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INCOMPATIBILITY-GOVERNED ELASTO-PLASTICITY FOR CONTINUA WITH DISLOCATIONS

SAMUEL AMSTUTZ AND NICOLAS VAN GOETHEM

ABSTRACT. 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 compatibility modulus, that 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., [19]) the total strain ϵ is assumed to satisfy the following two conditions:

- There exists an additive decomposition $\epsilon = \epsilon^e + \epsilon^p$ where the elastic strain satisfies $\epsilon^e = \mathbb{A}^{-1}\sigma$ 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 is compatible, that is, there exists a displacement field u such that $\epsilon = \nabla^S u$.

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, ϵ^p) . It is not discussed here the fact that this approach has provided enough evidences 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 $\nabla^S u$ 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.

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- 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 $\text{inc } \epsilon = \text{Curl } \kappa$. Therefore plasticity is governed by strain incompatibility, which must be considered as a variable of the model equations.
- The second Principle of thermodynamics must hold, and possibly be at the heart of the model since 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 inc inc . A crucial scalar appearing in these equations is the newly-defined compatibility 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 functional¹. 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 increase 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

2.1. 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 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 2nd rank tensors are defined componentwise as follows with the summation convention on repeated indices:

$$\begin{aligned} (\text{div } E)_i &:= \partial_j E_{ij}, \\ (\text{Curl } T)_{ij} &:= (\nabla \times T)_{ij} = \epsilon_{jkm} \partial_k T_{im}, \\ (\text{inc } E)_{ij} &:= (\text{Curl } (\text{Curl } E)^t)_{ij} = \epsilon_{ikm} \epsilon_{jln} \partial_k \partial_l E_{mn}, \\ (N \times T)_{ij} &:= -(T \times N)_{ij} = \epsilon_{jkm} N_k T_{im}. \end{aligned}$$

Here, E and T are 2nd rank tensors, N is a vector, and ϵ is the Levi-Civita 3rd rank tensor. In two space dimensions, $N = N_1 e_1 + N_2 e_2$, hence the curl of T rewrites as

$$(\text{Curl } T)_{i1} = \partial_2 T_{i3}, \quad (\text{Curl } T)_{i2} = -\partial_1 T_{i3}, \quad (\text{Curl } T)_{i3} = \partial_1 T_{i2} - \partial_2 T_{i1}. \quad (2.1)$$

One also has

$$(T \times N)_{i1} = -N_2 T_{i3}, \quad (T \times N)_{i2} = N_1 T_{i3}, \quad (T \times N)_{i3} = N_2 T_{i1} - N_1 T_{i2}. \quad (2.2)$$

Note that by (2.2), $(\text{Curl } E)^t \times N = 0$ means that $(\text{Curl } E)^t e_3 = 0$.

2.2. Function spaces used and preliminary results. Define

$$\begin{aligned} \mathcal{H}(\Omega) &:= \{E \in H^2(\Omega, \mathbb{S}^3), \text{div } E = 0\}, \\ \mathcal{H}_0(\Omega) &:= \{E \in \mathcal{H}(\Omega) : E = (\partial_N E \times N)^t \times N = 0 \text{ on } \partial\Omega\}. \end{aligned} \quad (2.3)$$

These spaces are naturally endowed with the Hilbertian structure of $H^2(\Omega, \mathbb{S}^3)$. Note that $(\partial_N E \times N)^t \times N = 0$ exactly mean that the tangential components of $\partial_N E$ vanish. Furthermore, it is

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

proved in [3] (see also [25]) that the following holds on $\partial\Omega$:

$$E = (\partial_N E \times N)^t \times N = 0 \Rightarrow \text{Curl}^t E \times N = 0 \Rightarrow \text{inc } EN = 0. \quad (2.4)$$

Tensor $\text{Curl}^t E$ is called the Frank tensor (see [30–32]).

2.3. Basic properties. The next lemma is related to the Friedrich inequalities, and for planar domains, a proof can be found in [16]. It basically follows from the simple-connectedness of Ω , the smoothness of its boundary, and from regularity results of Dirichlet and Neumann Laplacian problems. Note that a general Lipschitz boundary is not sufficient, as counterexample show (the classical $\mathcal{C}^{1,1}$ is admissible, though). In 3D we refer to [15, 34] for the proof of such inequalities.

Lemma 1 (Friedrich inequality). *Let $E \in H_{\text{curl}}(\Omega; \mathbb{M}^3)$ be such that $\text{div } E = 0$ in Ω and $E \times N = 0$ on $\partial\Omega$. Then $E \in H^1(\Omega; \mathbb{M}^3)$ and it holds*

$$\|\nabla E\|_{L^2(\Omega)} \leq C \|\text{Curl } E\|_{L^2(\Omega)}. \quad (2.5)$$

The following results can be proven without major difficulty from Lemma 1. Details can be found in [3].

Lemma 2. *For all $E \in \mathcal{H}_0(\Omega)$ it holds*

$$\|E\|_{H^2(\Omega)} \leq C (\|E\|_{L^2(\Omega)} + \|\text{Curl } E\|_{L^2(\Omega)} + \|\text{inc } E\|_{L^2(\Omega)}).$$

Theorem 1 (Poincaré). *Let $\partial\Omega_0 \subset \partial\Omega$ be non flat with $\mathcal{H}^1(\partial\Omega_0) > 0$. There exists a constant $C > 0$ such that for each $u \in H^1(\Omega; \mathbb{R}^3)$,*

$$\|u\|_{L^2(\Omega)} \leq C \left(\|\nabla u\|_{L^2(\Omega)} + \int_{\partial\Omega_0} |u \times N| dS \right). \quad (2.6)$$

Theorem 2 (Coercivity). *Let Ω be a bounded and connected domain with \mathcal{C}^1 -boundary and let a non-flat subset $\partial\Omega_0 \subset \partial\Omega$ with $\mathcal{H}^1(\partial\Omega_0) > 0$. There exists a constant $C > 0$ s.t. for each $E \in \mathcal{H}_0(\Omega)$,*

$$\|E\|_{H^2(\Omega)} \leq C \|\text{inc } E\|_{L^2(\Omega)}. \quad (2.7)$$

2.4. Some important theorems. 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 3 (Beltrami decomposition [20]). *Assume that Ω is simply-connected and let $\partial\Omega_0 \subset \partial\Omega$ with $\mathcal{H}^1(\partial\Omega_0) > 0$. Let $p \in (1, +\infty)$ be a real number and let $d \in L^p(\Omega; \mathbb{S}^3)$. Then, for any $v_0 \in W^{1/p,p}(\partial\Omega_0)$, there exists a unique $v \in W^{1,p}(\Omega; \mathbb{R}^3)$ with $v = v_0$ on $\partial\Omega_0$ and a unique $F \in L^p(\Omega; \mathbb{S}^3)$ with $\text{Curl } F \in L^p(\Omega; \mathbb{R}^{3 \times 3})$, $\text{inc } F \in L^p(\Omega; \mathbb{S}^3)$, $\text{div } F = 0$ and $FN = 0$ on $\partial\Omega$ such that*

$$d = \nabla^S v + \text{inc } F. \quad (2.8)$$

We call $\nabla^S v$ the compatible part and $\text{inc } F$ the (solenoidal) incompatible part of the Beltrami decomposition.

