdot \hat{F})\,\mathrm{d}x.$$

Hence, $f := -\operatorname{div}\mathbb{K}$ may be interpreted as a volume force (gravity for instance) and $g := \mathbb{K}N$ as a surface load. The loads $\mathbb{G} := \operatorname{inc}\mathbb{K}, g_0 := \mathcal{T}_0(\mathbb{K}), g_1 := \mathcal{T}_1(\mathbb{K})$ are generalized external forces that work against the incompatible part of $\hat{d}$. Although it is not straightforward to give a precise physical meaning to these quantities, one should remark that it is not possible to prescribe these loads independently. For instance, g and g_1 share common components of $\mathbb{K}$. In fact, the system

$$\left.\begin{aligned} -\operatorname{div}\mathbb{K} = f,\ \operatorname{inc}\mathbb{K} = \mathbb{G} \quad &\text{in } \Omega \\ \mathbb{K}N = g \quad &\text{on } \partial\Omega \end{aligned}\right\}$$

is well posed. This is easily seen with the decomposition $\mathbb{K} = \nabla^S\phi + \operatorname{inc}\mathbb{H}$. The system for ϕ is a Neumann elasticity system with unit elasticity tensor. The system for $\mathbb{H} \in \mathcal{H}_0$ was studied in [2] (note that $\mathbb{H}$ satisfies $\operatorname{inc}\mathbb{H}N = 0$ on $\partial\Omega$). Thus, one can prescribe f, $\mathbb{G}$ and g, but then g_0 and g_1 must be consistent with this choice. More details will be provided in §5c.

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(iii) Equilibrium equations

At this stage, the virtual power principle in weak form reads

$$\sum_{i=1}^{n}\int_{\Omega_i}(\sigma_i - \operatorname{div}\tau_i)\cdot\hat{d}\,\mathrm{d}x = \int_{\Omega}\mathbb{K}\cdot\hat{d}\,\mathrm{d}x, \tag{3.5}$$

for all kinematically admissible $\hat{d}$. This will be our gradient-elasticity model equation.

4. Constitutive laws

(a) General form

Let us concentrate on a set Ω_i and drop the index i. Tensor $\mathbb{A}$ is recognized as Hooke's tensor of linear elasticity. Assuming material isotropy, it admits the classical expression $\mathbb{A} = 2\mu\mathbb{I}_4 + \lambda\mathbb{I}_2$. Similarly, under the same assumption, it is shown in [13] that $\mathbb{B}$ derives from the quadratic form

$$\tfrac{1}{2}\mathbb{B}\nabla\epsilon\cdot\nabla\epsilon = c_1(\partial_j\epsilon_{ij})(\partial_k\epsilon_{ik}) + c_2(\partial_k\epsilon_{ii})(\partial_j\epsilon_{jk}) + c_3(\partial_k\epsilon_{ii})(\partial_k\epsilon_{jj}) + c_4(\partial_k\epsilon_{ij})(\partial_k\epsilon_{ij}) + c_5(\partial_k\epsilon_{ij})(\partial_i\epsilon_{jk})$$

where $c_1, \dots, c_5$ are real numbers. Componentwise, this reads

$$\sigma_{ij} = \lambda\delta_{ij}\epsilon_{kk} + 2\mu\epsilon_{ij} \tag{4.1}$$

and

$$\begin{aligned}\tau_{ijk} = {} & c_1(\delta_{ki}\partial_l\epsilon_{lj} + \delta_{kj}\partial_l\epsilon_{li}) + \frac{c_2}{2}(\delta_{ki}\partial_j\epsilon_{ll} + \delta_{kj}\partial_i\epsilon_{ll} + 2\delta_{ij}\partial_l\epsilon_{lk}) + 2c_3\delta_{ij}\partial_k\epsilon_{ll}\\ & + 2c_4\partial_k\epsilon_{ij} + c_5(\partial_i\epsilon_{jk} + \partial_j\epsilon_{ik}).\end{aligned} \tag{4.2}$$

(b) Consistency with classical linear elasticity

Let us again restrict ourselves to the domain Ω_i. In order to be consistent with standard models, i.e. with models for continua without dislocations, one imposes that the hyperstress τ does not produce any virtual intrinsic power as soon as the strain d is compatible. This means

$$\operatorname{inc}\epsilon = 0 \Rightarrow \int_{\Omega}\tau\cdot\nabla\hat{d}\,\mathrm{d}x = 0, \quad \forall\,\hat{d}\in C_0^{\infty}(\Omega).$$

Integrating by parts yields $\operatorname{inc}\epsilon = 0 \Rightarrow -\operatorname{div}\tau = 0$ in Ω. One obtains from (4.2)

$$(\operatorname{div}\tau)_{ij} = (c_1 + c_5)(\partial_{ik}\epsilon_{jk} + \partial_{jk}\epsilon_{ik}) + c_2(\partial_{ij}\epsilon_{ll} + \delta_{ij}\partial_{kl}\epsilon_{kl}) + 2c_3\delta_{ij}\partial_{kk}\epsilon_{ll} + 2c_4\partial_{kk}\epsilon_{ij}. \tag{4.3}$$

For $\epsilon = \nabla^{\mathrm{S}}u$, one finds

$$\operatorname{div}\tau = (c_1 + c_2 + c_5)\nabla^2\operatorname{div}u + (c_1 + 2c_4 + c_5)\nabla^{\mathrm{S}}\Delta u + (c_2 + 2c_3)\Delta\operatorname{div}u\mathbb{I}_2.$$

This vanishes for every $u\in C_0^{\infty}(\Omega)$ if and only if $c_1 + c_2 + c_5 = 0$, $c_1 + 2c_4 + c_5 = 0$, $c_2 + 2c_3 = 0$. The above system is equivalent to the existence of a scalar ℓ such that $c_1 + c_5 = -\ell$, $c_2 = \ell$,

$c_3 = -\ell/2$, $c_4 = \ell/2$. Plugging this into (4.3) yields

$$(\operatorname{div}\tau)_{ij} = -\ell(\partial_{ik}\epsilon_{jk} + \partial_{jk}\epsilon_{ik}) + \ell(\partial_{ij}\epsilon_{ll} + \delta_{ij}\partial_{kl}\epsilon_{kl}) - \ell\delta_{ij}\partial_{kk}\epsilon_{ll} + \ell\partial_{kk}\epsilon_{ij}.$$

This expression is identical to that found by Lazar & Maugin in [10] (with different arguments), and rewrites as

$$-\operatorname{div}\tau = \ell \operatorname{inc}\epsilon. \tag{4.4}$$

Remark that ℓ has the dimension of a force. Moreover, ℓ can take values in $[0, +\infty[$. It will be called the incompatibility modulus: it is a force that governs strain incompatibility, namely that opposes to incompatibility: if ℓ increases then resistance to incompatibility increases, and in the limit $\ell = +\infty$ classical compatible elasticity is recovered as $\operatorname{inc}\epsilon = 0$. On the contrary, decreasing the value of ℓ means that incompatibility can increase more freely, and the limit $\ell = 0$ corresponds to perfect plasticity because there is no more limit for incompatibility. This interpretation will become clear once the model equations are established.

We emphasize that so far ℓ is taken constant. Indeed, taking ℓ constant in space and time means that we consider a high-order model of elasticity to account for incompatible deformations (which Mindlin has modelled as taking place with specific displacements at a lower scale, but we prefer to simply consider the Beltrami decomposition). We will show in the sequel that our elasto-plasticity model is based on the possibility that ℓ varies in space and time. As a matter of fact, the chosen constitutive law for ℓ will determine our plasticity model. Indeed, plasticity is modelled, as varying ℓ implies by the governing equations that the strain incompatibility varies accordingly, the latter being related to the motion of dislocations, i.e. their mobility.

