A SECOND-ORDER MODEL OF SMALL-STRAIN INCOMPATIBLE ELASTICITY

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Abstract. This work deals with the modeling of solid continua undergoing incompatible deformations due to the presence of microscopic defects like dislocations. Our approach relies on a geometrical description of the medium by the strain tensor and the representation of internal efforts using zero-th and second-order strain gradients in an infinitesimal framework. At the same time, energetic arguments allow to monitor the corresponding moduli. We provide mathematical and numerical results to support these ideas in the framework of isotropic constitutive laws.

1. Introduction

We propose this contribution in the wake of previous work on this topic, and with the purpose to eventually settle a firm framework for the macroscopic description of elasto-plastic behaviors of deformable solids based on the strain incompatibility concept. The starting point of this approach is Kröner's celebrated work [24] on geometric elasticity with defects showing the link between strain incompatibility and the density of dislocations (see also [38]). Indeed, plasticity is a phenomenon of deformation of metals made possible by the motion and/or creation or annihilation of dislocation loops inside the crystal, on or outside specific glide planes. As soon as dislocations are non-homogeneously distributed inside the crystal, the strain incompatibility ceases to vanish and thus we prospect a model where strain incompatibility, besides strain itself, plays a central role. The choice of the strain field as main kinematical variable is also a specificity of our approach, and is similar in spirit to Ph. Ciarlet's and coauthors' recent works on intrinsic elasticity [14]. By this choice we intentionally depart from the conventional standpoint of considering the displacement (or the deformation map) as the main kinematical variable. Indeed, in our approach, it is crucial to base the model on objective quantities, such as the strain rate or the strain increment, instead of the displacement which relies on the existence of a one-to-one and smooth enough deformation with respect to some reference configuration. Also, by this choice we adopt a geometric setting for the kinematical descriptors, with the strain understood as a metric and the incompatibility as the linearization of the associated Riemann curvature tensor (see [8,13,27]). The derivation of the model will be based on the principle of virtual work exposed in a systematic way by d'Alembert in his *Traité de dynamique* of 1758. Indeed, it appears to us as the most natural in its expression, due to its generality, rigor in its application if attention is paid to the notion of objective descriptors (here we follow the approach advocated by Germain [18] and Maugin [28]), and appropriateness to the mathematical treatment since a variational or weak form is readily obtained. Moreover, to infer strong forms and prescribe relevant boundary conditions and loads, it is required to carefully study the associated functional spaces, as we have done in [6,9], including orthogonal decompositions of these spaces in the spirit of Leray's projection which is classically used in fluid mechanics. The interpretation of these boundary conditions was until now an open problem that we also address here through a mesoscopic analysis, that is at a scale where the dislocations are singularity lines, the so-called Volterra dislocations [1,39]. Indeed, we propose interpretations in terms of "micro-hard" and "micro-free" in the spirit of Gurtin and Needleman [20], though our models diverge from the start. However, in our general macroscopic setting, as opposed to other works by the second author (e.g., [32,33]), dislocations are not represented by geometric field singularities. This

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is also in contrast to Gurtin and Needleman's crystal plasticity model where local slip systems are prescribed. We also display a construction of the strain we deal with from a mesoscopic analysis, basically adding to the displacement symmetric gradient a correction term in order to account for the highly nonlinear deformations and the decohesion effects concentrated in dislocation cores.

We emphasize that at the averaged macroscopic scale the body is a continuum medium filled with dislocations at a smaller scale, represented by a tensor field called the density of dislocations (in the spirit of Kröner and our previous works). However, the model itself does not directly involve the dislocation density field, but its effect on constitutive laws. Moreover, in this work we assume that plasticity is driven by the motion of dislocations only, neglecting disclinations at all scales. Further, infinitesimal deformations are considered, thereby justifying to linearize also the Riemann curvature tensor, yielding the strain incompatibility, $\operatorname{inc} E$, that will be considered as a kinematic variable besides the strain itself, E.

Our mechanical model belongs to the class of higher grade theories of Generalized Continuum Mechanics, with the incorporation of an internal variable to describe dissipative effects[1]. Internal efforts are described using zeroth and second-order strain gradients in a linearized framework, with isotropic constitutive laws. First-order models show a strong form involving E and $\operatorname{inc} E$, whereas second-order models involve E and $\operatorname{inc}(\mathbb{D} \operatorname{inc} E)$ with $\mathbb{D}$ a material-dependent tensor. First-order model were addressed in [7], but the present formalism leads to a better interpretation of boundary conditions and is more tractable from a numerical standpoint due to its variational form. At the same time, energetic arguments allow us to monitor the corresponding tangent moduli that generalize the Lamé coefficients to this second-order model, and this is what we substitute to flow rules. In conventional plasticity, the effective tangent moduli are also byproducts of the flow rules (see [23]), but in our approach where the notion of plastic strain is absent, they may be decomposed in elastic and plastic parts (in our modeling example we chose an harmonic decomposition). Note that other approaches, also with the purpose to avoid the use of any reference configuration, both in finite and linearized elasto-plasticity with dislocations, are currently developed with success [2,12]. Though, our approach, based on a unique strain field to describe both elastic and plastic effects, is, to our knowledge, novel.

From a mathematical standpoint, the main tool we repeatedly use is the so-called Beltrami decomposition[2], applied either to the kinematical variable E itself, or to the virtual field $\hat{E}$. Therefore we report on functional analysis concepts. Moreover, we also provide thermodynamical considerations and numerical simulations to assess the validity of our model on some simple test cases. However, a complete incremental scheme is the purpose of future works.

The paper is organized as follows. The geometrical setting and the modeling of internal efforts are described in Section 2. The prescription of boundary conditions of Dirichlet type is investigated in Section 3 with the help of a kinematical analysis at the mesoscopic scale. Preliminary mathematical results are collected in Section 4. In Section 5 we interpret the strain at the mesoscopic scale. The modeling of external efforts is addressed in Section 6. Mathematical properties of the model for given tangent moduli are established in Section 7, while the evolution of these moduli is discussed in Section 8. Numerical analysis aspects and simulations are reported in Sections 9 through 11.

2. Construction of a second-order model of incompatible elasticity

2.1. **Virtual work principle.** Let us consider a body $\Omega = \Omega(t)$ at time t that undergoes internal deformations under the action of a system of external forces. The model we propose is based on d'Alembert's principle of virtual work in a quasi-static regime, i.e., without inertial terms. This principle is based on the following assertion: if a certain type of internal deformation is imposed to the body, the body will in turn produce a reaction in the form of an internal virtual work. It is

[1] We refer the reader to [31] for this nomenclature and a review of plasticity models based on strain gradients (and plastic strain).

[2] whose precise mathematical statement can be found in [27].

called virtual because one should imagine any type of deformation, and not only the actual one, which will only be the outcome of problem solving. Let us call $\hat{E}$ the virtual strain field, namely a 3×3 symmetric tensor field representing the local metric change. Then $\mathcal{W}_i(\hat{E})$ denotes the internal (or intrinsic) work, typically consisting of the integral over Ω of a density of internal virtual work. Now, the external virtual work $\mathcal{W}_e$ is by definition the work exerted by the system of external efforts under the considered deformation. The principle of virtual work consists in writing that the balance law

$$\mathcal{W}_i(\hat{E}) = \mathcal{W}_e(\hat{E})$$

must hold for every kinematically admissible virtual strain $\hat{E}$. This principle also implicitly contains the assumption that both $\mathcal{W}_i(\hat{E})$ and $\mathcal{W}_e(\hat{E})$ be continuous and linear functionals of $\hat{E}$. However, the topology to be considered for continuity remains a modeling choice. Another major requirement is the fact that the internal work be an objective functional, namely that it does not involve any decomposition of $\hat{E}$ based on a reference configuration, boundary conditions, or other arbitrary choices possibly made by the observer. On the contrary, the external work may be non-objective (see [28]). This is natural, since it depends on the particular setting of the experiment.

In classical displacement-based formulations, the external work is a continuous linear functional on a subspace of $H^1(\Omega)$, therefore we assume in our intrinsic framework that it is a continuous linear functional on $L^2(\Omega, \mathbb{S}^3)$, where $\mathbb{S}^3$ is the set of symmetric 3×3 real matrices. By Riesz representation there exists a tensor field $\mathbb{K} \in L^2(\Omega, \mathbb{S}^3)$ such that

$$\mathcal{W}_e(\hat{E}) = \int_\Omega \mathbb{K} \cdot \hat{E} dx. \tag{2.1}$$

The tensor $\mathbb{K}$ may be non-objective. In order to represent classical body or boundary forces, the construction of $\mathbb{K}$ depends on the way a virtual displacement field can be associated with $\hat{E}$, which involves boundary conditions. All the modeling aspects raised above will be discussed in details in the next sections. In particular, we emphasize that it will not be needed for practical use to explicitly compute $\mathbb{K}$: we will express the external work against an orthogonal decomposition of $\hat{E}$, as explained in section 6, to arrive at a weak form appropriate for a finite element approximation, see section 9.

2.2. **Kinematical descriptors: a geometric approach.** Besides the virtual work principle, we strive to adopt a geometrical setting for the kinematical description of the medium. To this respect we consider the deformed body as a Riemannian manifold, thus equipped with geometrical quantities such as metric, curvature, connection and torsion. For simplicity we avoid introducing connection torsion in this work, hence we only allow for the Levi-Civita connection defined from the partial derivatives of the metric. Thus, we take as main kinematical descriptors the metric and the resulting curvature. They can be interpreted as follows.