Theorem 4 (Divergence-free lifting [3]). *Let $\mathbb{E} \in H^{3/2}(\partial\Omega; \mathbb{S}^3)$ with $\int_{\partial\Omega} \mathbb{E} N dS(x) = 0$, and $\mathbb{G} \in H^{1/2}(\partial\Omega; \mathbb{S}^3)$. There exists $E \in \mathcal{H}(\Omega)$ such that*

$$\begin{cases} E = \mathbb{E} & \text{on } \partial\Omega, \\ (\partial_N E)_T = \mathbb{G}_T & \text{on } \partial\Omega, \end{cases}$$

in the sense of traces.

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

$$\int_{\Omega} T \cdot \text{inc } \eta dx = \int_{\Omega} \text{inc } T \cdot \eta dx + \int_{\partial\Omega} \mathcal{T}_1(T) \cdot \eta dS(x) + \int_{\partial\Omega} \mathcal{T}_0(T) \cdot \partial_N \eta dS(x) \quad (2.9)$$

with the trace operators defined as

$$\mathcal{T}_0(T) := (T \times N)^t \times N, \quad (2.10)$$

$$\mathcal{T}_1(T) := (\text{Curl} (T \times N)^t)^S + ((\partial_N + k)T \times N)^t \times N + (\text{Curl}^t T \times N)^S, \quad (2.11)$$

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

Remark 1. Alternative expressions for $\mathcal{T}_1(T)$ are given in [3]. In particular,

$$\mathcal{T}_1(T) = - \sum_R k^R (T \times \tau^R)^t \times \tau^R + ((-\partial_N + k)T \times N)^t \times N - 2 \left(\sum_R (\partial_R T \times N)^t \times \tau^R \right)^S, \quad (2.12)$$

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 . In two space dimensions, one has

$$\mathcal{T}_1(T) = -k(T \times \tau)^t \times \tau + ((-\partial_N + k)T \times N)^t \times N - 2((\partial_\tau T \times N)^t \times \tau)^S \quad (2.13)$$

$$= k(T \times \tau)^t \times \tau - ((\partial_N + k)T \times N)^t \times N - 2\partial_\tau ((T \times N)^t \times \tau)^S, \quad (2.14)$$

where ∂_τ stands for the derivative along the tangent vector τ .

Remark 2. It is not hard to see that every $E \in \mathcal{H}_0(\Omega)$ satisfies $\text{div} (\text{Curl } E)^t = 0$ in Ω and $\partial_N E = 0$ on $\partial\Omega$. Moreover,

$$\int_\Omega \text{inc } E \cdot F dx = \int_\Omega E \cdot \text{inc } F dx,$$

for every $E, F \in \mathcal{H}_0(\Omega)$.

2.5. 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. [3]). For a general symmetric tensor T , one has in this basis:

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

$$(T \times N)^t \times N = \begin{pmatrix} T_{BB} & -T_{AB} & 0 \\ -T_{AB} & T_{AA} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.15)$$

In the same token,

$$(T \times \tau^A)^t \times \tau^A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & T_{NN} & -T_{BN} \\ 0 & -T_{NB} & T_{BB} \end{pmatrix}, \quad (T \times \tau^B)^t \times \tau^B = \begin{pmatrix} T_{NN} & 0 & -T_{AN} \\ 0 & 0 & 0 \\ -T_{NA} & 0 & T_{AA} \end{pmatrix}, \quad (2.16)$$

and,

$$(T \times \tau^A)^t \times \tau^B = \begin{pmatrix} 0 & 0 & 0 \\ -T_{NN} & 0 & T_{AN} \\ T_{NB} & 0 & -T_{AB} \end{pmatrix}, \quad (T \times \tau^B)^t \times \tau^A = \begin{pmatrix} 0 & -T_{NN} & T_{BN} \\ 0 & 0 & 0 \\ 0 & T_{NA} & -T_{BA} \end{pmatrix}. \quad (2.17)$$

Similarly,

$$(T \times N)^t \times \tau^A = \begin{pmatrix} 0 & T_{NB} & -T_{BB} \\ 0 & -T_{NA} & T_{BA} \\ 0 & 0 & 0 \end{pmatrix}, \quad (T \times N)^t \times \tau^B = \begin{pmatrix} -T_{NB} & 0 & T_{AB} \\ T_{NA} & 0 & -T_{AA} \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.18)$$

3. CONSTRUCTION OF THE MODEL EQUATIONS FOR A CONTINUUM WITH DISLOCATIONS

3.1. 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. This procedure is originally attributed to the French mechanician J. Le Rond d'Alembert [18], as based on the first thoughts on this concept by Aristotle [5] (see also the Cossera brothers works [6]). A certain revival of the method was experienced in the 70ies thanks to three other French mechanicians P. Germain [11–13], P. Suquet [28] and G. Maugin [21], following the theory of distributions by L. Schwartz [26] and its consequences for mathematical modelling. Since then, it has been rather seldom used in theoretical works, being preferred by Hamiltonian variational principles. Yet, this principle is still considered for the construction of elasto-plastic models (see e.g., [8, 23]), in the Russian school with a slightly different formalism by Sedov [27] and more recently by Zubov [35] in the context of dislocations, and also by the Italian school of Mechanics [8, 9, 24].

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 $\mathcal{V} = \mathcal{V}_0 \times \dots \times \mathcal{V}_N$ 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 must not be a displacement or a velocity, but in general it is the rate of some well-defined deformation field (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 \mathcal{V}_i . In the following we consider a family of virtual fields $v = (v^0, \dots, v^N) \in \mathcal{V}_0 \times \dots \times \mathcal{V}_N$.

3.1.1. Virtual external power. These linear functionals represent on the one hand the virtual power of external volume and contact forces. The virtual power of these external forces writes as (with summation convention on i),

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

where $\langle \cdot, \cdot \rangle$ stands for the duality pairing in \mathcal{V}_i . In the traditional presentation of the method, the given (data) fields Φ^i represent either the generalized bulk or contact forces, respectively. The former have their origin in distant systems interacting with the system under analysis, whereas the latter are generalized loads exerted on the boundary. One should bear in mind that being generalized means that these need not be Newtonian forces, and also need not have the dimension of a force. Furthermore, note that we are at liberty to set Φ^i vanishing for certain $0 \leq i \leq N$, if there is no physical evidence for the associated volume and contact forces Φ^i . It is crucial to have in mind that this choice together with the selection of virtual rate fields will determine the model ingredient and associated governing equations.