5. Incompatibility-governed linearized elasticity system

(a) Weak formulation of generalized elasticity

By the above constitutive laws, (3.5) rewrites as

$$\sum_{i=1}^{n} \int_{\Omega_i} (\mathbb{A}_i\epsilon + \ell_i \operatorname{inc}\epsilon)\cdot \hat{d}\,\mathrm{d}x = \int_{\Omega} \mathbb{K}\cdot\hat{d}\,\mathrm{d}x,$$

for all kinematically admissible $\hat{d}$. Defining the functions

$$\mathbb{A} = \sum_{i=1}^{n} \mathbb{A}_i\chi_{\Omega_i}, \quad \ell = \sum_{i=1}^{n} \ell_i\chi_{\Omega_i},$$

with χ_{Ω_i} the characteristic function of Ω_i, we arrive at

$$\int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc}\epsilon)\cdot \hat{d}\,\mathrm{d}x = \int_{\Omega} \mathbb{K}\cdot\hat{d}\,\mathrm{d}x, \tag{5.1}$$

for all kinematically admissible $\hat{d}$. It is a second-gradient model of elasticity, because the operator inc involves two derivatives of the strain. Then, Beltrami's decomposition of $\hat{d}$ yields the coupled system

$$\left.\begin{aligned} \int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc}\epsilon)\cdot \nabla^{\mathrm{S}}\hat{v}\,\mathrm{d}x &= \int_{\Omega} \mathbb{K}\cdot\nabla^{\mathrm{S}}\hat{v}\,\mathrm{d}x \quad \forall\,\hat{v} \qquad (5.2)\\ \int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc}\epsilon)\cdot \operatorname{inc}\hat{F}\,\mathrm{d}x &= \int_{\Omega} \mathbb{K}\cdot\operatorname{inc}\hat{F}\,\mathrm{d}x \quad \forall\,\hat{F}. \qquad (5.3)\end{aligned}\right\}$$

Write the Beltrami decomposition of ϵ as $\epsilon = \nabla^{\mathrm{S}}u + \epsilon^0$, with $\epsilon^0 = \operatorname{inc}E$ and where E is called the internal variable of incompatibility. A typical kinematical framework could be the following. Split the boundary $\partial\Omega$ as the disjoint union of a Dirichlet boundary $\partial\Omega_{\mathrm{D}}$ and a Neumann boundary $\partial\Omega_{\mathrm{N}}$. On $\partial\Omega_{\mathrm{D}}$ fix $u = 0$ and $E = (\partial_{\mathrm{N}}E \times N)^{\mathrm{t}} \times N = 0$. Recall that this latter condition implies $\epsilon^0 N = \operatorname{inc}EN = 0$. This means that the incompatible strain can only be tangential to the Dirichlet boundary. Said otherwise, incompatible (plastic) sliding tangent to the boundary can occur. This is in contrast with the compatible (elastic) strain which has no purely tangential component on the Dirichlet boundary. Let us emphasize that plastic slip is permitted on the Dirichlet part of the boundary even if the deformation is in L^2 and not in a measure space.[2] Of course, the same kinematic restrictions apply to the test fields $\hat{v}$ and $\hat{F}$. With the notations of §3c(ii) we arrive at

$$\left.\begin{aligned} \int_{\Omega} (\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon)\cdot\nabla^{\mathrm{S}}\hat{v}\,\mathrm{d}x &= \int_{\Omega} f\cdot\hat{v}\,\mathrm{d}x + \int_{\partial\Omega_{\mathrm{N}}} g\cdot\hat{v}\,\mathrm{d}x \quad \forall\,\hat{v} \qquad (5.4)\\ \int_{\Omega} (\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon)\cdot\,\mathrm{inc}\,\hat{F}\,\mathrm{d}x &= \int_{\Omega} \mathbb{G}\cdot\hat{F}\,\mathrm{d}x + \int_{\partial\Omega_{\mathrm{N}}} (g_0\cdot\partial_{\mathrm{N}}\hat{F} + g_1\cdot\hat{F})\,\mathrm{d}x \quad \forall\,\hat{F}. \qquad (5.5)\end{aligned}\right\}$$

(b) Strong forms of generalized elasticity

The classical procedure consists in selecting various particular cases of admissible virtual fields $\hat{v}$ and $\hat{F}$. By admissible it is intended from a physical as well as a mathematical standpoint. In particular, appropriate boundary lifting results as well as Gauss–Green-type of formulae must first been established (see [2]). A case study will now be done.

Taking $\hat{v}$ arbitrary in $\bar{\Omega}$, (5.4) classically yields

$$\left.\begin{aligned} -\,\mathrm{div}\,(\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon) &= f \quad \text{a.e. in } \Omega\\ \text{and} \qquad (\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon)N &= g \quad \text{a.e. on } \partial\Omega_{\mathrm{N}}.\end{aligned}\right\} \qquad (5.6)$$

By boundary lifting (i.e. theorem 2.3), one can select $\hat{F}$, $(\partial_{\mathrm{N}}\hat{F})_{\mathrm{T}}$ arbitrary on $\partial\Omega_{\mathrm{N}}$ up to the condition that $\int_{\partial\Omega_{\mathrm{N}}}\hat{F}N\,\mathrm{d}S(x) = 0$. Then, (5.5) yields the additional model equation

$$\left.\begin{aligned} \mathrm{inc}\,(\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon) &= \mathbb{G} \quad \text{a.e. in } \Omega,\\ \mathcal{T}_0(\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon) &= g_0 \quad \text{a.e. on } \partial\Omega_{\mathrm{N}}\\ \text{and} \qquad \mathcal{T}_1(\mathbb{A}\epsilon + \ell\,\mathrm{inc}\,\epsilon) &= g_1 \quad \text{a.e. on } \partial\Omega_{\mathrm{N}}.\end{aligned}\right\} \qquad (5.7)$$

We emphasize that in general equations (5.6) and (5.7) are coupled. In this paper, we do not study existence of solutions for such a system. Furthermore, we observe that if ℓ is constant in space then (5.6) simplifies to the classical elasticity system with the extra boundary force $-\ell\,\mathrm{inc}\,\epsilon N$.

(c) Coupling between external forces

We now investigate the precise relations between the boundary source terms $g = \mathbb{K}N$, $g_0 = \mathcal{T}_0(\mathbb{K})$, $g_1 = \mathcal{T}_1(\mathbb{K})$.