2.2.1. *Modeling the deformation field through the metric.* We assume that within the medium we can identify and follow infinitesimal fibers. Denote by a_1, a_2, a_3 three such fibers which at time t originate from point x and are oriented along the axes of a Cartesian coordinate system and of length ε. Then the strain rate at x can be intrinsically defined by

$$d_{ij}(t) := \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon^2} \left(\frac{d}{dt}(a_i \cdot a_j) \right)_t, \tag{2.2}$$

where d/dt stands for the total (or material) derivative. It is immediately recognized that the diagonal components of d_{ij} represent the relative elongation rate of the fibers, whereas the off-diagonal terms represent minus one-half the rate of the mutual angular variations. This formula corresponds to the classical definition from a velocity field v, namely $d_{ij} = (\partial_i v_j + \partial_j v_i)/2$ (see, e.g., [19, Section 11.2] and [15, Eq. (I.51)]), which is valid in finite as well as in infinitesimal elasticity, provided the existence of a transformation is assumed from a reference configuration to the current one. However it is an essential aspect of the present framework to allow the strain rate to be defined independently of any such velocity field. Given a time increment Δt, we will rather work with the strain increment

$$E_{ij}(t) = \frac{1}{2}\left(\lim_{\varepsilon\to 0}\frac{(a_i\cdot a_j)_{t+\Delta t}}{\varepsilon^2} - \delta_{ij}\right),$$

so that (2.2) is retrieved as the limit of $E_{ij}(t)/\Delta t$ when $\Delta t \to 0$, assuming that the limits in space and time can be interchanged.

Following infinitesimal fibers such that $a_i \cdot a_j = \varepsilon^2\delta_{ij}$ at time $t = 0$, we also define the metric

$$g_{ij}(t) = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon^2}(a_i\cdot a_j)_t.$$

In this work we will focus our attention on a small and single increment and simply call $E_{ij} := E_{ij}(0)$ the strain. We immediately obtain the strain-metric relation

$$g_{ij} := g_{ij}(\Delta t) = \delta_{ij} + 2E_{ij}.$$

The smallness assumption will be crucial to define (2.1) in the fixed domain $\Omega = \Omega(0)$. We emphasize again that the strain tensor is not constructed from a deformation field as in classical continuum mechanics, which specifically enables curvature. This generalized framework will allow the modeling of some phenomena which in principle occur below the continuum scale. We only assume that E behaves like a second order symmetric tensor under a change of basis, which means that it encodes the behavior of arbitrary fibers in a bilinear algebra format.

2.2.2. *Modeling strain incompatibility through the Riemannian curvature and its linearization.* From the metric and the Levi-Civita connection we classically define the Riemannian curvature tensor that we denote by $\mathrm{Riem}(g)$. Expanding $\mathrm{Riem}(g)$ in terms of E we obtain an expression of form [27]

$$(\mathrm{Riem}(g))_{ijkl} = c_{ijklpq}(\,\mathrm{inc}\;E)_{pq} + o(\nabla\nabla E),$$

for some constants c_{ijklpq}, and where the incompatibility operator is defined as

$$\mathrm{inc}\;E = \;\mathrm{Curl}\;\;\mathrm{Curl}^t\;E, \qquad (\,\mathrm{inc}\;E)_{ij} = \epsilon_{ikl}\epsilon_{jmn}\partial_{km}E_{nl}.$$

We use the convention that the Curl of a tensor is computed row-wise, whereby $\mathrm{Curl}^t\;E$ computes the Curl column-wise whenever E is symmetric. It is well known that the incompatibility of a symmetric tensor is symmetric, and that the incompatibility of a symmetric gradient vanishes, i.e. $\mathrm{inc}\;\nabla^S u = 0$. Therefore, in the small strain setting encompassing the fact that the remainder $o(\nabla\nabla E)$ can be neglected, we will use $\mathrm{inc}\;E$ as a representation of the Riemannian curvature.

Remark 1. *Notice that in $3d$ the Riemann curvature tensor can be written algebrically by means of the Ricci or even the Einstein tensor. It is interesting to observe as in [25] that the Einstein tensor, as the incompatibility tensor, is symmetric and divergence free. Therefore our geometric approach can be understood as grounded on the metric and the Einstein tensors, the latter being linearized for our purposes.*

2.3. **The internal work.** On the basis of this geometrical setting, the internal efforts will manifest themselves in the form of work expended against virtual deformations described by a pair $(\hat{E},\,\mathrm{inc}\;\hat{E})$. Therefore we distinguish between two contributions with their own geometrical interpretations. On the one hand, the efforts acting against $\hat{E}$ are a reaction against an arbitrary deformation, represented by stretching and rotation of material fibers, being compatible or not. On the other hand, the efforts acting against $\mathrm{inc}\;\hat{E}$ are a specific reaction against a virtual bending of the manifold, i.e., when departing from a flat manifold through microstructural modifications, including creation, motion and rearrangements of defects at the micro-scale. The impossibility of such phenomena is characterized by an infinite stiffness against bending, as we will mathematically analyze later.

Therefore we introduce two symmetric second order tensors Σ and Λ, the former one working against $\hat{E}$ and the latter one working against $\operatorname{inc}\hat{E}$. We write the internal work as the linear functional

$$\mathcal{W}_i(\hat{E}) := \int_\Omega \left(\Sigma \cdot \hat{E} + \Lambda \cdot \operatorname{inc}\hat{E}\right) dx.$$

Thus the principle of virtual work is expressed as

$$\mathcal{W}_i(\hat{E}) := \int_\Omega \left(\Sigma \cdot \hat{E} + \Lambda \cdot \operatorname{inc}\hat{E}\right) dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx = \mathcal{W}_e(\hat{E}),$$

for every admissible $\hat{E}$.

2.4. **Linear constitutive laws.** The generalized forces Σ and Λ depend on the physical state of the medium. In the linear and essentially geometric model which we aim at, we assume that they are related to the geometrical quantities E and $\operatorname{inc} E$ by constitutive laws of form

$$\Sigma = \mathbb{A}E + \mathbb{B}\operatorname{inc} E \text{ and } \Lambda = \mathbb{C}E + \mathbb{D}\operatorname{inc} E,$$

where $\mathbb{A}$, $\mathbb{B}$, $\mathbb{C}$, $\mathbb{D}$ are fourth-order tensors possibly spatially dependent. As a consequence, the internal work reads

$$\mathcal{W}_i(\hat{E}) = \int_\Omega \left(\mathbb{A}E \cdot \hat{E} + \mathbb{B}\operatorname{inc} E \cdot \hat{E} + \mathbb{C}E \cdot \operatorname{inc}\hat{E} + \mathbb{D}\operatorname{inc} E \cdot \operatorname{inc}\hat{E}\right) dx.$$

The model obtained from the first two terms has been studied in [7–9]. It is appealing in that the mixed term in the simplified form $\ell \operatorname{inc} E \cdot \hat{E}$ can be derived by integration by parts from a first gradient (with respect to strain) model with natural assumptions, it leads to well-posed governing equations, and it is consistent with compatible elasticity at the limit $\ell \to \pm\infty$ in the absence of kinematical constraint. However, Dirichlet-type boundary conditions cannot be easily incorporated, and the natural boundary condition leaves the incompatibility flux across the boundary as a free variable. Similar conclusions can be obtained by considering the third term $\mathbb{C}E \cdot \operatorname{inc}\hat{E}$. Therefore, in the present model, we drop the two mixed terms and choose $\mathbb{B} = \mathbb{C} = 0$. Another justification for this choice is to assume that, for consistence with standard elasticity, the internal work reduces to the first term as soon as either $\operatorname{inc} E = 0$ or $\operatorname{inc}\hat{E} = 0$. We arrive at the balance law

$$\mathcal{W}_i(\hat{E}) = \int_\Omega \left(\mathbb{A}E \cdot \hat{E} + \mathbb{D}\operatorname{inc} E \cdot \operatorname{inc}\hat{E}\right) dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx = \mathcal{W}_e(\hat{E}), \tag{2.3}$$

valid for any kinematically admissible virtual strain tensor field $\hat{E}$.

2.5. **Isotropy.** We assume that the matrix fields $\mathbb{A}$ and $\mathbb{D}$ are piecewise smooth, and we consider an arbitrary point $z \in \Omega$ at which they are continuous. We choose a ball $B \subset \Omega$ centered at z and small enough so that $\mathbb{A}$ and $\mathbb{D}$ can be seen as constant in B. Actually, continuous variations can be treated by passing to the limit in the radius, but we prefer to avoid this technicality. Up to a shift of the coordinate system, we assume for simplicity that $z = 0$. We rewrite the internal work expended within B as

$$\mathcal{W}_i(B; E, \hat{E}) = \int_B \left(\mathbb{A}E \cdot \hat{E} dx + \mathbb{D}\operatorname{inc} E \cdot \operatorname{inc}\hat{E}\right) dx.$$

Given a pair $(E, \hat{E})$ and an orthogonal matrix Q, we define another strain field E^* obtained after rotation of E by Q, namely

$$E^*(x) = Q^t E(Qx)Q, \quad E^*_{ij}(x) = Q_{pi}E_{pq}(Q_{uv}x_v)Q_{qj},$$

and likewise another virtual strain field $\hat{E}^*$. The material is isotropic if

$$\mathcal{W}_i(B; E, \hat{E}) = \mathcal{W}_i(B; E^*, \hat{E}^*)$$

for every triple $(E, \hat{E}, Q)$. Since equalizing two symmetric bilinear forms is equivalent to equalizing the corresponding quadratic forms, we define

$$\mathcal{Q}_{\mathbb{A}}(E) = \int_B \mathbb{A}E \cdot E dx, \quad \mathcal{Q}_{\mathbb{D}}(E) = \int_B \mathbb{D} \operatorname{inc} E \cdot \operatorname{inc} E dx.$$