3.1.2. Virtual intrinsic power. On the other hand, another family of linear and continuous maps are defined, defining the virtual internal power, that is the power exerted by matter on itself. It is written as

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

The functional structure, i.e., the chosen scalar product, will determine whether v^k alone, or also some of its derivatives will be taken into account in the model equations.

3.1.3. General conservation law. D'Alembert principle in the absence of inertia is then stated as

$$\mathcal{P}_{(i)}(v, \Omega) = \mathcal{P}_{(e)}(v, \Omega), \quad (3.1)$$

for all $v \in \mathcal{V}$ satisfying some kinematic assumptions. The latter ones amount to choosing a subspace of \mathcal{V} , thus they could have been directly incorporated in \mathcal{V} . However, it is sometimes useful to define the internal power on a larger space, since it is associated to the matter itself

and not to a particular configuration. Upon incorporating in \mathcal{V} fields accounting to heat transfer, D'Alembert principle is equivalent to the First Principle of thermodynamics.

Note that it is redundant to state D'Alembert principle in any subset $\Pi \subset \Omega$, since the virtual fields might be taken as arbitrary, that is, might be taken vanishing in the complementary set of any such Π . Note also that in some cases there is no need to define the internal and external powers independently, since prescribing the external first and considering invariance, among other principles, is sufficient to construct the model equations (see [8]). Nevertheless the general procedure described above (see [21] for detail) is interesting because it allows one to construct new models, and not only to recover known ones. This is mainly due to the selection of the kinematic variables in \mathcal{V} , which if chosen as nonstandard will automatically provide nonstandard laws. Furthermore, this procedure is not only elegant, it also bears a mathematical structure, that of duality, which is of interest for modelling purposes. In fact, since the procedure is based on functional duality, the larger \mathcal{V} , the finer will be the knowledge of the generalized forces, that is, of the mechanisms acting on the continuum and its microstructure.

3.1.4. Objectivity. The virtual internal 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. In the classical theory of continuum mechanics [21], it is postulated that rigid virtual deformations of the body do not generate internal power. A convenient formulation of this statement is to select spaces $\{\mathcal{V}_i, i \in I_{\text{obj}}\}$ of objective fields, that is, fields that vanish whenever a rigid deformation is considered, and to set $\Lambda^i = 0$ for all $i \notin I_{\text{obj}}$. As an example, it is well-known that the virtual field “velocity” is not objective, and nor is its gradient, whereas its symmetric part is objective.

However, our concern is that it is not always possible to define a velocity field in an intrinsic manner. Classically, the velocity is the time derivative of the displacement field, and hence any reference configuration has disappeared from its definition. Our standpoint is that the displacement cannot be considered as a first model variable, even for eventually defining a symmetric velocity gradient, which would be objective in a classical sense². Indeed, in the presence of crystal defects like dislocations the traditional approaches of continuum mechanics based on material transformations do not apply [17], and the notion of intrinsic velocity is not clearly defined at any scale. For instance, at the microscopic (atomic) scale, bonds can move while atoms remain fixed. For us the velocity field is the name given to one element of the Beltrami decomposition [20] of a symmetric tensors d , i.e., $d = \nabla^S v + \text{inc } F$, which is a mere mathematical decomposition of d .

3.2. Model objective tensors: strain and strain rate. In our model, we consider the deformation rate d as the principal objective field. In classical continuum mechanics, in a Galilean frame, and for an absolute Newtonian chronology, the value of d is intrinsic, i.e., it is univoquely defined and determined for any two observers in relative motion (but still considering the same origin of time). Specifically, it is a symmetric tensor whose components at point x can be defined in the following manner. Identify three fibers 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 (see, e.g., [10])

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

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

²For us, the displacement is even “less objective” because integrating a rigid velocity $v(P) = v(O) + \omega \times \overline{OP}$, where O is a reference point and P any other point while ω is the instantaneous angular velocity, would require to fix a reference point in a reference configuration. Of course the displacement gradient and even its symmetric part are not objective, because something which is not intrinsic, viz., the arbitrary choice of the reference configuration, is required for its definition.

the coordinate directions. In the presence of defects, the above definition can still be used at the microscopic scale, and permits to define its mesoscopic (defects are kinematic singularities) and macroscopic (defects are distributed) counterparts by local averaging (outside the defects in the first case, everywhere in the second case).

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

$$d(t) = \nabla^S v(t) + \text{inc } F(t). \quad (3.3)$$

For a compatible deformation one has $\text{inc } d = \text{inc } F = 0$ hence v is determined up to rigid motions [20]. 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 [20]. However, in the incompatible case, as for instance in the presence of dislocations, the incompatible strain rate $\text{inc } F$ is nonvanishing due to the volumic source $\text{inc } d$, and hence, the velocity field appears in conjunction with the symmetric and solenoidal tensor F , which we call the incompatibility tensor field.

It is now crucial to remark that neither $\nabla^S v$ nor $\text{inc } F$ are objective, simply because they follow from a decomposition which is nonunique. Uniqueness would indeed require to fix boundary conditions for v and F in the Beltrami decomposition, which is by definition dependent on external constraints.

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

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

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

3.3. Generalized rate fields for continua with dislocations.

3.3.1. 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 $\mathcal{V}^0 := L^2(\Omega, \mathbb{S}^3)$ as single space of virtual objective fields. Therefore, by the Riesz representation theorem, the internal power generated by the virtual strain rate \hat{d} takes the form

$$\mathcal{P}_{(i)}(\hat{d}, \Omega) = \int_{\Omega_i} \sigma \cdot \hat{d} \, dx,$$

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 distorsion which we consider as crucial in the modeling of continua with dislocations.

Here, we assume that there exists a partition of Ω as $\Omega = \Omega_1 \sqcup \dots \sqcup \Omega_N$ in mutually disjoint subsets Ω_i , such that, in each Ω_i , the material is homogeneous and linear in the sense that the internal power generated by the virtual strain $\hat{d} \in \mathcal{C}_0^\infty(\Omega_i, \mathbb{S}^3)$ is the classical Mindlin model [22]

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

where \mathbb{A}_i and \mathbb{B}_i are constant second and third order tensors, respectively. In the literature [17, 22], $\sigma_i := \mathbb{A}_i \epsilon$ 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

$$\mathcal{P}_{(i)}(\hat{d}, \Omega_i) = \int_{\Omega_i} (\sigma_i - \text{div } \tau_i) \cdot \hat{d} \, dx.$$

Supposing that $\sigma_i - \operatorname{div} \tau_i \in L^2(\Omega, \mathbb{R}^{3 \times 3})$, 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 $\hat{d} \in L^2(\Omega, \mathbb{S}^3)$

$$\mathcal{P}_{(i)}(\hat{d}, \Omega) = \sum_{i=1}^N \mathcal{P}_{(i)}(\hat{d}, \Omega_i) = \sum_{i=1}^N \int_{\Omega_i} (\sigma_i - \operatorname{div} \tau_i) \cdot \hat{d} \, dx.$$

3.3.2. 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 [21]) allows to use 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 since the two fields are combined at every point. Therefore, we suppose that the external power is a linear functional of \hat{d} , that is,

$$\mathcal{P}_{(e)}(\hat{d}, \Omega) = \int_{\Omega} \mathbb{K} \cdot \hat{d} \, dx,$$

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 3 yields

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

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

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

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 [3] (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 detail will be provided in Section 5.3.