First, we observe that $\mathbb{K}N$ and $\mathcal{T}_0(\mathbb{K})$ have uncoupled components, as this latter only involves the tangential components of $\mathbb{K}$. As for $\mathbb{K}N$ and $\mathcal{T}_1(\mathbb{K})$, one should consider expression (2.7). Let us write g in the local basis (τ^A, τ^B, N) as $g = (g_A, g_B, g_{\mathrm{N}})$. Then, the first curvature-dependent term of (2.7) writes by (2.8) as

$$-\sum_R \kappa^R(\mathbb{K}\times\tau^R)^{\mathrm{t}}\times\tau^R = -\kappa^A\begin{pmatrix}0 & 0 & 0\\ 0 & g_{\mathrm{N}} & -g_B\\ 0 & -g_B & \mathbb{K}_{BB}\end{pmatrix} - \kappa^B\begin{pmatrix}g_{\mathrm{N}} & 0 & -g_A\\ 0 & 0 & 0\\ -g_A & 0 & \mathbb{K}_{AA}\end{pmatrix}. \qquad (5.8)$$

The second curvature-dependent term of (2.7) is $\kappa\mathcal{T}_0(\mathbb{K})$ while two other terms are $-\mathcal{T}_0(\partial_{\mathrm{N}}\mathbb{K})$, and, by (2.9),

$$-2\sum_R(\partial_R\mathbb{K}\times N)^{\mathrm{t}}\times\tau^R = -2\begin{pmatrix}0 & \partial_A g_B & -\partial_A\mathbb{K}_{BB}\\ 0 & -\partial_A g_A & \partial_A\mathbb{K}_{BA}\\ 0 & 0 & 0\end{pmatrix} - 2\begin{pmatrix}-\partial_B g_B & 0 & \partial_B\mathbb{K}_{AB}\\ \partial_B g_A & 0 & -\partial_B\mathbb{K}_{AA}\\ 0 & 0 & 0\end{pmatrix}. \qquad (5.9)$$

From these relations we observe that for a flat boundary, the only coupling is due to the tangential variations of g in (5.9). That is, spatial fluctuations of g (and in the extreme case, discontinuities)

[2] As found in other formulations if the displacement is taken of bounded deformation, see [14–16].

can be considered as sources on incompatibility. For a curved boundary, all terms of g and of the tangential variations of its tangential components will act as source terms for the incompatibility. It is interesting to note that the magnitudes of these terms increase with the curvature. All other source terms, i.e. the tangential components of $\mathbb{K}$ and their tangential derivatives, are not explicitly coupled with the boundary load g. As an example, assume that g_N is the only non-vanishing component of g. Then, the incompatibility source terms vanish for a flat boundary, and increase with the curvature. The limit case of a corner is a particular source of incompatibility.

(d) Interpretation of the incompatibility modulus in terms of dislocation mobility and macroscopic plasticity

When $\ell = 0$, the incompatible part of ϵ is not controlled. On the contrary, when $\ell \to \infty$, (5.3) formally shows that $\operatorname{inc} \epsilon \to 0$. This also holds locally. Now, by Kröner's formula, $\operatorname{inc} \epsilon = \operatorname{Curl} \kappa$ (see [17] for a proof) where κ is the dislocation contortion (or its density) defined by $\kappa = \Lambda - (\mathbb{I}_2/2) \operatorname{tr} \Lambda$, with Λ the dislocation density (with the conservation property $\operatorname{div} \Lambda = 0$). Take a reference value ℓ_∞ large enough so that the incompatible part of the strain is negligible. If ℓ is decreased in some region $\omega \Subset \Omega$, then $\operatorname{inc} \epsilon$ is likely to increase in ω, meaning that κ varies in space so as to increase its curl. This means that motion of dislocations has taken place at a microscopic level, i.e. that plastic effects are observed at a macroscopic level.

(e) Selected examples

Let us recall that in Cartesian coordinates and components, the incompatibility of ε reads *in extenso* as follows

$$\left.\begin{aligned}
T_{xx} &= \partial_y^2 \epsilon_{zz} + \partial_z^2 \epsilon_{yy} - 2\partial_{yz}\epsilon_{yz}\\
T_{yy} &= \partial_x^2 \epsilon_{zz} + \partial_z^2 \epsilon_{xx} - 2\partial_{xz}\epsilon_{xz}\\
T_{zz} &= \partial_x^2 \epsilon_{yy} + \partial_y^2 \epsilon_{xx} - 2\partial_{xy}\epsilon_{xy}\\
T_{xy} &= \partial_z(\partial_y \epsilon_{xz} + \partial_x \epsilon_{yz} - \partial_z \epsilon_{xy}) - \partial_{xy}\epsilon_{zz}\\
T_{xz} &= \partial_y(\partial_x \epsilon_{yz} + \partial_z \epsilon_{xy} - \partial_y \epsilon_{xz}) - \partial_{xz}\epsilon_{yy}\\
\text{and}\quad T_{yz} &= \partial_x(\partial_z \epsilon_{xy} + \partial_y \epsilon_{xz} - \partial_x \epsilon_{yz}) - \partial_{yz}\epsilon_{xx}.
\end{aligned}\right\} \tag{5.10}$$

In this section, we will consider 2*D* elasticity, meaning that the strain ϵ only depends on the coordinates (x, y) and is independent of the vertical coordinate z. Moreover, the stress and strain tensors represented by 3×3 matrices. The geometry is that of a vertical cylinder. We consider an homogeneous material, i.e. ℓ is constant. In this case, (5.10) is rewritten as

$$\left.\begin{aligned}
T_{xx} &= \partial_y^2 \epsilon_{zz}\\
T_{yy} &= \partial_x^2 \epsilon_{zz} + \partial_z^2 \epsilon_{xx} - 2\partial_{xz}\epsilon_{xz}\\
T_{zz} &= \partial_x^2 \epsilon_{yy} - 2\partial_{xy}\epsilon_{xy}\\
T_{xy} &= -\partial_{xy}\epsilon_{zz}\\
T_{xz} &= \partial_y(\partial_x \epsilon_{yz} - \partial_y \epsilon_{xz})\\
\text{and}\quad T_{yz} &= \partial_x(\partial_y \epsilon_{xz} - \partial_x \epsilon_{yz}).
\end{aligned}\right\} \tag{5.11}$$

Furthermore, note that in 2*D*, $T := \operatorname{inc} \epsilon$ vanishes if and only if componentwise $\varepsilon_{ikm}\varepsilon_{jln}\partial_k\partial_l\epsilon_{mn} = 0$, that is, if and only if there exists real numbers K, a_α and b such that [4] $\varepsilon_{\alpha\gamma}\varepsilon_{\beta\delta}\partial_\alpha\partial_\beta\epsilon_{\gamma\delta} = 0$, $\varepsilon_{\alpha\beta}\partial_\alpha\epsilon_{\beta z} = K$, $\epsilon_{zz} = a_\alpha x_\alpha + b$.

(i) Planar strain and edge dislocations

Assume that the strain and stress tensors are of the form

$$\epsilon = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & 0 \\ \epsilon_{xy} & \epsilon_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix},$$

with

$$\left.\begin{array}{ll} \sigma_{xx} = (\lambda + 2\mu)\epsilon_{xx} + \lambda\epsilon_{yy}, & \sigma_{yy} = (\lambda + 2\mu)\epsilon_{yy} + \lambda\epsilon_{xx} \\ \sigma_{xy} = \lambda\epsilon_{xy}, & \sigma_{zz} = \lambda(\epsilon_{xx} + \epsilon_{yy}). \end{array}\right\} \tag{5.12}$$

and

We infer

$$T = \operatorname{inc}\epsilon = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & T_{zz} \end{pmatrix}, \quad \text{with } T_{zz} = \partial_{xx}\epsilon_{yy} - 2\partial_{xy}\epsilon_{xy} + \partial_{yy}\epsilon_{xx}.$$

We find

$$\operatorname{inc}(\sigma + \ell T) = \begin{pmatrix} \partial_{yy}(\sigma_{zz} + \ell T_{zz}) & -\partial_{xy}(\sigma_{zz} + \ell T_{zz}) & 0 \\ -\partial_{xy}(\sigma_{zz} + \ell T_{zz}) & \partial_{xx}(\sigma_{zz} + \ell T_{zz}) & 0 \\ 0 & 0 & \partial_{xx}\sigma_{yy} - 2\partial_{xy}\sigma_{xy} + \partial_{yy}\sigma_{xx} \end{pmatrix},$$

thus $\operatorname{inc}(\sigma + \ell T) = 0$ is equivalent to $\sigma_{zz} + \ell T_{zz}$ affine, and $\operatorname{inc}\sigma_{\text{plan}} := \partial_{xx}\sigma_{yy} - 2\partial_{xy}\sigma_{xy} + \partial_{yy}\sigma_{xx} = 0$. Using (5.12), we get $\sigma_{zz} = (1/2(\lambda + \mu))(\sigma_{xx} + \sigma_{yy})$, whereby we deduce T_{zz}.