The series of computations

$$\partial_l E^*_{ij}(x) = Q_{pi} \partial_s E_{pq}(Q_{uv} x_v) Q_{sl} Q_{qj},$$

$$\partial_{kl} E^*_{ij}(x) = Q_{pi} \partial_{rs} E_{pq}(Q_{uv} x_v) Q_{rk} Q_{sl} Q_{qj},$$

$$(\operatorname{inc} E^*)_{mn}(x) = \epsilon_{mli} \epsilon_{nkj} \partial_{kl} E^*_{ij} = \epsilon_{mli} \epsilon_{nkj} Q_{pi} Q_{rk} Q_{sl} Q_{qj} \partial_{rs} E_{pq}(Qx),$$

$$\begin{aligned} Q_{um}(\operatorname{inc} E^*)_{mn}(x) Q_{vn} &= (\epsilon_{mli} Q_{um} Q_{sl})(\epsilon_{nkj} Q_{vn} Q_{rk}) Q_{pi} Q_{qj} \partial_{rs} E_{pq}(Qx) \\ &= (\epsilon_{usa} Q_{ai})(\epsilon_{vrb} Q_{bj}) Q_{pi} Q_{qj} \partial_{rs} E_{pq}(Qx) = \epsilon_{usa} \epsilon_{vrb} (Q_{ai} Q_{pi})(Q_{bj} Q_{qj}) \partial_{rs} E_{pq}(Qx) \\ &= \epsilon_{usp} \epsilon_{vrq} \partial_{rs} E_{pq}(Qx) = (\operatorname{inc} E(Qx))_{uv} \end{aligned}$$

result in

$$\operatorname{inc} E^*(x) = Q^t \operatorname{inc} E(Qx) Q. \tag{2.4}$$

Thus, the isotropy condition

$$\mathcal{Q}_{\mathbb{A}}(E) + \mathcal{Q}_{\mathbb{D}}(E) = \mathcal{Q}_{\mathbb{A}}(E^*) + \mathcal{Q}_{\mathbb{D}}(E^*) = \mathcal{Q}_{\mathbb{A}}(Q^t E(Qx) Q) + \mathcal{Q}_{\mathbb{D}}(Q^t \operatorname{inc} E(Qx) Q)$$

formulates after a change of variables as

$$\int_B \mathbb{A}E \cdot E dx + \int_B \mathbb{D} \operatorname{inc} E \cdot \operatorname{inc} E dx = \int_B \mathbb{A}(Q^t E Q) \cdot (Q^t E Q) dx + \int_B \mathbb{D}(Q^t \operatorname{inc} E Q) \cdot (Q^t \operatorname{inc} E Q) dx.$$

Choosing first E constant then $\operatorname{inc} E$ constant, it follows from a classical result of linear algebra that $\mathcal{Q}_{\mathbb{A}}$ and $\mathcal{Q}_{\mathbb{D}}$ only depend on the scalar invariants of E and $\operatorname{inc} E$. The three invariants of a 3×3 matrix A are $\mathrm{I}(A) := \operatorname{tr} A, \mathrm{II}(A) := \frac{1}{2}\left((\operatorname{tr} A)^2 - \operatorname{tr}(A^2)\right)$ and $\mathrm{III}(A) := \det A$, hence we can write

$$\mathcal{Q}_{\mathbb{A}}(E) = \hat{\mathcal{Q}}_{\mathbb{A}}(\mathrm{I}(E), \mathrm{II}(E), \mathrm{III}(E)).$$

Being quadratic we have

$$\mathcal{Q}_{\mathbb{A}}(E) = \frac{1}{2} D^2 \mathcal{Q}_{\mathbb{A}}(0)(E, E).$$

Using $D\mathrm{I}(E) = \mathbb{I},\ D\mathrm{II}(E) = \mathrm{I}(E)\mathbb{I} - E$ and the chain rule we get

$$\mathcal{Q}_{\mathbb{A}}(E) = \frac{1}{2}\left(D_{\mathrm{I},\mathrm{I}} \hat{\mathcal{Q}}_{\mathbb{A}}(0)(\operatorname{tr} E)^2 + D_{\mathrm{II}} \hat{\mathcal{Q}}_{\mathbb{A}}(0)((\operatorname{tr} E)^2 - \operatorname{tr}(E^2))\right).$$

This can be formulated as

$$\mathcal{Q}_{\mathbb{A}}(E) = \alpha_{\mathbb{A}} \mathrm{I}(E)^2 + \beta_{\mathbb{A}} \mathrm{II}(E),$$

for some scalars $\alpha_{\mathbb{A}}$ and $\beta_{\mathbb{A}}$, and of course a similar expression holds for $\mathcal{Q}_{\mathbb{D}}$. The 4th order tensor $\mathbb{A}$ is obtained by differentiating twice $\mathcal{Q}_{\mathbb{A}}$, namely

$$\mathbb{A} = \frac{1}{2} D^2 \mathcal{Q}_{\mathbb{A}}(E) = (\alpha_{\mathbb{A}} + \frac{\beta_{\mathbb{A}}}{2}) \mathbb{I} \otimes \mathbb{I} - \frac{\beta_{\mathbb{A}}}{2} \mathbb{I}_4,$$

where the 4th order identity tensor $\mathbb{I}_4$ is defined indice-wise as $(\mathbb{I}_4)_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. To summarize we arrive at the constitutive linearized laws

$$\mathbb{A} = 2\mu_{\mathbb{A}} \mathbb{I}_4 + \lambda_{\mathbb{A}} \mathbb{I} \otimes \mathbb{I}, \quad \mathbb{D} = 2\mu_{\mathbb{D}} \mathbb{I}_4 + \lambda_{\mathbb{D}} \mathbb{I} \otimes \mathbb{I}. \tag{2.5}$$

Of course we recognize the standard Hooke's tensor $\mathbb{A}$, with corresponding Lamé moduli $\lambda_{\mathbb{A}}$ and $\mu_{\mathbb{A}}$, and the new tensor $\mathbb{D}$ is its incompatible counterpart.

2.6. **Deviatoric-volumetric decomposition.** Since typical incompatible deformations occur in shear due to the presence of dislocations moving along glide planes, it is natural to use the following decompositions for Σ and Λ:

$$\Sigma = \mathbb{A}E = 2\mu_{\mathbb{A}}\mathrm{dev}(E) + \kappa_{\mathbb{A}}\,\mathrm{tr}(E)\mathbb{I}, \quad \Lambda = \mathbb{D}\,\mathrm{inc}\,E = 2\mu_{\mathbb{D}}\mathrm{dev}(\,\mathrm{inc}\,E) + \kappa_{\mathbb{D}}\,\mathrm{tr}(\,\mathrm{inc}\,E)\mathbb{I},$$

where the deviatoric part of E and the elastic / incompatible bulk moduli are defined by

$$\mathrm{dev}E := E - \frac{1}{3}\,\mathrm{tr}(E)\mathbb{I}, \qquad \kappa_{\mathbb{A}/\mathbb{D}} = \frac{2}{3}\mu_{\mathbb{A}/\mathbb{D}} + \lambda_{\mathbb{A}/\mathbb{D}}. \tag{2.6}$$

2.7. **The tangent model and the flow rules.** As already said, in our linearized approach, E is to be understood as an increment of strain over a certain time interval in a quasi-static evolution. The tangent tensors $\mathbb{A}$ and $\mathbb{D}$ may change over time, following a process which will substitute to the flow rules of conventional elasto-plasticity models. There, a similar effective Hooke's tensor often appears in an implicit manner, see e.g. [23, Eq. (63)]. Our choices for evolution procedures will be discussed in details later. We will also present an implicit approach, in which $\mathbb{A}$ and $\mathbb{D}$ will, on the basis of thermodynamic arguments, themselves indirectly depend on E.

3. Burgers tensor, Frank tensor and micro-hard condition

3.1. **Frank and Burgers tensors.** Here, as opposed to the previous section, we consider linearized elasticity at the mesoscopic scale, i.e., a continuum scale where the dislocations and disclinations are modeled as singularity lines, namely either loops, or straight lines with endpoint at the crystal boundary. We denote by ε the strain outside singularities and glide planes, which is classically considered as the elastic strain. Following the formalism introduced in [40], there are two basic tensors that allow to compute the jump of the rotation and displacement fields, namely the Frank tensor

$$\mathbb{F} = \,\mathrm{Curl}^t\,\varepsilon, \qquad \mathbb{F}_{ij} = \epsilon_{ikl}\partial_k\varepsilon_{jl}, \tag{3.1}$$

and the Burgers tensor[3], given a reference point x_0,

$$\mathbb{B}(x) = \varepsilon(x) + \left((x - x_0)\times\,\mathrm{Curl}\,\varepsilon(x)\right)^t, \qquad \mathbb{B}_{ij} = \varepsilon_{ij} + \epsilon_{ipq}(x_p - x_{0p})\mathbb{F}_{qj}. \tag{3.2}$$

These definitions are justified by the observation that, in the compatible framework where the strain tensor, the rotation vector and the Burgers field can be respectively defined by

$$\varepsilon = \nabla^S u, \qquad \omega = \frac{1}{2}\,\mathrm{Curl}\,u, \qquad b = u - \omega\times(x - x_0),$$

we have the relations

$$\partial_j\omega_i = \frac{1}{2}\epsilon_{ikl}\partial_{jk}u_l = \epsilon_{ikl}\partial_k\varepsilon_{jl} = \mathbb{F}_{ij},$$

$$\partial_j b_i = \partial_j u_i - \epsilon_{ilm}\partial_j\omega_l(x_m - x_{0m}) - \epsilon_{ilj}\omega_l = \partial_j u_i + \epsilon_{iml}\partial_j\omega_l(x_m - x_{0m}) + \frac{1}{2}\epsilon_{lij}\epsilon_{lkm}\partial_k u_m = \mathbb{B}_{ij}.$$

This provides by integration along a path from x_0 to x

$$\omega_i(x) - \omega_i(x_0) = \int_{x_0}^{x}\partial_j\omega_i(\xi)d\xi_j = \int_{x_0}^{x}\mathbb{F}_{ij}(\xi)d\xi_j, \tag{3.3}$$

$$b_i(x) - b_i(x_0) = \int_{x_0}^{x}\partial_j b_i(\xi)d\xi_j = \int_{x_0}^{x}\mathbb{B}_{ij}(\xi)d\xi_j, \tag{3.4}$$

and obviously the above integrals vanish along a closed loop. Turning now to the incompatible case, when ε and ω are not constructed from a displacement, the rightmost integrals in (3.3)-(3.4) are still well-defined using (3.1) and (3.2), but they may be non-vanishing on closed loops. Moreover,

[3]Our meaning of the Burgers tensor is different from Gurtin and Needleman's one [20], which for us would be the dislocation density tensor.

if we consider a circuit C which encloses dislocations and / or disclinations, then we can define the Frank and Burgers vectors associated with C as

$$\Omega_i[C] = \int_C \mathbb{F}_{ij} dx_j, \qquad B_i[C] = \int_C \mathbb{B}_{ij} dx_j.$$

We note that the above-defined Frank and Burgers vectors are independent of the so-called Burgers' circuit C that encloses the line singularities (this is called the Weingarten's lemma, see, e.g., [40]).