3.3.3. Equilibrium equations. At this stage the virtual power principle in weak form reads

$$\sum_{i=1}^N \int_{\Omega_i} (\sigma_i - \operatorname{div} \tau_i) \cdot \hat{d} \, dx = \int_{\Omega} \mathbb{K} \cdot \hat{d} \, dx, \quad (3.5)$$

for all kinematically admissible \hat{d} .

4. CONSTITUTIVE LAWS

4.1. 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 [22] that \mathbb{B} derives from the quadratic form

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

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

$$\sigma_{ij} = \lambda \delta_{ij} \epsilon_{kk} + 2\mu \epsilon_{ij} \quad (4.1)$$

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

4.2. 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

$$\text{inc } \epsilon = 0 \Rightarrow \int_{\Omega} \tau \cdot \nabla \hat{d} \, dx = 0 \quad \forall \hat{d} \in \mathcal{C}_0^\infty(\Omega).$$

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

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

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

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

This vanishes for every $u \in \mathcal{C}_0^\infty(\Omega)$ 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 $c_1 + c_5 = -\ell$, $c_2 = \ell$, $c_3 = -\frac{\ell}{2}$, $c_4 = \frac{\ell}{2}$. Plugging this into (4.3) yields

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

This expression is identical to that found by Lazar and Maugin in [17] (with different arguments), and rewrites as

$$-\text{div } \tau = \ell \text{inc } \epsilon. \quad (4.4)$$

Remark that ℓ has the dimension of a force. Moreover ℓ can take values in $[0, +\infty[$. It will be called the compatibility modulus: it is a force that opposes to incompatibility. If ℓ increases then the resistance to compatibility increases, that is, incompatibility decreases, and in the limit $\ell = +\infty$ classical compatible elasticity is recovered, since $\text{inc } \epsilon = 0$. On the contrary decreasing values of ℓ means that incompatibility increases more freely, and in the limit, $\ell = 0$ means perfect plasticity, since there is no more limit for incompatibility. This interpretation will become clear once the model equations will be 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 modeled 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, since 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. THE GENERALIZED ELASTICITY SYSTEM

5.1. Weak formulation. By the above constitutive laws, (3.5) rewrites as

$$\sum_{i=1}^N \int_{\Omega_i} (\mathbb{A}_i \epsilon + \ell_i \text{inc } \epsilon) \cdot \hat{d} \, dx = \int_{\Omega} \mathbb{K} \cdot \hat{d} \, dx \quad \forall \hat{d},$$

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

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

we arrive at

$$\int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) \cdot \hat{d} \, dx = \int_{\Omega} \mathbb{K} \cdot \hat{d} \, dx \quad \forall \hat{d}, \quad (5.1)$$

for all kinematically admissible \hat{d} . Then, Beltrami's decomposition of \hat{d} yields the coupled system

$$\int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) \cdot \nabla^S \hat{v} \, dx = \int_{\Omega} \mathbb{K} \cdot \nabla^S \hat{v} \, dx \quad \forall \hat{v}, \quad (5.2)$$

$$\int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) \cdot \operatorname{inc} \hat{F} \, dx = \int_{\Omega} \mathbb{K} \cdot \operatorname{inc} \hat{F} \, dx \quad \forall \hat{F}. \quad (5.3)$$

Write the Beltrami decomposition of ϵ as $\epsilon = \nabla^S u + \epsilon^0$, 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 $\partial\Omega_D$ and a Neumann boundary $\partial\Omega_N$. On $\partial\Omega_D$ fix $u = 0$ and $E = (\partial_N E \times N)^t \times N = 0$. 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 to 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 space³. Of course, the same kinematic restrictions apply to the test fields \hat{v} and \hat{F} . With the notations of section 3.3.2 we arrive at

$$\int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) \cdot \nabla^S \hat{v} \, dx = \int_{\Omega} f \cdot \hat{v} \, dx + \int_{\partial\Omega} g \cdot \hat{v} \, dx \quad \forall \hat{v}, \quad (5.4)$$

$$\int_{\Omega} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) \cdot \operatorname{inc} \hat{F} \, dx = \int_{\Omega} \mathbb{G} \cdot \hat{F} \, dx + \int_{\partial\Omega} (g_0 \cdot \partial_N \hat{F} + g_1 \cdot \hat{F}) \, dx \quad \forall \hat{F}. \quad (5.5)$$

5.2. Derivation of the strong forms. 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 [3]). A case study will now be done.

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

$$\begin{cases} -\operatorname{div} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) &= f & \text{a.e. in } \Omega, \\ (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon)N &= g & \text{a.e. on } \partial\Omega_N. \end{cases} \quad (5.6)$$

By boundary lifting (i.e., Theorem 4) one can select $\hat{F}, \partial_N \hat{F}$ arbitrary on $\partial\Omega$ up to the condition that $\int_{\partial\Omega} \hat{F} N dS(x) = 0$. Then, (5.5) yields the additional model equation

$$\begin{cases} \operatorname{inc} (\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) &= \mathbb{G} & \text{a.e. in } \Omega, \\ \mathcal{T}_0(\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) &= g_0 & \text{a.e. on } \partial\Omega_N, \\ \mathcal{T}_1(\mathbb{A}\epsilon + \ell \operatorname{inc} \epsilon) &= g_1 & \text{a.e. on } \partial\Omega_N. \end{cases} \quad (5.7)$$

We emphasize that in general Eqs. (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 $-\ell \operatorname{inc} \epsilon N$.

5.3. Coupling between external forces. We now investigate the precise relation between the boundary source terms $g = \mathbb{K}N$, $g_0 = T_0(\mathbb{K})$, $g_1 = T_1(\mathbb{K})$.

First we observe that $\mathbb{K}N$ and $\mathcal{T}_0(\mathbb{K})$ are obviously decoupled, since this latter only involves the tangent components of \mathbb{K} . As for $\mathbb{K}N$ and $\mathcal{T}_1(\mathbb{K})$, one should consider expression (2.12). Let us

³as found in other formulations if the displacement is taken of bounded deformation, see [7, 28, 29].

write g in the local basis (τ^A, τ^B, N) as $g = (g_A, g_B, g_N)$. Then the first curvature-dependent term of (2.12) writes by (2.16) as

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

The second curvature-dependent term of (2.12) is $\kappa \mathcal{T}_0(\mathbb{K})$ while two other terms are $-\mathcal{T}_0(\partial_N \mathbb{K})$, and, by (2.18),

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

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), 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 notice 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 explicetely coupled with the boundary load g .