If $\ell \to +\infty$ then $T_{zz} \to 0$ and the standard solution is retrieved. Note also that by (5.12) $\operatorname{inc}\sigma_{\text{plan}} = \lambda\Delta\operatorname{tr}\epsilon + 2\mu(\operatorname{inc}\epsilon)_{zz} = \lambda\operatorname{tr}\operatorname{inc}\epsilon + 2\mu\operatorname{inc}\epsilon_{zz} = (\lambda + 2\mu)T_{zz} = 0$. If $\ell \to 0$ then T_{zz} is not controlled.

Following [4] and classical textbooks [18], the edge dislocation in 2D corresponds to a planar strain. At the mesoscopic scale (dislocations are modelled as kinematical singularities), according to [4], the strain associated with a straight line along the z-axis, with Burgers vector $B = B_y e_y$ reads in Cartesian components and polar coordinates as

$$\epsilon_{\text{edge}} = \frac{-B_y}{2\pi r}\begin{pmatrix} \cos\theta & \sin\theta & 0 \\ \sin\theta & -\cos\theta & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

(ii) Transverse strain (3D shear) and screw dislocation

Assume now that the strain and the Cauchy stress read

$$\epsilon = \begin{pmatrix} 0 & 0 & \epsilon_{xz} \\ 0 & 0 & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & 0. \end{pmatrix}, \quad \sigma = 2\mu\epsilon,$$

The incompatibility is purely transverse, namely,

$$T = \operatorname{inc}\epsilon = \begin{pmatrix} 0 & 0 & \partial_{xy}\epsilon_{yz} - \partial_{yy}\epsilon_{xz} \\ 0 & 0 & \partial_{xy}\epsilon_{xz} - \partial_{xx}\epsilon_{yz} \\ \partial_{xy}\epsilon_{yz} - \partial_{yy}\epsilon_{xz} & \partial_{xy}\epsilon_{xz} - \partial_{xx}\epsilon_{yz} & 0 \end{pmatrix}.$$

Following [4,18], the screw dislocation in 2D corresponds to a 3D shear. According to [4], the strain associated with a straight line along the z-axis, with Burgers vector $B = B_z e_z$ reads in Cartesian components and polar coordinates as

$$\epsilon_{\text{screw}} = \frac{B_z}{4\pi r}\begin{pmatrix} 0 & 0 & \sin\theta \\ 0 & 0 & -\cos\theta \\ \sin\theta & -\cos\theta & 0 \end{pmatrix}.$$

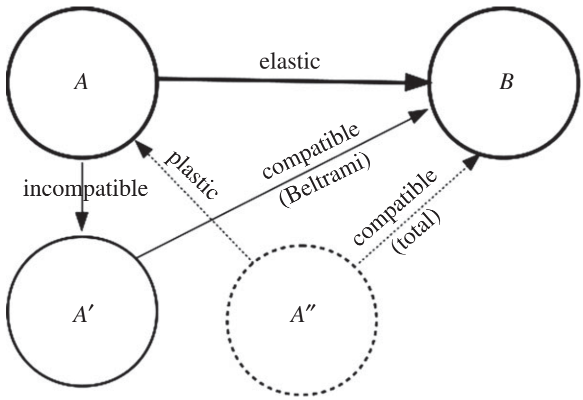

Figure 1. The Beltrami decomposition ($A \longrightarrow A' \longrightarrow B$) versus the standard elastic/plastic decomposition ($A'' \longrightarrow A \longrightarrow B$).

(f) Link with classical elasto-plasticity models

Recall that classical elasto-plasticity models are based on the *a priori* decomposition $\epsilon^{\mathrm{tot}} = \epsilon^{\mathrm{e}} + \epsilon^{\mathrm{p}}$, where the total strain ϵ^{tot} is compatible ($\operatorname{inc} \epsilon^{\mathrm{tot}} = 0$), the elastic strain ϵ^{e} is derived from the Cauchy stress by Hooke's law and the plastic strain ϵ^{p} obeys so-called flow rules. We now compare this decomposition with the Beltrami decomposition $\epsilon = \nabla^{\mathrm{S}} u + \epsilon^0$. As $\operatorname{inc} \epsilon^{\mathrm{tot}} = \operatorname{inc} \nabla^{\mathrm{S}} u = 0$, there exists a vector field w (see [7]) such that $\epsilon^{\mathrm{tot}} = \nabla^{\mathrm{S}} u - \nabla^{\mathrm{S}} w$ and we can write

$$\epsilon^{\mathrm{tot}} = \nabla^{\mathrm{S}} u - \nabla^{\mathrm{S}} w = -(\epsilon^0 + \nabla^{\mathrm{S}} w) + (\nabla^{\mathrm{S}} u + \epsilon^0).$$

We then recognize $\nabla^{\mathrm{S}} u + \epsilon^0$ as the strain ϵ.

The interpretation is the following (figure 1): for us, ϵ represents the deformation from a reference state, say state A to a neighbour state B of the same material. It can be viewed as the composition of the incompatible deformation ϵ^0 from state A to an intermediate state A', and the compatible deformation $\nabla^{\mathrm{S}} u$ from A' to B. In the classical approach, another configuration A'' serves as reference configuration. The total deformation ϵ^{tot} from A'' to B is the sum of the plastic deformation $\epsilon^{\mathrm{p}} = -(\epsilon^0 + \nabla^{\mathrm{S}} w)$ from A'' to A and the elastic deformation $\epsilon^{\mathrm{e}} = \epsilon$ from A to B. Of course, choosing $w = 0$ (thus $A'' = A'$) would be a choice of simplicity, but it would be too restrictive because in that case ϵ^{p} would be identified with $-\epsilon^0$, hence it would not be trace-free and it could not comply with the flow rules.

6. Energy dissipation by incompatibility

(a) Time-rate formulation

For the purpose of evaluating energy dissipation, it is crucial to involve time. Knowing that (5.2) and (5.3) represent a linearized elasticity system (small strain with respect to a natural configuration), their time-rate counterparts in the general case are

$$\left.\begin{aligned} \int_{\Omega} (\mathbb{A}\dot{\epsilon} + \ell \operatorname{inc} \dot{\epsilon}) \cdot \nabla^{\mathrm{S}} \hat{v}\, \mathrm{d}x &= \int_{\Omega} \dot{\mathbb{K}} \cdot \nabla^{\mathrm{S}} \hat{v}\, \mathrm{d}x \qquad (6.1)\\ \int_{\Omega} (\mathbb{A}\dot{\epsilon} + \ell \operatorname{inc} \dot{\epsilon}) \cdot \operatorname{inc} \hat{F}\, \mathrm{d}x &= \int_{\Omega} \dot{\mathbb{K}} \cdot \operatorname{inc} \hat{F}\, \mathrm{d}x, \qquad (6.2) \end{aligned}\right\}$$

with $\dot{\epsilon} = \nabla^{\mathrm{S}} \dot{u} + \dot{\epsilon}^0$, $\dot{\epsilon}^0 = \operatorname{inc} \dot{E}$. In this formulation, $\mathbb{A}$ and ℓ play the role of tangent moduli and only the rates $\dot{\epsilon}$, $\dot{u}$ and $\dot{E}$ are the unknowns of the model. We emphasize that at a given time the solution of (6.1) and (6.2) are not the time derivatives of the solution of (5.2) and (5.3), because $\mathbb{A}$ and ℓ

may vary with time in this general formulation of the model (according to the material stress–strain and hyperstress-incompatibility curves). Indeed, (6.1) and (6.2) should be understood as the time-rate equations of state for a nonlinear model of gradient-elasticity.