The Burgers field, tensor and vector, in contrast to the Frank tensor and vector, depend a priori on the prescription of an arbitrary point x_0. However, if $\Omega_i[C] = 0$, i.e., C does not enclose disclinations, then it is immediately seen that the Burgers vector is independent of the point x_0. In this work, we make the assumption that there are no disclinations. Now, having locally defined the rotation and Burgers field by the path integrals (3.3)-(3.4), a displacement can also be locally constructed by $u_{x_0} = b + \omega \times (x - x_0)$, and the jump of u around C at x_0 equals the Burgers vector. Note that u_{x_0} defines a multi-valued vector field at the mesoscopic scale, as it may jump on any Burgers circuit around a dislocation loop. To make it single-valued we can first define S_L as a surface enclosed by the dislocation loop L and $S_{\mathcal{L}} = \cup S_L$ as the union of all S_L over all dislocation loops $\mathcal{L}$, then define the vector field $\bar{u} = u_{x_0}$ on $\Omega \setminus S_{\mathcal{L}}$. It can be shown that the jump of $\bar{u}$ is equal to B on $S_{\mathcal{L}}$, or, equivalently that the circulation of $\nabla \bar{u}$ is a concentrated measure on $\mathcal{L}$ (see [34, 35] for details). To obtain a macroscopic single-valued displacement field on Ω we will consider below the Beltrami decomposition complemented by a set of boundary conditions. We will analyze the connection between the two scales, in particular between ε and E, in section 5. We recall that at the macroscopic scale that we mostly consider in the paper, the dislocations are not present in the form of line singularities but modeled through a diffuse density field. Therefore all fields are square-integrable with no concentration effects. It will nevertheless prove useful for both scales to pursue the mesoscopic analysis towards the derivation of boundary conditions directly applicable to E.

3.2. **Relation between the Burgers vector and the incompatibility field.** In order to evaluate the displacement jump, we can use the Stokes theorem to rewrite the line integral as a surface integral. To this respect we first compute

$$\begin{aligned}
(\,\mathrm{Curl}\,\mathbb{B})_{ik}(x) &= \epsilon_{klj}\partial_l \mathbb{B}_{ij}(x) = \epsilon_{klj}\partial_l \varepsilon_{ij} + \epsilon_{klj}\epsilon_{imp}\partial_l\big((\,\mathrm{Curl}\,\varepsilon)_{jp}(x_m - x_{0m})\big)\\
&= \epsilon_{klj}\partial_l \varepsilon_{ij} + \epsilon_{klj}\epsilon_{imp}\big(\partial_l(\,\mathrm{Curl}\,\varepsilon)_{jp}(x_m - x_{0m}) + (\,\mathrm{Curl}\,\varepsilon)_{jp}\delta_{ml}\big)\\
&= \epsilon_{klj}\partial_l \varepsilon_{ij} + \epsilon_{klj}\epsilon_{imp}\partial_l(\epsilon_{pqr}\partial_q\varepsilon_{jr})(x_m - x_{0m}) + \epsilon_{klj}\epsilon_{imp}(\epsilon_{pqr}\partial_q\varepsilon_{jr})\delta_{ml}\\
&= \epsilon_{klj}\partial_l \varepsilon_{ij} + \epsilon_{klj}\epsilon_{imp}\epsilon_{pqr}\partial_{lq}\varepsilon_{jr}(x_m - x_{0m}) + \epsilon_{klj}\epsilon_{ilp}\epsilon_{pqr}\partial_q\varepsilon_{jr}\\
&= \epsilon_{klj}\partial_l \varepsilon_{ij} + \epsilon_{imp}\epsilon_{klj}\epsilon_{pqr}\partial_{lq}\varepsilon_{jr}(x_m - x_{0m}) + \epsilon_{klj}(\delta_{iq}\delta_{lr} - \delta_{ir}\delta_{lq})\partial_q\varepsilon_{jr}\\
&= \epsilon_{klj}\partial_l \varepsilon_{ij} + \epsilon_{imp}(\,\mathrm{inc}\,\varepsilon)_{kp}(x_m - x_{0m}) + \epsilon_{klj}(\partial_i\varepsilon_{jl} - \partial_l\varepsilon_{ji})\\
&= \epsilon_{imp}(\,\mathrm{inc}\,\varepsilon)_{kp}(x_m - x_{0m}).
\end{aligned}$$

Hence, if S is a surface of boundary C (i.e., $\partial S = C$) and unit normal N, then we have at each point of S

$$(\,\mathrm{Curl}\,\mathbb{B}(x)N)_i = (\,\mathrm{Curl}\,\mathbb{B}(x))_{ik}N_k = \epsilon_{imp}(\,\mathrm{inc}\,\varepsilon)_{kp}(x_m - x_{0m})N_k,$$

which reads

$$\mathrm{Curl}\,\mathbb{B}(x)N = (x - x_0) \times (\,\mathrm{inc}\,\varepsilon N).$$

This formulates the resultant Burgers vector associated with a density of defect lines inside C, or equivalently crossing S, as

$$B[C] = \int_S (x - x_0) \times (\,\mathrm{inc}\,\varepsilon N) dS(x). \tag{3.5}$$

3.3. **Micro-hard condition.** We say that a surface S satisfies the micro-hard condition if

$$\text{inc}\ \varepsilon N = 0 \text{ on } S. \tag{3.6}$$

By (3.5), this is equivalent to saying that the resultant Burgers vector $B[C']$ of defect lines enclosed in any circuit $C' = \partial S' \subset S$ vanishes. In particular, no individual dislocation line can emerge across S.

Note that the condition $(\text{ Curl } \mathbb{B})N = 0$ can be obtained by imposing $\mathbb{B} \times N = 0$ on S. This is exactly the micro-hard condition of Gurtin and Needleman [20], thus which is stronger than ours. Similarly, imposing $\text{Curl}^t\ \varepsilon \times N = 0$ also yields $\text{inc}\ \varepsilon N = 0$.

3.4. **Macroscopic boundary condition.** In Section 5 we will show that the strain E can be defined in such a way that $\text{inc}\ E = -\text{inc}\ \varepsilon$ at the mesoscopic scale. Its macroscopic counterpart is defined by local averaging, thus we formulate the micro-hard condition at the macroscale as

$$\text{inc}\ EN = 0 \text{ on } S. \tag{3.7}$$

We will see below that $\text{div inc}\ E = 0$, whereby the incompatibility flux $\text{inc}\ EN$ has no jump in the space (4.5). Hence (3.7) is satisfied at the interface between Ω and a fictitious outer compatible phase when the two phases form a continuum from the point of view of the present framework.

4. Green formula, Beltrami decomposition and consequences

4.1. **Green formula and related function spaces.** Throughout the paper we assume that Ω is a bounded domain of $\mathbb{R}^3$ with $\mathcal{C}^1$ boundary.

Lemma 1 (Green formula for the incompatibility [6]). *Suppose that $E \in \mathcal{C}^2(\overline{\Omega}, \mathbb{S}^3)$ and $\eta \in H^2(\Omega, \mathbb{S}^3)$. Then*

$$\int_\Omega E \cdot \text{inc}\ \eta dx = \int_\Omega \text{inc}\ E \cdot \eta dx + \int_{\partial\Omega} \mathcal{T}_1(E) \cdot \eta\ dS(x) + \int_{\partial\Omega} \mathcal{T}_0(E) \cdot \partial_N \eta\ dS(x) \tag{4.1}$$

with the trace operators defined as

$$\mathcal{T}_0(E) := (E \times N)^t \times N, \tag{4.2}$$

$$\mathcal{T}_1(E) := \left(\text{Curl } (E \times N)^t\right)^S + ((\partial_N + k)E \times N)^t \times N + \left(\text{Curl}^t\ E \times N\right)^S, \tag{4.3}$$

where $k := \kappa^A + \kappa^B$ is twice the mean curvature of $\partial\Omega$, $E^S := (E + E^t)/2$ is the symmetric part of E, and cross products are computed row-wise. In addition, it holds

$$\int_{\partial\Omega} \mathcal{T}_1(E) N dS(x) = 0. \tag{4.4}$$

In particular, choosing compactly supported test functions, (4.1) allows to recover the distributional formulation of the inc operator, which satisfies $\text{inc}\ \nabla^S u = 0$ for all $u \in L^1_{\text{loc}}(\Omega, \mathbb{R}^3)$ and $\text{div inc}\ E = 0$ for all $E \in L^1_{\text{loc}}(\Omega, \mathbb{S}^3)$. The main function space on which we will build our analysis is

$$H^{\text{inc}}(\Omega, \mathbb{S}^3) = \left\{E \in L^2(\Omega, \mathbb{S}^3) : \text{inc}\ E \in L^2(\Omega, \mathbb{S}^3)\right\}. \tag{4.5}$$

It is naturally endowed with an Hilbertian structure for the norm

$$\|E\|_{H^{\text{inc}}(\Omega,\mathbb{S}^3)} = \left(\|E\|_{L^2(\Omega,\mathbb{S}^3)} + \|\text{ inc } E\|_{L^2(\Omega,\mathbb{S}^3)}\right)^{1/2}.$$

The traces $\mathcal{T}_0(E)$ and $\mathcal{T}_1(E)$ extend by duality to every function $E \in H^{\text{inc}}(\Omega, \mathbb{S}^3)$, with $\mathcal{T}_0(E) \in H^{-1/2}(\partial\Omega, \mathbb{S}^3)$ and $\mathcal{T}_1(E) \in H^{-3/2}(\partial\Omega, \mathbb{S}^3)$, so as to generalize (4.1). An alternative definition of the boundary trace operators using divergence-free test functions and corresponding liftings has been considered in [6]. Throughout we will denote duality pairings by integrals.

We next define $H^{\text{inc}}_0(\Omega, \mathbb{S}^3)$ as the closure of $\mathcal{C}^\infty_c(\Omega, \mathbb{S}^3)$ in $H^{\text{inc}}(\Omega, \mathbb{S}^3)$. The following properties are proved in [9].