As an example, assume that g_N is the only nonvanishing 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.

5.4. Interpretation of the compatibility modulus in terms of dislocation mobility and macroscopic plasticity. When $\ell = 0$, the incompatible part of ϵ is not controlled. On the contrary, when $\ell \rightarrow \infty$, (5.3) formally shows that $\text{inc } \epsilon \rightarrow 0$. This also holds locally. Now, by Kröner's formula, $\text{inc } \epsilon = \text{Curl } \kappa$ where κ is the dislocation contortion (or its density) defined by $\kappa = \Lambda - \frac{1}{2} \text{tr} \Lambda$, with Λ the dislocation density (with the conservation property $\text{div } \Lambda = 0$).

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 $\text{inc } \epsilon$ 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.

5.5. Selected examples. Let us recall that in Cartesian coordinates and components, the incompatibility of ϵ reads in extenso as follows

$$\begin{cases} T_{xx} = & \partial_y^2 \epsilon_{zz} + \partial_z^2 \epsilon_{yy} - 2\partial_{yz} \epsilon_{zy} \\ T_{yy} = & \partial_x^2 \epsilon_{zz} + \partial_z^2 \epsilon_{xx} - 2\partial_{xz} \epsilon_{zx} \\ T_{zz} = & \partial_x^2 \epsilon_{yy} + \partial_y^2 \epsilon_{xx} - 2\partial_{xy} \epsilon_{xy} \\ T_{xy} = & \partial_z (\partial_y \epsilon_{xz} + \partial_x \epsilon_{yz} - \partial_z \epsilon_{xy}) - \partial_{xy} \epsilon_{zz} \\ T_{xz} = & \partial_y (\partial_x \epsilon_{yz} + \partial_z \epsilon_{xy} - \partial_y \epsilon_{xz}) - \partial_{xz} \epsilon_{yy} \\ T_{yz} = & \partial_x (\partial_z \epsilon_{xy} + \partial_y \epsilon_{xz} - \partial_x \epsilon_{yz}) - \partial_{yz} \epsilon_{xx}. \end{cases} \quad (5.10)$$

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

$$\begin{cases} T_{xx} = & \partial_y^2 \epsilon_{zz} \\ T_{yy} = & \partial_x^2 \epsilon_{zz} + \partial_z^2 \epsilon_{xx} - 2\partial_{xz} \epsilon_{zx} \\ T_{zz} = & \partial_x^2 \epsilon_{yy} - 2\partial_{xy} \epsilon_{xy} \\ T_{xy} = & -\partial_{xy} \epsilon_{zz} \\ T_{xz} = & \partial_y (\partial_x \epsilon_{yz} - \partial_y \epsilon_{xz}) \\ T_{yz} = & \partial_x (\partial_y \epsilon_{xz} - \partial_x \epsilon_{yz}). \end{cases} \quad (5.11)$$

Furthermore, note that in $2D$, $T := \text{inc } \varepsilon$ vanishes iff componentwise $\epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l\varepsilon_{mn} = 0$, that is, iff there exists real numbers K, a_α and b such that [32]

$$\begin{cases} \epsilon_{\alpha\gamma}\epsilon_{\beta\delta}\partial_\alpha\partial_\beta\varepsilon_{\gamma\delta} &= 0 \\ \epsilon_{\alpha\beta}\partial_\alpha\varepsilon_{\beta z} &= K \\ \varepsilon_{zz} &= a_\alpha x_\alpha + b. \end{cases} \quad (5.12)$$

5.5.1. Planar strain and edge dislocations. Consider a two-dimensional problem where the strain is of form

$$\varepsilon = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

By Hooke's law it follows

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

with

$$\begin{aligned} \sigma_{xx} &= (\lambda + 2\mu)\varepsilon_{xx} + \lambda\varepsilon_{yy}, & \sigma_{yy} &= (\lambda + 2\mu)\varepsilon_{yy} + \lambda\varepsilon_{xx}, \\ \sigma_{xy} &= \lambda\varepsilon_{xy}, & \sigma_{zz} &= \lambda(\varepsilon_{xx} + \varepsilon_{yy}). \end{aligned} \quad (5.13)$$

We infer

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

We have

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

thus $\text{inc } (\sigma + \ell T) = 0$ is equivalent to

$$\sigma_{zz} + \ell T_{zz} \text{ affine, and } \text{inc } \sigma_{plan} := \partial_{xx}\sigma_{yy} - 2\partial_{xy}\sigma_{xy} + \partial_{yy}\sigma_{xx} = 0. \quad (5.14)$$

Using (5.13) we get

$$\sigma_{zz} = \frac{1}{2(\lambda + \mu)}(\sigma_{xx} + \sigma_{yy}).$$

From (5.14), we deduce T_{zz} . Furthermore, $(\text{div } \sigma + \ell \text{inc } \varepsilon)_z = 0$ hence f_z must vanish to maintain planar strains, whatever the value of ℓ .

If $\ell \rightarrow +\infty$ then $T_{zz} \rightarrow 0$ and the standard solution is retrieved. Note that by (5.13) $\text{inc } \sigma_{plan} = \lambda\Delta \text{tr } \varepsilon + 2\mu(\text{inc } \varepsilon)_{zz} = \lambda \text{tr inc } \varepsilon + 2\mu \text{inc } \varepsilon_{zz} = (\lambda + 2\mu)T_{zz} = 0$. If $\ell \rightarrow 0$ then T_{zz} is not controlled.

Following [32] and classical textbooks [14] the edge dislocation in $2D$ corresponds to a planar strain. At the mesoscopic scale, according to [32], the strain associated to a straight line along the z -axis, with Burgers vector $B = B_y e_y$ reads in Cartesian components and polar coordinates as

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

5.5.2. Pure vertical compression/dilation. Consider a two-dimensional problem where the strain and the Cauchy stress read

$$\varepsilon = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}, \quad \sigma = \begin{pmatrix} \lambda\varepsilon_{zz} & 0 & 0 \\ 0 & \lambda\varepsilon_{zz} & 0 \\ 0 & 0 & (\lambda + 2\mu)\varepsilon_{zz} \end{pmatrix}.$$

The incompatibility is purely planar, i.e.,

$$T = \text{inc } \varepsilon = \begin{pmatrix} \partial_{yy}\varepsilon_{zz} & -\partial_{xy}\varepsilon_{zz} & 0 \\ -\partial_{xy}\varepsilon_{zz} & \partial_{xx}\varepsilon_{zz} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

For $N = (0, 0, 1)^t$ we have

$$(T \times N)^t \times N = \begin{pmatrix} \partial_{xx}\varepsilon_{zz} & \partial_{xy}\varepsilon_{zz} & 0 \\ \partial_{xy}\varepsilon_{zz} & \partial_{yy}\varepsilon_{zz} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (5.15)$$

hence the conditions $\mathcal{T}_0(T) = \mathcal{T}_1(T) = 0$ are equivalent to ε_{zz} and σ affine, and thus $T = 0$.