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(b) Mechanical dissipation

The work of the external load in the time interval $[t_1, t_2]$ is

$$W_{t_1,t_2} = \int_{t_1}^{t_2} \mathrm{d}t \int_{\Omega} (\mathbb{K} \cdot \nabla^{\mathrm{S}} \dot{u} + \mathbb{K} \cdot \operatorname{inc} \dot{E})\, \mathrm{d}x.$$

Suppose first that ℓ is constant in space and tends to infinity so as to enforce $\operatorname{inc} \dot{\epsilon} = 0$ in the interval $[t_1, t_2]$. Hence, there is no motion of dislocations, that is, no dissipation. This transformation is thus said to be isentropic or reversible. In this case, we have $\dot{\epsilon}_{\mathrm{rev}} = \nabla^{\mathrm{S}} \dot{u}_{\mathrm{rev}}$ and (6.1) becomes

$$\int_{\Omega} \mathbb{A} \dot{\epsilon}_{\mathrm{rev}} \cdot \nabla^{\mathrm{S}} \hat{v}\, \mathrm{d}x = \int_{\Omega} \dot{\mathbb{K}} \cdot \nabla^{\mathrm{S}} \hat{v}\, \mathrm{d}x. \tag{6.3}$$

We assume that $\mathbb{A}$ is time invariant. A standard calculation leads to

$$W^{\mathrm{rev}}_{t_1,t_2} = \int_{t_1}^{t_2} \mathrm{d}t \int_{\Omega} \mathbb{K} \cdot \nabla^{\mathrm{S}} \dot{u}_{\mathrm{rev}}\, \mathrm{d}x = \left[\int_{\Omega} \left(\mathbb{K} \cdot \nabla^{\mathrm{S}} u_{\mathrm{rev}} - \frac{1}{2} \mathbb{A} \nabla^{\mathrm{S}} u_{\mathrm{rev}} \cdot \nabla^{\mathrm{S}} u_{\mathrm{rev}} \right) \mathrm{d}x \right]_{t_1}^{t_2},$$

with $[X]_{t_1}^{t_2} := X(t_2) - X(t_1)$. This quantity corresponds to the increment of free energy Ψ in the time interval $[t_1, t_2]$. The free energy rate is

$$\dot{\Psi} = \int_{\Omega} \mathbb{K} \cdot \nabla^{\mathrm{S}} \dot{u}_{\mathrm{rev}}\, \mathrm{d}x.$$

Let us now come back to a general transformation. The global dissipation rate is defined as the difference between the power provided to the system by external loads and the rate of free energy, i.e. $\mathcal{D} := \dot{W} - \dot{\Psi}$. The power of the external forces is

$$\dot{W} = \int_{\Omega} \mathbb{K} \cdot (\nabla^{\mathrm{S}} \dot{u} + \dot{\epsilon}^0)\, \mathrm{d}x.$$

Still assuming $\mathbb{A}$ time invariant, we obtain

$$\mathcal{D} = \int_{\Omega} \mathbb{K} \cdot (\nabla^{\mathrm{S}} \dot{u} + \dot{\epsilon}^0 - \nabla^{\mathrm{S}} \dot{u}_{\mathrm{rev}})\, \mathrm{d}x. \tag{6.4}$$

We emphasize that the reversible field $\dot{u}_{\mathrm{rev}}$ is independent of ℓ, hence it will not play any role in our subsequent sensitivity analysis.

The dissipation rate can be rewritten in a more classical manner (e.g. [1]) in the following case: consider a time interval in which $\mathbb{A}$ and ℓ are constant (as in an incremental formulation). For simplicity (and without loss of generality), we assume that $\mathbb{K}$ vanishes at $t = 0$. We define $u_{\mathrm{rev}}(t) := \int_0^t \dot{u}_{\mathrm{rev}}(s)\, \mathrm{d}s$ and $\epsilon(t) := \int_0^t \dot{\epsilon}(s)\, \mathrm{d}s$. Integrating in time, the relations (6.1) and (6.2) yield

$$\mathcal{D} = \int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) \cdot (\nabla^{\mathrm{S}}(\dot{u} - \dot{u}_{\mathrm{rev}}) + \dot{\epsilon}^0)\, \mathrm{d}x.$$

This expression shows the dissipation rate as the power of the flux $\dot{\epsilon} - \nabla^{\mathrm{S}} \dot{u}_{\mathrm{rev}}$ against the force $\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon$. By definition, the dissipation rate vanishes when $\ell \to \infty$. Some standard models of plasticity can be written in the form of the principle of maximum dissipation, namely, plasticity occurs so as to maximize the dissipation rate among a given set of internal variable rates [19]. At least, by the second principle of thermodynamics, the dissipation rate must be positive. Thus, in order to model a time-dependent experiment, an evolution law for ℓ has to be determined in such a way that this principle is satisfied. In an incremental formulation, ℓ is constant in each time interval $[t_i, t_{i+1}]$, but the values (they depend on space) need to be fixed. The analysis of the behaviour of $\mathcal{D}$ with respect to the spatial distribution of ℓ is the object of the next sections.

7. Topological sensitivity analysis

(a) Framework

The coupled system (5.4)–(5.5) (or equivalently, (6.1)–(6.2)) seems highly involved from the mathematical point of view. In fact, in this paper dedicated to the presentation of the new model, we have not proven the existence of a solution. In the subsequent analysis, we will restrict ourselves to a simplified model assuming that

(1) the principal part of (6.1)–(6.2) is predominant,
(2) full homogeneous Dirichlet conditions are prescribed.

These assumptions lead to the problem: find $E \in \mathcal{H}_0$ such that

$$\int_\Omega \ell \operatorname{inc} E \cdot \operatorname{inc} F \,\mathrm{d}x = \int_\Omega \mathbb{G} \cdot F \,\mathrm{d}x, \quad \forall F \in \mathcal{H}_0. \tag{7.1}$$

According to [2], this problem is well posed as long as $\ell \in L^\infty(\Omega)$, $\inf_\Omega \ell > 0$, $\mathbb{G} \in L^2(\Omega)$, $\operatorname{div} \mathbb{G} = 0$. Note that from this section on, in comparison with (6.1)–(6.2), E plays the role of $\dot\epsilon^0$ and F that of $\hat F$. In [2], it is also shown that the problem: find $E \in \mathcal{H}_0$ such that

$$\int_\Omega \alpha \mathbb{M}^\star \operatorname{inc} E \cdot \operatorname{inc} F \,\mathrm{d}x = \int_\Omega \mathbb{G} \cdot F \,\mathrm{d}x, \quad \forall F \in H_0, \tag{7.2}$$

with $\mathbb{M}^\star$ a fixed symmetric positive definite fourth-rank tensor, is well posed if $\alpha \in L^\infty(\Omega)$, $\inf_\Omega \alpha > 0$. We will focus on (7.2), choosing

$$\mathbb{M}^\star := \gamma \mathbb{I}_4 + \beta \mathbb{I}_2 \otimes \mathbb{I}_2.$$

Obviously, (7.1) is recovered from (7.2) by taking $\alpha \mathbb{M}^\star = \ell \mathbb{I}_4$.