Proposition 2. (1) $H^{\text{inc}}_0(\Omega, \mathbb{S}^3) = \left\{E \in H^{\text{inc}}(\Omega, \mathbb{S}^3) : \mathcal{T}_0(E) = \mathcal{T}_1(E) = 0 \textit{ on } \partial\Omega\right\}$.

(2) *Let Γ be a relatively open subset of $\partial\Omega$. If $E \in H^{\text{inc}}(\Omega, \mathbb{S}^3)$ satisfies $\mathcal{T}_0(E) = \mathcal{T}_1(E) = 0$ on Γ then $\text{inc}\ EN = 0$ on Γ.*

4.2. **Beltrami decomposition and related function spaces.** We define the function spaces

$$\mathcal{V} = \left\{E \in L^2(\Omega, \mathbb{S}^3) : \text{inc } E = 0\right\},$$
$$\mathcal{W} = \left\{E \in L^2(\Omega, \mathbb{S}^3) : \text{div } E = 0\right\},$$
$$\mathcal{Z} = \left\{E \in H^{\text{inc}}(\Omega, \mathbb{S}^3) : \text{div } E = 0, EN = 0 \text{ on } \partial\Omega\right\},$$

and, given subsets Γ_1, Γ_2 of $\partial\Omega$ with Γ_1 relatively open, $\Gamma_1 \cup \Gamma_2 = \partial\Omega$, $\Gamma_1 \cap \Gamma_2 = \emptyset$,

$$\mathcal{V}^0_{\Gamma_1} = \{E \in \mathcal{V} : \mathcal{T}_0(E) = \mathcal{T}_1(E) = 0 \text{ on } \Gamma_1\},$$
$$\mathcal{V}^{00}_{\Gamma_1} = \left\{\nabla^S v : v \in H^1(\Omega, \mathbb{R}^3), v = 0 \text{ on } \Gamma_1\right\},$$
$$\mathcal{W}^0_{\Gamma_2} = \{E \in \mathcal{W} : EN = 0 \text{ on } \Gamma_2\}.$$

We refer to [9] for the precise meaning of this latter condition and for the proof of the following result.

Theorem 3. *Assume Ω is simply-connected.*

(1) *We have the representations*
$$\mathcal{V} = \left\{\nabla^S v, v \in H^1(\Omega, \mathbb{R}^3)\right\}, \qquad \mathcal{W} = \{\text{ inc } F, F \in \mathcal{Z}\}.$$
(2) *If $E \in L^2(\Omega, \mathbb{S}^3)$ satisfies* inc $E = 0$ *in Ω and $\mathcal{T}_0(E) = \mathcal{T}_1(E) = 0$ on $\partial\Omega$ then there exists $v \in H^1_0(\Omega, \mathbb{R}^3)$ such that $E = \nabla^S v$.*
(3) *Let $v \in H^1(\Omega, \mathbb{R}^3)$. If $v = r$ on Γ_1 in the sense of traces, with r a rigid displacement field, then $\mathcal{T}_0(\nabla^S v) = \mathcal{T}_1(\nabla^S v) = 0$ on Γ_1. The converse statement holds true if $\Gamma_1 = \partial\Omega$.*
(4) *We have the L^2-orthogonal sums (variants of the Beltrami decomposition)*
$$L^2(\Omega, \mathbb{S}^3) = \mathcal{V}^{00}_{\Gamma_1} \oplus \mathcal{W}^0_{\Gamma_2}, \qquad H^{\text{inc}}(\Omega, \mathbb{S}^3) = \mathcal{V} \oplus \mathcal{Z}.$$
(5) *We have the Poincaré inequality*
$$\|E\|_{H^1(\Omega,\mathbb{S}^3)} \leq c\|\text{ inc } E\|_{L^2(\Omega,\mathbb{S}^3)} \qquad \forall E \in \mathcal{Z},$$
for some positive constant c.

Note that Theorem 3 implies $\mathcal{V}^{00}_{\Gamma_1} \subset \mathcal{V}^0_{\Gamma_1}$, with equality if $\Gamma_1 = \partial\Omega$.

For later purpose, we provide two additional results related to the set

$$\mathcal{Y} = \left\{E \in H^{\text{inc}}(\Omega, \mathbb{S}^3) : \text{div } E \in L^2(\Omega, \mathbb{R}^3), EN = 0 \text{ on } \partial\Omega\right\}. \tag{4.6}$$

Theorem 4. *If Ω is simply-connected, then there exists $c > 0$ such that*

$$\|E\|_{L^2(\Omega,\mathbb{S}^3)} \leq c\left(\|\text{ inc } E\|_{L^2(\Omega,\mathbb{S}^3)} + \|\text{ div } E\|_{L^2(\Omega,\mathbb{R}^3)}\right) \qquad \forall E \in \mathcal{Y}.$$

Proof. We define the auxiliary space

$$\mathcal{X} = \left\{(F, h) \in L^2(\Omega, \mathbb{S}^3) \times L^2(\Omega, \mathbb{R}^3) : \text{div } F = 0, \int_\Omega h dx = \int_\Omega h \times x dx = 0\right\}$$

and the continuous linear map

$$\Phi : E \in \mathcal{Y} \mapsto (\text{ inc } E, \text{ div } E) \in \mathcal{X}.$$

We equip $\mathcal{X}$ and $\mathcal{Y}$ with the norms

$$\|(F, h)\|_{\mathcal{X}} = (\|F\|^2_{L^2(\Omega,\mathbb{S}^3)} + \|h\|^2_{L^2(\Omega,\mathbb{R}^3)})^{1/2},$$
$$\|E\|_{\mathcal{Y}} = (\|E\|^2_{L^2(\Omega,\mathbb{S}^3)} + \|\text{ inc } E\|^2_{L^2(\Omega,\mathbb{S}^3)} + \|\text{ div } E\|^2_{L^2(\Omega,\mathbb{R}^3)})^{1/2},$$

whereby $\mathcal{X}$ and $\mathcal{Y}$ are Banach spaces. If $\Phi(E) = 0$ then E is a symmetric gradient by Theorem 3, and the conditions div $E = 0$, $EN = 0$ on $\partial\Omega$ yield $E = 0$. Given a pair $(F, h) \in \mathcal{X}$, setting $E = -\nabla^S w + G$ with $G \in \mathcal{Z}$ such that inc $G = F$, which is possible by Theorem 3 since $F \in \mathcal{W}$, and w a weak solution of

$$\begin{cases} -\text{div } \nabla^S w = h & \text{in } \Omega \\ \nabla^S w N = 0 & \text{on } \partial\Omega \end{cases}$$

results in $\operatorname{div} E = \operatorname{div} \nabla^S w = h$, $\operatorname{inc} E = \operatorname{inc} G = F$ and $EN = 0$ on $\partial\Omega$. We conclude that Φ is an isomorphism. The open mapping theorem yields that Φ^{-1} is continuous, thence the result. □

Theorem 5. *If Ω is simply-connected, then $\mathcal{Y}$ is a dense subspace of $H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$.*

Proof. We will prove that $\mathcal{Y}^\perp = \{0\}$, where orthogonality is meant for the inner product of $H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$. This will yield $\overline{\mathcal{Y}} = \mathcal{Y}^{\perp\perp} = H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$. Let $E \in \mathcal{Y}^\perp$. We have by definition

$$\int_\Omega (E \cdot F + \operatorname{inc} E \cdot \operatorname{inc} F)\, dx = 0 \qquad \forall F \in \mathcal{Y}.$$

We use the Beltrami decomposition from Theorem 3 as

$$E = E_c + E_i \in \mathcal{V} \oplus \mathcal{Z},$$

to obtain

$$\int_\Omega E_c \cdot F dx + \int_\Omega (E_i \cdot F + \operatorname{inc} E_i \cdot \operatorname{inc} F)\, dx = 0 \qquad \forall F \in \mathcal{Y}. \tag{4.7}$$

Choosing $F = E_i$ in (4.7), using $\mathcal{Z} \subset \mathcal{Y}$ and the L^2-orthogonality of E_c and E_i, yields $E_i = 0$. It remains

$$\int_\Omega E_c \cdot F dx = 0 \qquad \forall F \in \mathcal{Y}.$$

We can choose in particular arbitrary test functions in $\mathcal{C}_c^\infty(\Omega, \mathbb{S}^3)$, showing that $E_c = 0$. □

Recall that the Beltrami decomposition is not objective, therefore it has not been used to describe internal efforts. It will be used later to recover a displacement field from the strain and to describe external efforts when applied to virtual fields.

4.3. **Hard boundary condition.** In view of Proposition 2, claim (1), we call hard boundary condition the condition $\mathcal{T}_0(E) = \mathcal{T}_1(E) = 0$. By Theorem 3, claims (2) and (3), it naturally extends the clamped condition to the possibly incompatible case. Proposition 2, claim (2), means that the hard condition implies the micro-hard one (3.7).

5. Multiscale definition of the strain at the mesoscopic scale based on the Beltrami and Radon-Nikodým decompositions

In this section we will show how the strain E, basic ingredient of our approach, can be interpreted in a coherent way with the Beltrami decomposition.