5.5.3. Transverse strain (3D shear) and screw dislocation. Assume now that the strain and the Cauchy stress read

$$\varepsilon = \begin{pmatrix} 0 & 0 & \varepsilon_{xz} \\ 0 & 0 & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & 0 \end{pmatrix}, \quad \sigma = 2\mu\varepsilon,$$

and where the independent variables are the planar x and y only. The incompatibility is purely transverse, i.e.,

$$T = \text{inc } \varepsilon = \begin{pmatrix} 0 & 0 & \partial_{xy}\varepsilon_{yz} - \partial_{yy}\varepsilon_{xz} \\ 0 & 0 & \partial_{xy}\varepsilon_{xz} - \partial_{xx}\varepsilon_{yz} \\ \partial_{xy}\varepsilon_{yz} - \partial_{yy}\varepsilon_{xz} & \partial_{xy}\varepsilon_{xz} - \partial_{xx}\varepsilon_{yz} & 0 \end{pmatrix},$$

and for $N = (0, 0, 1)^t$, the condition $(T \times N)^t \times N = 0$ is automatically satisfied.

Following [14, 32] the screw dislocation in $2D$ corresponds to a $3D$ shear. According to [32], the strain associated to a straight line along the z -axis, with Burgers vector $B = B_z e_z$ reads in Cartesian components and polar coordinates as

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

6. ENERGY DISSIPATION BY INCOMPATIBILITY

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

$$\int_{\Omega} (\mathbb{A}\dot{\epsilon} + \ell \text{inc } \dot{\epsilon}) \cdot \nabla^S \hat{v} \, dx = \int_{\Omega} \dot{\mathbb{K}} \cdot \nabla^S \hat{v} \, dx, \quad (6.1)$$

$$\int_{\Omega} (\mathbb{A}\dot{\epsilon} + \ell \text{inc } \dot{\epsilon}) \cdot \text{inc } \hat{F} \, dx = \int_{\Omega} \dot{\mathbb{K}} \cdot \text{inc } \hat{F} \, dx, \quad (6.2)$$

with $\epsilon = \nabla^S u + \epsilon^0$, $\epsilon^0 = \text{inc } E$. The work of the external load in the time interval $[t_1, t_2]$ is

$$W_{t_1}^{t_2} = \int_{t_1}^{t_2} dt \int_{\Omega} (\mathbb{K} \cdot \nabla^S \dot{u} + \mathbb{K} \cdot \text{inc } \dot{E}) \, dx.$$

Suppose first that ℓ is constant in space and tends to infinity so as to enforce $\text{inc } \dot{E} = 0$ in the interval $[t_1, t_2]$. Hence, there is no motion of dislocations, that is, no dissipation. This transformation is thus said isentropic. We also assume that \mathbb{A} is time invariant. Integration by parts in time entails that

$$W_{t_1}^{t_2} = \int_{t_1}^{t_2} dt \int_{\Omega} \mathbb{K} \cdot \nabla^S \dot{u} \, dx = \left[\int_{\Omega} \mathbb{K} \cdot \nabla^S u \, dx \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \int_{\Omega} \dot{\mathbb{K}} \cdot \nabla^S u \, dx.$$

Using (6.1) we obtain

$$W_{t_1}^{t_2} = \left[\int_{\Omega} \mathbb{K} \cdot \nabla^S u \, dx \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \int_{\Omega} (\mathbb{A} \dot{\epsilon} + \ell \operatorname{inc} \dot{\epsilon}) \cdot \nabla^S u \, dx.$$

Since $\dot{\epsilon} = \nabla^S \dot{u}$ we get

$$W_{t_1}^{t_2} = \left[\int_{\Omega} \mathbb{K} \cdot \nabla^S u \, dx \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \int_{\Omega} \mathbb{A} \nabla^S \dot{u} \cdot \nabla^S u \, dx = \left[\int_{\Omega} \left(\mathbb{K} \cdot \nabla^S u - \frac{1}{2} \mathbb{A} \nabla^S u \cdot \nabla^S u \right) dx \right]_{t_1}^{t_2}.$$

Recalling the relation $\delta W = d\Psi$ for a reversible process, we define the free energy as

$$\Psi := \int_{\Omega} \left(\mathbb{K} \cdot \nabla^S u - \frac{1}{2} \mathbb{A} \nabla^S u \cdot \nabla^S u \right) dx.$$

It determines how much work the system can produce. Of course, Ψ is defined up to an additive constant. Here it is chosen so that $\Psi = 0$ corresponds to the reference state $u = 0$.

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,

$$\mathcal{D} := \dot{W} - \dot{\Psi}.$$

The power of the external forces is

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

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

$$\mathcal{D} = \int_{\Omega} \left(\mathbb{K} \cdot \dot{\epsilon}^0 - \dot{\mathbb{K}} \cdot \nabla^S u + \mathbb{A} \nabla^S \dot{u} \cdot \nabla^S u \right) dx,$$

which by (6.1) yields

$$\mathcal{D} = \int_{\Omega} \left(\mathbb{K} \cdot \dot{\epsilon}^0 - (\mathbb{A}(\nabla^S \dot{u} + \dot{\epsilon}^0) + \ell \operatorname{inc} \dot{\epsilon}^0) \cdot \nabla^S u + \mathbb{A} \nabla^S \dot{u} \cdot \nabla^S u \right) dx,$$

and after simplification

$$\mathcal{D} = \int_{\Omega} \left(\mathbb{K} \cdot \dot{\epsilon}^0 - (\mathbb{A} \dot{\epsilon}^0 + \ell \operatorname{inc} \dot{\epsilon}^0) \cdot \nabla^S u \right) dx. \quad (6.3)$$

Comparing with classical formulae for the dissipation (cf. e.g. [19]), one recognizes $\dot{\epsilon}^0$ as the counterpart of the rate of plastic strain. The other quantities are specific for incompatibility-based models.

By definition, the dissipation rate vanishes when $\ell \rightarrow \infty$, since $\dot{\epsilon}^0 \rightarrow 0$. Some standard models of plasticity postulate that plasticity occurs so as to maximize the dissipation. At least, by the Second Principle of thermodynamics, it has to 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 behavior of \mathcal{D} with respect to the spatial distribution of ℓ is the object of the next sections.