(b) Preliminaries

Let $\omega \subset \mathbb{R}^d$ with smooth boundary $\partial\omega$ and outward unit normal N. For $\omega_\epsilon := \hat{x} + \epsilon\omega \subset\subset \Omega$, $\epsilon > 0$, we define

$$\alpha_\epsilon = \begin{cases} \alpha_0 & \text{in } \Omega \backslash \omega_\epsilon \\ \alpha_1 & \text{in } \omega_\epsilon \end{cases},$$

with α_0, α_1 two positive constants. We consider a cost functional of form

$$J(E) = \int_\Omega \mathbb{H} \cdot E \,\mathrm{d}x,$$

for a given tensor field $\mathbb{H} \in L^2(\Omega)$, $\operatorname{div} \mathbb{H} = 0$. In particular, choosing $\mathbb{H} = \mathbb{K}$ gives the contribution of the incompatible strain to the dissipation (6.4). Furthermore, the transmission conditions are as follows. If a solenoidal tensor field T satisfies $\operatorname{inc}(\alpha T) = 0$ weakly in a neighbourhood of $\partial\omega$, then it is shown in [2] that the following transmission conditions hold on $\partial\omega_\epsilon$

$$[\![\mathcal{T}_0(\alpha T)]\!] = 0, \quad [\![\mathcal{T}_1(\alpha T)]\!] = 0, \quad [\![TN]\!] = 0. \tag{7.3}$$

By convention, $[\![T]\!] = T_{\mathrm{ext}} - T_{\mathrm{int}}$.

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(c) Formal derivation

The background solution E_0 satisfies

$$a_0(E_0, F) = l(F) := \int_\Omega \mathbb{G} \cdot F \, \mathrm{d}x, \quad \forall F \in \mathcal{H}_0(\Omega), \tag{7.4}$$

with $a_0(E_0, F) := \int_\Omega \alpha_0 \mathbb{M}^\star \operatorname{inc} E_0 \cdot \operatorname{inc} F \, \mathrm{d}x$. Moreover, the perturbed solution E_ϵ satisfies

$$a_\epsilon(E_\epsilon, F) = l(F), \quad \forall F \in \mathcal{H}_0(\Omega), \tag{7.5}$$

with $a_\epsilon(E_\epsilon, F) := \int_\Omega \alpha_\epsilon \mathbb{M}^\star \operatorname{inc} E_\epsilon \cdot \operatorname{inc} F \, \mathrm{d}x$. The cost functional reads

$$j(\epsilon) := J(E_\epsilon) = \int_\Omega \mathbb{H} \cdot E_\epsilon \, \mathrm{d}x, \tag{7.6}$$

and the associated adjoint state $\hat{E}_\epsilon$ satisfies

$$a_\epsilon(E, \hat{E}_\epsilon) = -\int_\Omega \mathbb{H} \cdot E \, \mathrm{d}x, \quad \forall E \in \mathcal{H}_0(\Omega). \tag{7.7}$$

These definitions entail

$$\begin{aligned} \Sigma_\epsilon := j(\epsilon) - j(0) = \int_\Omega \mathbb{H} \cdot (E_\epsilon - E_0) &= -a_\epsilon(E_\epsilon - E_0, \hat{E}_\epsilon) \\ &= -a_\epsilon(E_\epsilon, \hat{E}_\epsilon) + a_\epsilon(E_0, \hat{E}_\epsilon). \end{aligned}$$

Using that $a_\epsilon(E_\epsilon, \hat{E}_\epsilon) = l(\hat{E}_\epsilon) = a_0(E_0, \hat{E}_\epsilon)$, we get

$$\begin{aligned} \Sigma_\epsilon &= -a_0(E_0, \hat{E}_\epsilon) + a_\epsilon(E_0, \hat{E}_\epsilon) = (a_\epsilon - a_0)(E_0, \hat{E}_\epsilon) \\ &= \int_\Omega (\alpha_\epsilon - \alpha_0) \mathbb{M}^\star \operatorname{inc} E_0 \cdot \operatorname{inc} \hat{E}_\epsilon \, \mathrm{d}x. \end{aligned} \tag{7.8}$$

Let us introduce the variation of the adjoint state

$$\tilde{E}_\epsilon := \hat{E}_\epsilon - \hat{E}_0. \tag{7.9}$$

By (7.3), one has

$$\left. \begin{aligned} &\operatorname{inc}(\alpha \mathbb{M}^\star \operatorname{inc} \tilde{E}_\epsilon) = 0 && \text{in } \omega \cup (\Omega \backslash \bar{\omega}) \\ &[\![\alpha_\epsilon \mathcal{T}_i(\mathbb{M}^\star \operatorname{inc} \tilde{E}_\epsilon)]\!] = -(\alpha_0 - \alpha_1) \mathcal{T}_i(\operatorname{inc} \hat{E}_0) && \text{on } \partial\omega, \quad (i = 0, 1) \\ \text{and} \quad &[\![(\mathbb{M}^\star \operatorname{inc} \tilde{E}_\epsilon) N]\!] = \beta [\![\operatorname{tr}(\operatorname{inc} \tilde{E}_\epsilon) N]\!] && \text{on } \partial\omega. \end{aligned} \right\} \tag{7.10}$$

Moreover, (7.8) yields

$$\Sigma_\epsilon = \int_\Omega (\alpha_\epsilon - \alpha_0) \mathbb{M}^\star \operatorname{inc} E_0 \cdot \operatorname{inc} \hat{E}_0 \, \mathrm{d}x + \int_\Omega (\alpha_\epsilon - \alpha_0) \mathbb{M}^\star \operatorname{inc} E_0 \cdot \operatorname{inc} \tilde{E}_\epsilon \, \mathrm{d}x. \tag{7.11}$$

We now approximate $\operatorname{inc} E_0$ and $\operatorname{inc} \hat{E}_0$ in ω_ϵ by the constant tensors $\operatorname{inc} E_0(\hat{x})$ and $\operatorname{inc} \hat{E}_0(\hat{x})$, respectively. This yields

$$\Sigma_\epsilon \sim |\omega_\epsilon| (\alpha_1 - \alpha_0) \mathbb{M}^\star \operatorname{inc} E_0(\hat{x}) \cdot \operatorname{inc} E_0(\hat{x}) + (\alpha_1 - \alpha_0) \operatorname{inc} E_0(\hat{x}) \cdot \int_{\omega_\epsilon} \mathbb{M}^\star \operatorname{inc} \tilde{E}_\epsilon \, \mathrm{d}x.$$

We further approximate $\tilde{E}_\epsilon(x)$ by $\tilde{E}_\epsilon(x) \sim \epsilon^2 H(x/\epsilon)$, solution to the blown-up transmission problem

$$\left. \begin{aligned} &\operatorname{inc}(\mathbb{M}^\star \operatorname{inc} H) = 0 && \text{in } \mathbb{R}^2 \backslash \partial\omega \\ &[\![\alpha \mathcal{T}_i(\mathbb{M}^\star \operatorname{inc} H)]\!] = -(\alpha_0 - \alpha_1) \mathcal{T}_i(\operatorname{inc} \hat{E}_0(\hat{x})) && \text{on } \partial\omega, \quad (i = 0, 1) \\ \text{and} \quad &[\![(\mathbb{M}^\star \operatorname{inc} H) N]\!] = \beta [\![\operatorname{tr}(\operatorname{inc} H) N]\!] && \text{on } \partial\omega. \end{aligned} \right\} \tag{7.12}$$

We write

$$\Sigma_\epsilon \sim |\omega_\epsilon| (\alpha_1 - \alpha_0) \mathbb{M}^\star \operatorname{inc} E_0(\hat{x}) \cdot \operatorname{inc} E_0(\hat{x}) + (\alpha_1 - \alpha_0) \epsilon^2 \operatorname{inc} E_0(\hat{x}) \cdot \int_\omega \mathbb{M}^\star \operatorname{inc} H \, \mathrm{d}x. \tag{7.13}$$