5.1. **Mesoscopic construction.** We first place ourselves at the mesoscopic scale where glide surfaces lead to singularities in the geometrical descriptors. In this setting, if u is smooth enough outside a surface S of discontinuity, the Radon-Nikodým decomposition of $\nabla^S u$ writes

$$\nabla^S u = \bar{\nabla}^S u - [\![u]\!] \odot N \delta_S, \tag{5.1}$$

with δ_S denoting the two-dimensional Hausdorff mesure restricted to S. Here, $[\![u]\!]$ is the jump of u counting positively the contribution with outward normal, and $(b \odot N)_{ij} = (b_i N_j + b_j N_i)/2$. Note that the absolutely continuous part $\bar{\nabla}^S u$ of the symmetric distributional gradient $\nabla^S u$ is the symmetric part of an approximate gradient in the sense of geometric measure theory (see, e.g., [4, 5]). Moreover, at this scale, $\bar{\nabla}^S u$ is typically only in L^p for $p < 2$, since $\operatorname{Curl} \bar{\nabla} u$ is indeed a concentrated measure (namely, the dislocation density) only for $p < 2$ [32, 33]. Therefore we will make use of an L^p version of the Beltrami decomposition developed in [27]. We can nevertheless work with $p = 2$ upon choosing a gradually varying jump within the dislocation core, from 0 to the Burgers vector, as done in [2] and considered next in Proposition 7. Moreover, the natural framework where (5.1) holds is the space $SBD(\Omega)$ of special functions with bounded deformation (this space was introduced in [36], see also [4, 22, 37]). The proposition below provides an interpretation of the kinematic variable E at the mesoscopic scale. It is based on a Beltrami decomposition of the absolutely continuous (sometimes called elastic) part of $\nabla^S u$ in order to define a strain E made of a compatible plus a concentrated (sometimes called plastic) term. By doing so, the incompatibility of the absolutely continuous part will be compensated.

Proposition 6. *Let $\Omega \subset \mathbb{R}^3$ be simply connected, $u \in SBD(\Omega)$ with jump set S and jump b, with $u = 0$ on $\partial\Omega$. Denote by $\bar\nabla^S u$ the absolutely continuous part of $\nabla^S u$. We assume that $\bar\nabla^S u \in L^p(\Omega, \mathbb{S}^3)$ for some $p \in (1, \infty)$. There exists a unique $\bar u \in W_0^{1,p}(\Omega, \mathbb{R}^3)$ such that*

$$E := \nabla^S \bar u - b \odot N\delta_S$$

satisfies

$$\operatorname{div} E = \operatorname{div} \nabla^S u. \tag{5.2}$$

In addition, we have $\operatorname{div} \bar\nabla^S u = \operatorname{div} \nabla^S \bar u$, and $S = \emptyset$ implies $\bar u = u$ and $E = \nabla^S u$.

Proof. We write the Beltrami decomposition of $\bar\nabla^S u$ as

$$\bar\nabla^S u = \nabla^S \bar u + F, \qquad \bar u \in W_0^{1,p}(\Omega, \mathbb{R}^3),\ F \in L^p(\Omega, \mathbb{S}^3),\ \operatorname{div} F = 0.$$

We have

$$\nabla^S u = \bar\nabla^S u - b \odot N\delta_S = \nabla^S \bar u - b \odot N\delta_S + F,$$

hence $E := \nabla^S \bar u - b \odot N\delta_S$ satisfies

$$E = \nabla^S u - F = \bar\nabla^S u - b \odot N\delta_S - F, \text{ and } \operatorname{div} \nabla^S u = \operatorname{div} E,$$

completing the existence. For the uniqueness, consider two pairs $(\bar u_1, E_1)$ and $(\bar u_2, E_2)$. This yields $E_2 - E_1 = \nabla^S(\bar u_2 - \bar u_1)$. From $\operatorname{div} \nabla^S(\bar u_2 - \bar u_1) = 0$ we infer $\bar u_2 - \bar u_1 = 0$, and subsequently $E_2 - E_1 = 0$. Lastly, $S = \emptyset$ implies $\operatorname{div} \nabla^S \bar u = \operatorname{div} E = \operatorname{div} \nabla^S u$, whereby $\bar u = u$. □

The condition $\operatorname{div} \nabla^S \bar u = \operatorname{div} \bar\nabla^S u$ implies in particular that $[\![\nabla^S \bar u N]\!] = [\![\bar\nabla^S u N]\!]$ across S. Therefore, $\bar u$ encodes all compatible jumps from $\bar\nabla^S u$. Setting $F = \nabla^S u - E$ we have

$$\operatorname{div} F = 0, \qquad \operatorname{inc} E = -\operatorname{inc} F = \operatorname{inc}(-b \odot N\delta_S) = -\operatorname{inc} \bar\nabla^S u. \tag{5.3}$$

The field F accounts for singular deformations localized in the vicinity of dislocation cores. To illustrate this local feature, let us consider a 2d situation with a glide (half-)plane $S = \{(0, y, z), y \geq 0\}$ and a single straight edge dislocation line along the z-axis with a constant Burgers vector $b = |b|e_y$. By (5.3) we can write $F = \operatorname{inc} \Psi$, with $\operatorname{inc} \operatorname{inc} \Psi = \operatorname{inc}(b \odot N\delta_S) = -|b|\partial_x \delta_{x=y=0} e_z \otimes e_z$. Looking for $\Psi = \psi e_z \otimes e_z$ we arrive at the free space expression in cylindrical coordinates and Cartesian components

$$F = \frac{-|b|}{4\pi r} \begin{pmatrix} \cos\theta\cos 2\theta & \sin\theta\cos 2\theta & 0 \\ \sin\theta\cos 2\theta & \cos\theta(2 - \cos 2\theta) & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{-|b|}{4\pi r} \left(\cos\theta(e_r \otimes e_r + e_\theta \otimes e_\theta) + 2\sin\theta e_r \odot e_\theta \right).$$

Here r is the distance to the dislocation line and we observe the decay

$$F = O(\frac{|b|}{r}). \tag{5.4}$$

To better interpret the condition $\operatorname{div} E = \operatorname{div} \nabla^S u$, or equivalently $\operatorname{div} \nabla^S \bar u = \operatorname{div} \bar\nabla^S u$, it is useful to consider the aforementioned gradual dislocation model. We assume the same edge dislocation as above with the same yz glide (half-) plane S, but now with a jump $[\![u]\!] = f(y)e_y$ on S. Here f is a smooth function which is constant when $y \geq R$ and vanishes at the origin, i.e. $f(0) = 0$. In other words we obtain a classical dislocation only in the limit $R \to 0$, and as far as $R > 0$ the problem is regularized in a core around the dislocation, here given by the cylinder

$$C = \{x^2 + y^2 < R^2\}.$$

Proposition 7. *In the above situation we have*

$$\operatorname{inc} \bar\nabla^S u = [\![\mathcal{T}_0(\bar\nabla^S u)]\!]\partial_N \delta_S + [\![\mathcal{T}_1(\bar\nabla^S u)]\!]\delta_S = -f'(y) e_z \otimes e_z \partial_x \delta_S. \tag{5.5}$$

Proof. The first equality stems from the Green formula in Theorem 1. The second one results from

$$\text{inc } \bar{\nabla}^S u = \text{ inc } ([\![u]\!] \odot N\delta_S) = \text{ inc } (f(y)e_y \odot e_x\delta_S)$$

and an explicit calculation. Indeed the above distributional incompatibility is computed as

$$\int_S (f(y)e_y \odot e_x) \cdot \text{ inc } (\varphi e_z \otimes e_z) dS = -\int_S f(y)\partial_{xy}\varphi dS = \int_S f'(y)\partial_x\varphi dS + \int_L f(0)\partial_x\varphi(0,0,z)dz,$$

then we use that that $f = 0$ on the z-axis. □

By assumption on $[\![u]\!]$ (i.e., that u is of the order $f(y)$ along e_y), the component $(\bar{\nabla}^S u)_{yy}$ is of order $f'(y)$ within C, which by (5.5) is directly related to $\text{inc } \bar{\nabla}^S u$. In particular, if $f'(y) \to \infty$, both $(\bar{\nabla}^S u)_{yy}$ and $\text{inc } \bar{\nabla}^S u$ degenerate at the same speed. As a matter of fact, the correction field F defining E by $E = \nabla^S u - F = \bar{\nabla}^S u - [\![u]\!] \odot N\delta_S - F$ exactly compensates the incompatibility of $\bar{\nabla}^S u$. Therefore it serves to compensate the degeneracy of $(\bar{\nabla}^S u)_{yy}$, which is irrelevant to represent the highly nonlinear core deformations. Equivalently by (5.5) it compensates the tangential jumps $[\![\mathcal{T}_0(\bar{\nabla}^S u)]\!]$ and $[\![\mathcal{T}_1(\bar{\nabla}^S u)]\!]$, without modifying the compatible ones $[\![\bar{\nabla}^S uN]\!]$, specifically because F is chosen as divergence-free. Furthermore, by removing the correction term F, the incompatibility of E is only due to the concentrated shear $-[\![u]\!] \odot N\delta_S$.

It is shown in [2] that a limiting version of the classical plasticity theory for a shear band of vanishing thickness corresponds to the choices of the plastic and elastic strains as $E_p = -b \odot N\delta_S$, $E_e = \bar{\nabla}^S u$, respectively. Our construction is fundamentally different, since we rely on a single symmetric field E containing elastic and plastic strains, minus a local correction term, F, accounting for incompatibility, whose effect is taken into account in our model through $\text{inc } F = -\text{inc } E$ in order to bypass the direct modeling of large deformations and decohesion phenomena within dislocation cores. In contrast, the concentrated shear $-b \odot N\delta_S$, which is not restricted to dislocation cores, is kept in E. The change of the material response to shear deformations due to dislocations will be taken into account in the variation of the shear modulus $\mu_{\mathbb{A}}$. This will be developed in section 8.

Remark 2. *Note that if we consider S as the full xy-glide plane (instead of half-plane), then it still holds* $\text{inc } ([\![u]\!] \odot N\delta_S) = -f'(y)e_z \otimes e_z\partial_x\delta_S$ *(even without the condition $f(0) = 0$). Hence considering $f \equiv b$ on S yields a deformation with zero incompatibility, as the dislocation has glided along S from one extremity to the other, where it has left the crystal. These are compatible plastic effects, which are as previously taken into account in the effective tangent modulus $\mu_{\mathbb{A}}$.*

5.2. **From the mesoscale to the macroscale.** We turn to the macroscopic implications of the previous discussions. We now use the index η to denote mesoscopic quantities, where η is a characteristic length of the individual Burgers vectors involved. Therefore, we assume that we are given a displacement field u_η, and that we have constructed a strain field E_η such that $\text{div } E_\eta = \text{ div } \nabla^S u_\eta$, as in (5.2). We further assume that, when $\eta \to 0$, $u_\eta \to u$ and $E_\eta \to E$ in the sense of distributions, for some pair (u, E). Since they are defined by a local averaging process, we consider these limits as the macroscopic displacement and strain fields. It is then straightforward that $\text{div } E = \text{ div } \nabla^S u$. This relation justifies the use of the Beltrami decomposition, or more specifically item (4) of Theorem 3, as the cornerstone of our approach to connect the strain and the displacement. Indeed, this decomposition is not only needed to reconstruct u from E, but also to define the tensor $\mathbb{K}$ of external efforts as described in the next section. Moreover, if we define $F_\eta = \nabla^S u_\eta - E_\eta$ and $F = \nabla^S u - E$ then $F_\eta \to F$ in the sense of distributions. If dislocations are concentrated within a region U with resulting Burgers vector b, passing (5.4) to the macroscopic case yields $F = O(|b|/r)$ where r is the distance to U.