Consider a time increment starting from the reference configuration (or obtained from it by rigid displacement). Then the incompatibility-induced dissipation reads

$$\mathcal{D} = \int_{\Omega} \mathbb{K} \cdot \dot{\epsilon}^0 dx, \quad (6.4)$$

showing that the incompatible part of \mathbb{K} is a direct potential source of dissipation. More precisely, assuming homogeneous boundary condition for E , one has $\mathcal{D} = \int_{\Omega} \mathbb{G} \cdot \dot{E} dx$, where $\mathbb{G} := \operatorname{inc} \mathbb{K}$ is the thermodynamic force associated to the internal variable E (i.e., $\dot{\epsilon}^0 = \operatorname{inc} \dot{E}$).

7. TOPOLOGICAL SENSITIVITY ANALYSIS

7.1. 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 Dirichlet conditions are prescribed.

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

$$\int_{\Omega} \ell \operatorname{inc} E \cdot \operatorname{inc} F dx = \int_{\Omega} \mathbb{G} \cdot F dx \quad \forall F \in \mathcal{H}_0. \quad (7.1)$$

According to [3] 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 ϵ^0 and F that of \hat{F} .

In [3] it is also shown that the problem: find $E \in \mathcal{H}_0$ such that

$$\int_{\Omega} \alpha \mathbb{M}^* \operatorname{inc} E \cdot \operatorname{inc} F dx = \int_{\Omega} \mathbb{G} \cdot F dx \quad \forall F \in H_0, \quad (7.2)$$

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

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

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

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

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

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

$$J(E) = \int_{\Omega} \mathbb{H} \cdot E dx,$$

for a given tensor field $\mathbb{H} \in L^2(\Omega)$, $\operatorname{div} \mathbb{H} = 0$. In particular, choosing $\mathbb{H} = \mathbb{K}$, this gives 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 neighborhood of $\partial\omega$ then it is shown in [3] that the following transmission conditions hold on $\partial\omega_\epsilon$:

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

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

7.3. Formal derivation. The background solution E_0 satisfies

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

with

$$a_0(E_0, F) := \int_{\Omega} \alpha_0 \mathbb{M}^* \operatorname{inc} E_0 \cdot \operatorname{inc} F dx. \quad (7.5)$$

Moreover, the perturbed solution E_ϵ satisfies

$$a_\epsilon(E_\epsilon, F) = l(F) \quad \forall F \in \mathcal{H}_0(\Omega), \quad (7.6)$$

with

$$a_\epsilon(E_\epsilon, F) := \int_{\Omega} \alpha_\epsilon \mathbb{M}^* \operatorname{inc} E_\epsilon \cdot \operatorname{inc} F dx. \quad (7.7)$$

The cost functional reads

$$j(\epsilon) := J(E_\epsilon) = \int_{\Omega} \mathbb{H} \cdot E_\epsilon dx, \quad (7.8)$$

where the adjoint state \hat{E}_ϵ satisfies

$$a_\epsilon(E, \hat{E}_\epsilon) = - \int_{\Omega} \mathbb{H} \cdot E dx \quad \forall E \in \mathcal{H}_0(\Omega). \quad (7.9)$$

These definitions entail

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

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

$$\Sigma = -a_0(E_0, \hat{E}_\epsilon) + a_\epsilon(E_0, \hat{E}_\epsilon) = (a_\epsilon - a_0)(E_0, \hat{E}_\epsilon) = \int_{\Omega} (\alpha_\epsilon - \alpha_0) \mathbb{M}^* \text{inc } E_0 \cdot \text{inc } \hat{E}_\epsilon dx. \quad (7.10)$$

Let us introduce the variation of the adjoint state

$$\tilde{E}_\epsilon := \hat{E}_\epsilon - \hat{E}_0. \quad (7.11)$$

By (7.3), one has

$$\begin{cases} \text{inc } (\alpha \mathbb{M}^* \text{inc } \tilde{E}_\epsilon) &= 0 \quad \text{in } \omega \cup (\Omega \setminus \bar{\omega}), \\ \llbracket \alpha_\epsilon \mathcal{T}_i(\mathbb{M}^* \text{inc } \tilde{E}_\epsilon) \rrbracket &= -(\alpha_0 - \alpha_1) \mathcal{T}_i(\text{inc } \hat{E}_0) \quad \text{on } \partial\omega, \quad (i = 0, 1), \\ \llbracket (\mathbb{M}^* \text{inc } \tilde{E}_\epsilon) N \rrbracket &= \beta \llbracket \text{tr}(\text{inc } \tilde{E}_\epsilon) N \rrbracket \quad \text{on } \partial\omega. \end{cases} \quad (7.12)$$

Moreover (7.10) yields

$$\Sigma = \int_{\Omega} (\alpha_\epsilon - \alpha_0) \mathbb{M}^* \text{inc } E_0 \cdot \text{inc } \hat{E}_0 dx + \int_{\Omega} (\alpha_\epsilon - \alpha_0) \mathbb{M}^* \text{inc } E_0 \cdot \text{inc } \tilde{E}_\epsilon dx. \quad (7.13)$$

We now approximate $\text{inc } E_0$ and $\text{inc } \hat{E}_0$ in ω_ϵ by $\text{inc } E_0(\hat{x})$ and $\text{inc } \hat{E}_0(\hat{x})$, respectively, where \hat{x} is the center of ω_ϵ . This yields

$$\Sigma \sim |\omega_\epsilon| (\alpha_1 - \alpha_0) \mathbb{M}^* \text{inc } E_0(\hat{x}) \cdot \text{inc } E_0(\hat{x}) + (\alpha_1 - \alpha_0) \text{inc } E_0(\hat{x}) \cdot \int_{\omega_\epsilon} \mathbb{M}^* \text{inc } \tilde{E}_\epsilon dx.$$

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

$$\begin{cases} \text{inc } (\mathbb{M}^* \text{inc } H) &= 0 \quad \text{in } \mathbb{R}^2 \setminus \partial\omega, \\ \llbracket \alpha \mathcal{T}_i(\mathbb{M}^* \text{inc } H) \rrbracket &= -(\alpha_0 - \alpha_1) \mathcal{T}_i(\text{inc } \hat{E}_0(\hat{x})) \quad \text{on } \partial\omega, \quad (i = 0, 1), \\ \llbracket (\mathbb{M}^* \text{inc } H) N \rrbracket &= \beta \llbracket \text{tr}(\text{inc } H) N \rrbracket \quad \text{on } \partial\omega. \end{cases} \quad (7.14)$$

Recalling the notation $\Sigma := j(\epsilon) - j(0)$, we write

$$\Sigma \sim |\omega_\epsilon| (\alpha_1 - \alpha_0) \mathbb{M}^* \text{inc } E_0(\hat{x}) \cdot \text{inc } E_0(\hat{x}) + (\alpha_1 - \alpha_0) \epsilon^2 \text{inc } E_0(\hat{x}) \cdot \int_{\omega} \mathbb{M}^* \text{inc } H dx. \quad (7.15)$$