(d) Topological sensitivity

We consider two space dimensions as in §5e. In the sequel, we will denote

$$\mathbb{S} := \operatorname{inc} E_0(\hat{x}), \quad \hat{\mathbb{S}} := \operatorname{inc} \hat{E}_0(\hat{x}), \tag{7.14}$$

and the main unknown of (7.12) by

$$T := \mathbb{M}^\star \operatorname{inc} H, \tag{7.15}$$

where H will be called the scattered field. Our aim is now to compute the contribution

$$\Lambda := (\alpha_1 - \alpha_0) \operatorname{inc} E_0(\hat{x}) \cdot \int_\omega \mathbb{M}^\star \operatorname{inc} H \, dx = (\alpha_1 - \alpha_0)\hat{\mathbb{S}} \cdot \int_\omega T \, dx.$$

Assuming that $T = T^{\text{int}}$ is constant in the interior of the inclusion (this will be proved valid in the sequel for a disc inclusion, see [20]), this rewrites as $\Lambda = (\alpha_1 - \alpha_0)|\omega|\hat{\mathbb{S}} \cdot T^{\text{int}}$. By the problem linearity in $\hat{\mathbb{S}}$, there exists a fourth-rank tensor $\mathbb{P}^\omega_{\alpha_0,\alpha_1}$ such that $T^{\text{int}} = \mathbb{P}^\omega_{\alpha_0,\alpha_1}\hat{\mathbb{S}}$. Hence, (7.13) results in

$$j(\epsilon) - j(0) = \epsilon^2 \delta j + R(\epsilon), \tag{7.16}$$

with

$$\delta j := |\omega|(\alpha_1 - \alpha_0)\mathbb{S} \cdot (\mathbb{M}^\star + \mathbb{P}^\omega_{\alpha_0,\alpha_1})\hat{\mathbb{S}} \tag{7.17}$$

and $R(\epsilon)$ the remainder. The fourth-rank tensor $\mathbb{M}^\star + \mathbb{P}^\omega_{\alpha_0,\alpha_1}$ is called the polarization tensor. Following the lines of [21], it is proved that $R(\epsilon) = o(\epsilon^2)$, whereby δj is identified with the so-called topological derivative of j.

Let the centre of the inclusion $\hat{x}$ be the origin of the chosen coordinate system oriented in such a way that $\hat{\mathbb{S}}$ writes as $\hat{\mathbb{S}} = \hat{\mathbb{S}}^{\text{plan}} + \hat{\mathbb{S}}^{\text{uni}} + \hat{\mathbb{S}}^{\text{trans}}$, where in Cartesian coordinates,

$$\hat{\mathbb{S}}^{\text{plan}} = \begin{pmatrix} \hat{s}_1 & 0 & 0 \\ 0 & \hat{s}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{\mathbb{S}}^{\text{uni}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \hat{s}_3 \end{pmatrix}, \quad \hat{\mathbb{S}}^{\text{trans}} = \begin{pmatrix} 0 & 0 & \hat{s}_4 \\ 0 & 0 & \hat{s}_5 \\ \hat{s}_4 & \hat{s}_5 & 0 \end{pmatrix}. \tag{7.18}$$

In the same basis, we decompose $\mathbb{S}$ as $\mathbb{S} = \mathbb{S}^{\text{plan}} + \mathbb{S}^{\text{uni}} + \mathbb{S}^{\text{trans}}$ with

$$\mathbb{S}^{\text{plan}} = \begin{pmatrix} s_1 & s_{12} & 0 \\ s_{12} & s_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbb{S}^{\text{uni}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & s_3 \end{pmatrix}, \quad \mathbb{S}^{\text{trans}} = \begin{pmatrix} 0 & 0 & s_4 \\ 0 & 0 & s_5 \\ s_4 & s_5 & 0 \end{pmatrix}. \tag{7.19}$$

Lengthy calculations, detailed in [20], lead for ω the unit disc

$$\mathbb{S} \cdot \mathbb{P}^\omega_{\alpha_0,\alpha_1}\hat{\mathbb{S}} = \mathbb{S}^{\text{plan}} \cdot \mathbb{P}^{\text{plan}}_{\alpha_0,\alpha_1}\hat{\mathbb{S}}^{\text{plan}} + \mathbb{S}^{\text{uni}} \cdot \mathbb{P}^{\text{uni}}_{\alpha_0,\alpha_1}\hat{\mathbb{S}}^{\text{uni}} + \mathbb{S}^{\text{trans}} \cdot \mathbb{P}^{\text{trans}}_{\alpha_0,\alpha_1}\hat{\mathbb{S}}^{\text{trans}},$$

where

$$\left.\begin{aligned} &\mathbb{P}^{\text{plan}}_{\alpha_0,\alpha_1} = B\mathbb{I}_4 + \frac{C}{2}\mathbb{I}_2 \otimes \mathbb{I}_2, \\ &\text{with } B = \frac{\gamma(\alpha_0 - \alpha_1)}{\gamma\alpha_1 + (3 + 4\beta)\alpha_0}, \quad C = \frac{2\alpha_0(\alpha_0 - \alpha_1)(\gamma^2 + 5\gamma\beta + 4\beta^2)}{(\gamma\alpha_0 + (\gamma + 2\beta)\alpha_1)(\gamma\alpha_1 + (3\gamma + 4\beta)\alpha_0)}, \end{aligned}\right\} \tag{7.20}$$

$$\mathbb{P}^{\text{uni}}_{\alpha_0,\alpha_1} = -\frac{\alpha_1 - \alpha_0}{\alpha_1}\mathbb{I}_4, \quad \mathbb{P}^{\text{trans}}_{\alpha_0,\alpha_1} = -2\frac{\alpha_1 - \alpha_0}{\alpha_1 + \alpha_0}\mathbb{I}_4. \tag{7.21}$$

It is immediately observed that $\mathbb{P}^{\text{uni}}_{\alpha_0,\alpha_1}$ is degenerated in the sense of [21], i.e.

- — it does not depend on the shape of ω,
- — it does not remain bounded when $\alpha_1 \to 0$.

8. Discussion

(a) Interpretation of the topological derivative

On choosing $\mathbb{M}^\star = \mathbb{I}_4$, the analysis of the two previous sections deals with the situation where the incompatibility modulus $\ell = \alpha$ varies from its background value α_0 to its new value α_1 inside the inclusion.

However, our main goal is to evaluate the dissipation due to dislocation motion/creation, which is by definition an energetic comparison between the elasto-plastic transformation and its purely elastic counterpart. Therefore, we analyse here formula (7.16) when $\alpha_0 \to \infty$, keeping the tensor $\mathbb{M}^\star$ for the sake of generality. Recall the direct and adjoint state equations

$$\int_\Omega \alpha_0 \mathbb{M}^\star \operatorname{inc} E_0 \cdot \operatorname{inc} F = \int_\Omega \mathbb{G} \cdot F, \qquad \forall F \in \mathcal{H}_0,$$
$$\int_\Omega \alpha_0 \mathbb{M}^\star \operatorname{inc} E \cdot \operatorname{inc} \hat{E}_0 = -\int_\Omega \mathbb{H} \cdot E, \quad \forall E \in \mathcal{H}_0.$$