6. Generalized external forces

In view of the above construction, we are going to give alternative representations of the external work (2.1) using the decompositions from Theorem 3. Consider a partition $\partial\Omega = \Gamma_1 \cup \Gamma_2$. Let a virtual strain $\hat{E} \in L^2(\Omega, \mathbb{S}^3)$ be decomposed as

$$\hat{E} = \nabla^S \hat{v} + \text{inc } \hat{F} \in V^{00}_{\Gamma_1} \oplus \mathcal{W}^0_{\Gamma_2},$$

with $\hat{v} \in H^1(\Omega, \mathbb{R}^3)$, $\hat{v} = 0$ on Γ_1 and $\hat{F} \in H^{\text{inc}}(\Omega, \mathbb{S}^3)$, $\text{inc } \hat{F}N = 0$ on Γ_2. The Green formula yields

$$W_e(\hat{E}) = \int_\Omega \mathbb{K} \cdot (\nabla^S \hat{v} + \text{inc } \hat{F}) dx$$
$$= -\int_\Omega \text{div } \mathbb{K} \cdot \hat{v} dx + \int_{\partial\Omega} \mathbb{K}N \cdot \hat{v} dS(x) + \int_\Omega \text{inc } \mathbb{K} \cdot \hat{F} dx + \int_{\partial\Omega} \Big(\mathcal{T}_1(\mathbb{K}) \cdot \hat{F} + \mathcal{T}_0(\mathbb{K}) \cdot \partial_N \hat{F}\Big) dS(x).$$

We recall the following property proved in [9].

Lemma 8. *If* $\mathbb{K} \in \mathcal{V}^{00}_{\Gamma_1}$ *and* $\text{inc } \hat{F} \in \mathcal{W}^0_{\Gamma_2}$ *then*

$$\int_{\partial\Omega} \Big(\mathcal{T}_1(\mathbb{K}) \cdot \hat{F} + \mathcal{T}_0(\mathbb{K}) \cdot \partial_N \hat{F}\Big) dS(x) = 0.$$

Let $f \in L^2(\Omega, \mathbb{R}^3)$ and $g \in H^{-1/2}(\partial\Omega, \mathbb{R}^3)$ be given. Using Lemma 8 and restricting for simplicity to the reference case where $\text{inc } \mathbb{K} = 0$, i.e. $\mathbb{K} = \nabla^S w$ with $w \in H^1(\Omega, \mathbb{R}^3)$, a (weak) solution of

$$\begin{cases} -\text{div } \nabla^S w = f & \text{in } \Omega \\ w = 0 & \text{on } \Gamma_1 \\ \left(\nabla^S w\right) N = g & \text{on } \Gamma_2 \end{cases}$$

then we retrieve the conventional external work

$$W_e(\hat{E}) = \int_\Omega f \cdot \hat{v} dx + \int_{\Gamma_2} g \cdot \hat{v} dS(x). \tag{6.1}$$

We will subsequently assume that $\mathbb{K}$ is defined in this way.

7. Well-posedness and elastic limit

7.1. **Well-posedness.** We are now in position to address the well-posedness of (2.3). In order to encode a hard boundary condition on Γ_1 and a free boundary condition on Γ_2 we set

$$\mathcal{H} = \left\{E \in H^{\text{inc}}(\Omega, \mathbb{S}^3) : \mathcal{T}_0(E) = \mathcal{T}_1(E) = 0 \text{ on } \Gamma_1\right\}.$$

A straightforward application of the Lax-Milgram theorem yields the following existence result.

Theorem 9. *Let* $\mathbb{K} \in L^2(\Omega, \mathbb{S}^3)$ *and assume* $\mathbb{A}, \mathbb{D}$ *are uniformly positive definite. There exists a unique* $E \in \mathcal{H}$ *such that*

$$\int_\Omega \Big(\mathbb{A}E \cdot \hat{E} + \mathbb{D}\text{inc } E \cdot \text{inc } \hat{E}\Big) dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{H}. \tag{7.1}$$

7.2. **Free boundary condition and strong form.** Assuming sufficient regularity for E, integrating the left-hand side of (7.1) by parts yields by the Green formula

$$\int_\Omega (\mathbb{A}E + \text{inc } (\mathbb{D}\text{inc } E)) \cdot \hat{E} dx + \int_{\partial\Omega} \mathcal{T}_0(\mathbb{D}\text{inc } E) \cdot \partial_N \hat{E} dS(x) + \int_{\partial\Omega} \mathcal{T}_1(\mathbb{D}\text{inc } E) \cdot \hat{E} dS(x).$$

Taking first $\hat{E} \in \mathcal{C}^\infty_c(\Omega, \mathbb{S}^3)$ yields the strong form

$$\mathbb{A}E + \text{inc } (\mathbb{D}\text{inc } E) = \mathbb{K} \quad \text{in } \Omega,$$

with $\mathbb{K}$ the tensor of external force, Riesz representative of the efforts f and g by (6.1).

Remark that taking $\hat{E} = \nabla^S \hat{v}$ yields the classical relations

$$-\text{div } (\mathbb{A}E) = f \quad \text{in } \Omega, \qquad \mathbb{A}EN = g \quad \text{on } \Gamma_2,$$

whereby $\mathbb{A}E$ is interpreted as the Cauchy stress tensor, and accordingly will be later used to compute the von Mises stress. By classical lifting in $H^2(\Omega)$ one obtains the additional boundary condition

$$\mathcal{T}_0(\mathbb{D}\,\mathrm{inc}\ E) = \mathcal{T}_1(\mathbb{D}\,\mathrm{inc}\ E) = 0 \quad \text{on } \Gamma_2.$$

This is our version of the micro-free or microscopically powerless boundary condition, similar in spirit to [20] but different in its expression since the authors of [20] have another kinematical description with prescribed slip systems.

7.3. **Elastic limit.** We now show that compatible linear elasticity is recovered at the limit when the eigenvalues of $\mathbb{D}$ tend to infinity.

Theorem 10. *Assume that $\mathbb{A}$ and $\mathbb{D}_k$ are uniformly positive definite and denote by d_k the smallest eigenvalue of $\mathbb{D}_k$. Let $E_k \in \mathcal{H}$ be the solution of*

$$\int_\Omega \left(\mathbb{A}E_k \cdot \hat{E} + \mathbb{D}_k \,\mathrm{inc}\ E_k \cdot \mathrm{inc}\ \hat{E} \right) dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{H}. \tag{7.2}$$

If $d_k \to +\infty$ then $E_k \to E_\infty$ in $L^2(\Omega, \mathbb{S}^3)$ where E_∞ is the unique solution in $\mathcal{V}^0_{\Gamma_1}$ of

$$\int_\Omega \mathbb{A}E_\infty \cdot \hat{E} dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{V}^0_{\Gamma_1}. \tag{7.3}$$

Proof. Choosing $\hat{E} = E_k$ yields

$$\|E_k\|_{L^2(\Omega,\mathbb{S}^3)} \leq c, \quad \|\,\mathrm{inc}\ E_k\|_{L^2(\Omega,\mathbb{S}^3)} \to 0, \tag{7.4}$$

for some constant c. Therefore, there exists $E_\infty \in L^2(\Omega, \mathbb{S}^3)$ such that E_k weakly converges to E_∞ in $L^2(\Omega, \mathbb{S}^3)$, up to a non-relabeled subsequence. We have for all $\Phi \in \mathcal{C}^\infty_c(\Omega, \mathbb{S}^3)$

$$\int_\Omega E_\infty \cdot \mathrm{inc}\ \Phi dx = \lim_{k\to\infty} \int_\Omega E_k \cdot \mathrm{inc}\ \Phi dx = \lim_{k\to\infty} \int_\Omega \mathrm{inc}\ E_k \cdot \Phi dx = 0,$$

hence $\mathrm{inc}\ E_\infty = 0$. Let now $\varphi_0, \varphi_1 \in C^\infty(\partial\Omega, \mathbb{S}^3)$ be supported on Γ_1 and $\Phi \in H^2(\Omega, \mathbb{S}^3)$ such that $\Phi = \varphi_0$ and $\partial_N \Phi = \varphi_1$ on $\partial\Omega$. We have by the Green formula, since $E_k \in \mathcal{H}$, and by (7.4),

$$\int_\Omega (E_\infty \cdot \mathrm{inc}\ \Phi - \mathrm{inc}\ E_\infty \cdot \Phi) dx = \lim_{k\to\infty} \int_\Omega E_k \cdot \mathrm{inc}\ \Phi dx = \lim_{k\to\infty} \int_\Omega \mathrm{inc}\ E_k \cdot \Phi dx = 0,$$

hence $\mathcal{T}_0(E_\infty) = \mathcal{T}_1(E_\infty) = 0$ on Γ_1. We have shown that $E_\infty \in \mathcal{V}^0_{\Gamma_1}$. Using a test function $\hat{E} \in \mathcal{V}^0_{\Gamma_1}$ in (7.2) yields

$$\int_\Omega \mathbb{A}E_k \cdot \hat{E} dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx,$$

then passing to the limit reveals that E_∞ solves (7.3). By uniqueness of this cluster point, the whole sequence (E_k) is converging. It remains to prove the strong convergence. To do so we compute

$$\int_\Omega \mathbb{A}(E_k - E_\infty) \cdot (E_k - E_\infty) dx = \int_\Omega \mathbb{A}E_k \cdot E_k dx + \int_\Omega \mathbb{A}E_\infty \cdot E_\infty dx - 2 \int_\Omega \mathbb{A}E_k \cdot E_\infty dx.$$