7.4. Topological sensitivity. In the sequel we will denote

$$\mathbb{S} := \text{inc } E_0(\hat{x}), \quad \hat{\mathbb{S}} := \text{inc } \hat{E}_0(\hat{x}), \quad (7.16)$$

and the main unknown of (7.14) by

$$T := \mathbb{M}^* \text{inc } H, \quad (7.17)$$

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

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

Assuming that $T = T^{\text{int}}$ is constant in the interior of the inclusion (this will be proved valid in the sequel for a disk inclusion), 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 4th-rank tensor $\mathbb{P}_{\alpha_0, \alpha_1}^\omega$ such that $T^{\text{int}} = \mathbb{P}_{\alpha_0, \alpha_1}^\omega \hat{\mathbb{S}}$. Hence (7.15) results in

$$j(\epsilon) - j(0) = \epsilon^2 \delta j + R(\epsilon), \quad (7.18)$$

with

$$\delta j := |\omega|(\alpha_1 - \alpha_0)\mathbb{S} \cdot (\mathbb{M}^* + \mathbb{P}_{\alpha_0, \alpha_1}^\omega) \hat{\mathbb{S}} \quad (7.19)$$

and $R(\epsilon)$ the remainder. The 4th-rank tensor $\mathbb{M}^* + \mathbb{P}_{\alpha_0, \alpha_1}^\omega$ is called the polarization tensor. Following the lines of [2] it is proved that $R(\epsilon) = o(\epsilon^2)$, whereby δj is identified with the topological derivative of j .

Let the center 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,

$$\hat{\mathbb{S}}^{\text{plan}} = \begin{pmatrix} \hat{s}_1 & 0 & 0 \\ 0 & \hat{s}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{\mathbb{S}}^{\text{uni}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \hat{s}_3 \end{pmatrix}, \quad \hat{\mathbb{S}}^{\text{trans}} = \begin{pmatrix} 0 & 0 & \hat{s}_4 \\ 0 & 0 & \hat{s}_5 \\ \hat{s}_4 & \hat{s}_5 & 0 \end{pmatrix}. \quad (7.20)$$

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

$$\mathbb{S}^{\text{plan}} = \begin{pmatrix} s_1 & s_{12} & 0 \\ s_{12} & s_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbb{S}^{\text{uni}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & s_3 \end{pmatrix}, \quad \mathbb{S}^{\text{trans}} = \begin{pmatrix} 0 & 0 & s_4 \\ 0 & 0 & s_5 \\ s_4 & s_5 & 0 \end{pmatrix}. \quad (7.21)$$

Lengthy calculations, detailed in [4], lead for ω the unit disk,

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

where

$$\begin{aligned} \mathbb{P}_{\alpha_0, \alpha_1}^{\text{plan}} &= B\mathbb{I}_4 + \frac{C}{2}\mathbb{I}_2 \otimes \mathbb{I}_2, \\ B &= \frac{\gamma(\alpha_0 - \alpha_1)}{\gamma\alpha_1 + (3 + 4\beta)\alpha_0}, \quad C = \frac{2\alpha_0(\alpha_0 - \alpha_1)(\gamma^2 + 5\gamma\beta + 4\beta^2)}{(\gamma\alpha_0 + (\gamma + 2\beta)\alpha_1)(\gamma\alpha_1 + (3\gamma + 4\beta)\alpha_0)} \\ \mathbb{P}_{\alpha_0, \alpha_1}^{\text{uni}} &= -\frac{\alpha_1 - \alpha_0}{\alpha_1}\mathbb{I}_4, \quad \mathbb{P}_{\alpha_0, \alpha_1}^{\text{trans}} = -2\frac{\alpha_1 - \alpha_0}{\alpha_1 + \alpha_0}\mathbb{I}_4. \end{aligned} \quad (7.22)$$

It is immediately observed that $\mathbb{P}_{\alpha_0, \alpha_1}^{\text{uni}}$ is degenerated in the sense of [2], i.e.,

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

8. DISCUSSION

8.1. Interpretation of the topological derivative. On choosing $\mathbb{M}^* = \mathbb{I}_4$, the analysis of the two previous sections deals with the situation where the compatibility 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 (7.18) when $\alpha_0 \rightarrow \infty$, keeping the tensor \mathbb{M}^* for the sake of generality. Recall the direct and adjoint state equations

$$\begin{aligned} \int_{\Omega} \alpha_0 \mathbb{M}^* \text{inc } E_0 \cdot \text{inc } F &= \int_{\Omega} \mathbb{G} \cdot F \quad \forall F \in \mathcal{H}_0, \\ \int_{\Omega} \alpha_0 \mathbb{M}^* \text{inc } E \cdot \text{inc } \hat{E}_0 &= - \int_{\Omega} \mathbb{H} \cdot E \quad \forall E \in \mathcal{H}_0. \end{aligned}$$

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

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

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

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

Note that the rescaled 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 . Rewrite (7.19) as

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

From (7.22)-(7.23) we obtain

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

We arrive at

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

Therefore, it appears that our model is able to represent the effect of plastic nucleation when the strain incompatibility has a nonvanishing uniaxial component. This situation occurs in the presence of edge dislocations. Observe that when $\alpha_1 \rightarrow 0$ (perfectly plastic inclusion) the topological derivative δj is likely to diverge, revealing an unbounded dissipation rate.

Consider now a more complete case where the compatible strain is assumed to be fixed while \mathbb{A} is not neglected and varies in the inclusion (as well-known in plasticity). In the topological gradient we have the additional term

$$\delta j_{\mathbb{A}} = 2|\omega|(\mathbb{A}_1 - \mathbb{A}_0)E \cdot \hat{\mathbb{T}}.$$

In the typical situation of screw dislocations E and $\hat{\mathbb{T}}$ have transverse components, hence this term does not vanish.

By (8.2), we remark that in this 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.

8.2. 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 first a reference configuration in which $\ell = \ell_0$ has a background *large* value.
- (ii) Compute the topological derivative δj of the total dissipation.
- (iii) Identify the points where $\delta j \geq \eta$, where $\eta > 0$ is a material-dependent constant⁴ (in a complete model, left for future work, η would depend on $\mathbb{A}, \ell, \nabla^S u$ and ϵ^0).
- (iv) At these points, where plasticity occurs, choose a new (lower) value for the compatibility modulus ℓ .

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 compatibility modulus should rely on a constitutive law. For instance, 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 $\ell = \ell_0$ permits to recover the (almost) purely elastic case, as in unloading.

⁴Quasi-static growth of damage and crack had already been envisaged with the topological derivative in [1, 33].

8.3. 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

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

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

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

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

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

yields

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

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.

8.4. 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, since 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 compatibility 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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