Assume α_0 is constant and set $E_0^\star = \alpha_0 E_0$, $\hat{E}_0^\star = \alpha_0 \hat{E}_0$. It holds by definition

$$\alpha_0 \mathbb{S} = \mathbb{T} := \operatorname{inc} E_0^\star(\hat{x}), \quad \alpha_0 \hat{\mathbb{S}} = \hat{\mathbb{T}} := \operatorname{inc} \hat{E}_0^\star(\hat{x}),$$

while $E_0^\star$, $\hat{E}_0^\star$ are obviously solutions of

$$\int_\Omega \mathbb{M}^\star \operatorname{inc} E_0^\star \cdot \operatorname{inc} F = \int_\Omega \mathbb{G} \cdot F, \qquad \forall F \in \mathcal{H}_0,$$
$$\int_\Omega \mathbb{M}^\star \operatorname{inc} E \cdot \operatorname{inc} \hat{E}_0^\star = -\int_\Omega \mathbb{H} \cdot E, \qquad \forall E \in \mathcal{H}_0.$$

Note that the re-scaled fields $E_0^\star$ and $\hat{E}_0^\star$ are independent of α_0, hence $\mathbb{T}$ and $\hat{\mathbb{T}}$ are also independent of α_0. We rewrite (7.17) as

$$\delta j := |\omega| \left(\frac{\alpha_1}{\alpha_0} - 1\right) \mathbb{T} \cdot \left(\frac{\mathbb{M}^\star + \mathbb{P}^\omega_{\alpha_0,\alpha_1}}{\alpha_0}\right) \hat{\mathbb{T}}. \tag{8.1}$$

From (7.20)–(7.21), we obtain

$$\lim_{\alpha_0 \to \infty} \frac{\mathbb{P}^{\text{plan}}_{\alpha_0,\alpha_1}}{\alpha_0} = 0, \quad \lim_{\alpha_0 \to \infty} \frac{\mathbb{P}^{\text{uni}}_{\alpha_0,\alpha_1}}{\alpha_0} = \frac{\mathbb{I}_4}{\alpha_1}, \quad \lim_{\alpha_0 \to \infty} \frac{\mathbb{P}^{\text{trans}}_{\alpha_0,\alpha_1}}{\alpha_0} = 0.$$

We arrive at

$$\lim_{\alpha_0 \to \infty} \delta j = -\frac{|\omega|}{\alpha_1} \mathbb{T}^{\text{uni}} \cdot \hat{\mathbb{T}}^{\text{uni}}. \tag{8.2}$$

Upon choosing the dissipation rate as cost function, this limiting topological derivative can be viewed as the power done by a thermodynamic force that works against variations of ℓ to dissipate energy (the thermodynamic force tending to zero as $\alpha_0 \to \infty$ as to compensate the divergence of $\alpha_1 - \alpha_0$). It appears that our model is able to represent the effect of plastic nucleation when the strain incompatibility has a non-vanishing uniaxial component. This situation occurs in the presence of edge dislocations. Observe that when $\alpha_1 \to 0$ (perfectly plastic inclusion) the topological derivative δj is likely to diverge, revealing an unbounded dissipation rate. We emphasize that our sensitivity analysis has been restricted to a significantly simplified model. In the full model, additional terms are expected to appear due to the coupling between the incompatible and compatible parts of the strain and also due to the fact that the elasticity tensor $\mathbb{A}$ may take a different value in the inclusion. By (8.2), we remark that in the present model the total dissipation δj does not depend on the shape of the inclusion, but only on its volume. In particular, this means that a plastic crack cannot dissipate energy.

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(b) A quasi-static elasto-plastic evolution scheme

The results of this paper allow us to consider a novel elasto-plastic scheme based on an incremental formulation. Each increment might be computed as follows.

(i) Consider the current configuration as reference configuration and compute the *almost elastic* deformation rate by solving the elasto-plasticity model $\ell = \ell_\infty$ as a background *large* value.
(ii) Compute the topological derivative δj of the dissipation rate.
(iii) Identify the points where $\delta j \geq \eta$, where $\eta > 0$ is a material-dependent threshold[3] (η could be a constant or depend on local material properties).
(iv) At these points, where plasticity occurs, choose a new (lower) value for the incompatibility modulus ℓ.
(v) With this new value, solve the elasto-plasticity model from the reference configuration and update the full deformation.
(vi) Increment the (pseudo)-time and update the load.

This scheme is repeated while the external force $\mathbb{K}$ (whatever the exact meaning at this stage of model development) is increased. The values successively chosen for the incompatibility modulus ℓ and the threshold η should rely on constitutive laws. For instance, some standard elasto-plastic laws can be represented as constraints within the principle of maximum dissipation [19], which in turn could give rise to specific choices of η (as a function of space) through Lagrange multipliers [24]. Strain hardening occurs when the decrease of ℓ in a given region is slower and slower, while the load increases at a fixed speed. Perfect plasticity occurs when ℓ goes to 0 in finite time. Keeping $\ell = \ell_\infty$ permits to recover the (almost) purely elastic case, as in unloading.

(c) Final remark on equation decoupling

Let us finally comment on the coupling between the compatible and incompatible parts of the strain. Recall the full equation

$$\int_\Omega (\mathbb{A}\dot{\epsilon} + \ell \operatorname{inc} \dot{\epsilon}) \cdot \operatorname{inc} \hat{F} \, dx = \int_\Omega \dot{\mathbb{K}} \cdot \operatorname{inc} \hat{F} \, dx. \tag{8.3}$$

In the case of planar strain (as in the typical case of edge dislocations), $\operatorname{inc} \dot{\epsilon}$ is uniaxial. If $\lambda = 0$, then $\mathbb{A}\dot{\epsilon}$ and $\ell \operatorname{inc} \dot{\epsilon}$ have uncoupled components. In particular, taking $\hat{F}$ planar leads to

$$\int_\Omega \ell \operatorname{inc} \dot{\epsilon} \cdot \operatorname{inc} \hat{F} \, dx = \int_\Omega \dot{\mathbb{K}} \cdot \operatorname{inc} \hat{F} \, dx,$$

which is the equation we considered in the simplified model, applying to the incompatible part of $\dot{\epsilon}$. Note also that choosing $\nabla^S \hat{v}$ planar in

$$\int_\Omega (\mathbb{A}\dot{\epsilon} + \ell \operatorname{inc} \dot{\epsilon}) \cdot \nabla^S \hat{v} \, dx = \int_\Omega \dot{\mathbb{K}} \cdot \nabla^S \hat{v} \, dx \tag{8.4}$$

yields

$$\int_\Omega \mathbb{A}\dot{\epsilon} \cdot \nabla^S \hat{v} \, dx = \int_\Omega \dot{\mathbb{K}} \cdot \nabla^S \hat{v} \, dx.$$

If μ is constant, it is the standard linear elasticity system applied to the compatible part of $\dot{\epsilon}$. On the contrary, if $\dot{\epsilon}$ has transverse components, then $\dot{\epsilon}$ and $\operatorname{inc} \dot{\epsilon}$ share common components. Then, in (8.3) coupling occurs between the compatible and incompatible parts of $\dot{\epsilon}$ as soon as μ is not constant. Eventually, the two equations are coupled. This will be further studied in future work.

[3]Quasi-static growth of damage and crack had already been envisaged with the topological derivative in [22,23].

(d) Concluding remarks

In this paper, we have presented and developed from the ground up a novel model for elasto-plastic continua. It is based on the known fact that plasticity is related to dislocation motion, which itself is a source of strain incompatibility. In traditional models, this interdependence is not clear, because there is a superposition of the equilibrium equations (for the elastic strain) and the flow rules (for the plastic strain), as deriving from other arguments. In our model, strain incompatibility is incorporated already in the equilibrium equations, hence showing a more general system than classically adopted. Plastic laws are introduced as soon as a constitutive law for the newly introduced incompatibility modulus is provided. Of course, numerical simulations are now required in order to assess our model. This task is left for future works.

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