We have on the one hand

$$\int_\Omega \mathbb{A}E_k \cdot E_\infty dx \to \int_\Omega \mathbb{A}E_\infty \cdot E_\infty dx = \int_\Omega \mathbb{K} \cdot E_\infty dx,$$

and on the other hand,

$$\int_\Omega \mathbb{A}E_k \cdot E_k dx = \int_\Omega \mathbb{K} \cdot E_k dx - \int_\Omega \mathbb{D}_k \,\mathrm{inc}\ E_k \cdot \mathrm{inc}\ E_k dx \leq \int_\Omega \mathbb{K} \cdot E_k dx \to \int_\Omega \mathbb{K} \cdot E_\infty dx.$$

It follows that

$$\limsup_{k\to\infty} \int_\Omega \mathbb{A}(E_k - E_\infty) \cdot (E_k - E_\infty) dx = 0,$$

from which we infer the strong convergence. $\square$

In view of Theorem 3, we can rephrase (7.3) in a fully standard form, at least in the following two cases:

(1) if $\Gamma_1 = \emptyset$ (free boundary condition on $\partial\Omega$) then $\mathcal{V}^0_{\Gamma_1} = \mathcal{V} = \{\nabla^S v, v \in H^1(\Omega, \mathbb{R}^3)\}$ and the Neumann linear elasticity problem is retrieved;
(2) if $\Gamma_1 = \partial\Omega$ (hard boundary condition on $\partial\Omega$) then $\mathcal{V}^0_{\Gamma_1} = \mathcal{V}^{00}_{\partial\Omega} = \{\nabla^S v, v \in H^1_0(\Omega, \mathbb{R}^3)\}$ and the Dirichlet linear elasticity problem is retrieved.

8. Dissipation and evolution rules

We aim here at studying evolution rules for the tangent moduli $\kappa_{\mathbb{A}}, \mu_{\mathbb{A}}, \kappa_{\mathbb{D}}, \mu_{\mathbb{D}}$ in order to obtain a thermodynamically consistent model. We begin with a continuous time framework.

8.1. **Continuous time evolution framework.** Going back to the general notation from subsection 2.3, the Clausius-Duhem inequality [19, 26] reads in the present case

$$\mathcal{R} = \Sigma \cdot \dot{E} + \Lambda \cdot \operatorname{inc} \dot{E} - \rho(\dot{\psi} + s\dot{T}) - \frac{q \cdot \nabla T}{T} \geq 0. \tag{8.1}$$

Here, $\mathcal{R}$ is the dissipation rate, ρ is the density, ψ, s are the specific Helmholtz free energy and entropy, respectively, q is the heat flux and T is the temperature. We postulate that the specific free energy is of form

$$\psi = \psi(E, \operatorname{inc} E, \theta, T),$$

where θ is a scalar internal variable accounting for dissipative phenomena. We can rewrite (8.1) as

$$\mathcal{R} = \left(\Sigma - \rho\frac{\partial\psi}{\partial E}\right) \cdot \dot{E} + \left(\Lambda - \rho\frac{\partial\psi}{\partial \operatorname{inc} E}\right) \cdot \operatorname{inc} \dot{E} - \rho\left(s + \frac{\partial\psi}{\partial T}\right)\dot{T} - \rho\frac{\partial\psi}{\partial\theta}\dot{\theta} - \frac{q \cdot \nabla T}{T} \geq 0.$$

A classical physical argument [26] leads to

$$\Sigma = \rho\frac{\partial\psi}{\partial E}, \qquad \Lambda = \rho\frac{\partial\psi}{\partial \operatorname{inc} E}, \qquad s = -\frac{\partial\psi}{\partial T}, \tag{8.2}$$

and we arrive at

$$\mathcal{R} = \mathcal{R}_M + \mathcal{R}_T, \qquad \mathcal{R}_M = -\rho\frac{\partial\psi}{\partial\theta}\dot{\theta}, \qquad \mathcal{R}_T = -\frac{q \cdot \nabla T}{T}.$$

In our mechanical approach we will neglect the thermal dissipation rate $\mathcal{R}_T$, and limit our study to the mechanical dissipation rate $\mathcal{R}_M$. A classical way to automatically satisfy $\mathcal{R}_M \geq 0$ is to postulate the existence of a dissipation potential ϕ minimal at 0 such that

$$\dot{\theta} \text{ maximizes } -\rho\frac{\partial\psi}{\partial\theta}\dot{\theta} - \phi(\dot{\theta}). \tag{8.3}$$

Indeed, this implies

$$\mathcal{R}_M = \left(-\rho\frac{\partial\psi}{\partial\theta}\dot{\theta} - \phi(\dot{\theta})\right) + \phi(\dot{\theta}) \geq -\phi(0) + \phi(\dot{\theta}) \geq 0.$$

Upon convexity and lower-semicontinuity of ϕ, we infer a flow rule for θ based on the equivalences [10, 11, 16]

$$(8.3) \Leftrightarrow -\rho\frac{\partial\psi}{\partial\theta} \in \partial\phi(\dot{\theta}) \Leftrightarrow \dot{\theta} \in \partial\phi^*(-\rho\frac{\partial\psi}{\partial\theta}),$$

where $\partial\phi$ is the subdifferential of ϕ and ϕ^* is the Legendre-Fenchel transform of ϕ. Choosing a positively homogeneous dissipation potential of form

$$\phi(s) = \begin{cases} +\infty & \text{if } s < 0 \\ \gamma s & \text{if } s \geq 0 \end{cases} \qquad \text{yields} \qquad \phi^*(p) = \begin{cases} 0 & \text{if } p \leq \gamma \\ +\infty & \text{if } p > \gamma. \end{cases}$$

This leads to $\partial\phi^*(p) = \{0\}$ for $p < \gamma$ and $\partial\phi^*(p) = [0, +\infty)$ for $p = \gamma$. On the one hand this is relevant to represent the threshold effect typical of perfect plasticity, in relation with the more general framework of rate independent systems, see [30] and the references therein. On the other hand it implies $\dot{\theta} \geq 0$, so that dissipation is characterized by an increase of θ. We believe that other dissipation potentials may encode hardening phenomena, but we leave this to further study.

However we will not use convex calculus in the sequel. We will directly translate (8.3) to the discrete time setting that will be of interest for practical implementation, in the spirit of Hencky's model of conventional plasticity (see e.g. [29]).

8.2. **Incremental framework.** In order to analyze the incremental procedure in a practical setting we adapt the previous considerations. Since we assume linear constitutive laws within each increment, we directly address the question of the evolution of the tangent tensors $\mathbb{A}$ and $\mathbb{D}$. We focus on a first increment $[0, t_1]$ where we assume a time-dependent load of form

$$\mathbb{K}(t) = t\mathbb{K}$$

and constant tangent tensors. Then the strain rate is also constant in the time interval. We will work with this quantity, rather than the strain itself, and we simply denote it by E. We take $t_1 = 1$ for simplicity. The total work expended during the increment is

$$W = \int_0^{t_1} \int_\Omega \mathbb{K}(t) \cdot E dx dt = \frac{1}{2} \int_\Omega \mathbb{K} \cdot E dx.$$

The balance law (2.3) yields the reformulation

$$W = \frac{1}{2} \int_\Omega (\mathbb{A} E \cdot E + \mathbb{D} \operatorname{inc} E \cdot \operatorname{inc} E)\, dx.$$

We assume the isotropic constitutive laws (2.5), where we choose $\lambda_\mathbb{D} = 0$ for simplicity. Together with (2.6) this yields

$$W = \frac{1}{2} \int_\Omega \left(\kappa_\mathbb{A} (\operatorname{tr} E)^2 + 2\mu_\mathbb{A} |\operatorname{dev} E|^2 + 2\mu_\mathbb{D} |\operatorname{inc} E|^2\right) dx.$$

In the same way as in the previous subsection we introduce an internal variable θ, but we bypass the free energy and the relations (8.2) to directly assume that $\mu_\mathbb{A}$ and $\kappa_\mathbb{D}$ are functions of θ. We stress that this θ is the incremental counterpart of $\dot\theta$ from the time continuous setting, therefore we will assume that $\theta \geq 0$. Because it is not expected to play any role in plasticity, the bulk modulus $\kappa_\mathbb{A}$ is assumed constant. We assume a constant temperature. Moreover, we fix by convention $\theta = (2\mu_\mathbb{D})^{-1}$, as by Theorem 10, linear elasticity corresponds to the limit $\theta \to 0$. We call θ the compatibility modulus. We assume that the effective shear and compatibility moduli are related by a constitutive law $\mu_\mathbb{A} = \mu_\mathbb{A}(\theta)$. For consistence we denote $\mu_\mathbb{D}(\theta) = (2\theta)^{-1}$.

Call $E(\theta) \in \mathcal{H}$ the solution of

$$\int_\Omega \left(\kappa_\mathbb{A} \operatorname{tr} E(\theta) \operatorname{tr} \hat{E} + 2\mu_\mathbb{A}(\theta) \operatorname{dev} E(\theta) \cdot \operatorname{dev} \hat{E} + 2\mu_\mathbb{D}(\theta) \operatorname{inc} E(\theta) \cdot \operatorname{inc} \hat{E}\right) dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx, \qquad \forall \hat{E} \in \mathcal{H}, \tag{8.4}$$

and $W(\theta)$ the work

$$W(\theta) = \frac{1}{2} \int_\Omega \mathbb{K} \cdot E(\theta) dx.$$

The global dissipation for the increment under consideration is the difference between the actual work and the corresponding elastic work for the same loading, equal to the variation of free energy, i.e.,

$$\mathcal{D}(\theta) = W(\theta) - W(0).$$

Obviously we have the variational formulation

$$-W(\theta) = \inf_{E \in \mathcal{H}} \left\{ \frac{1}{2} \int_\Omega \left(\kappa_\mathbb{A} \operatorname{tr}^2 E + 2\mu_\mathbb{A}(\theta) |\operatorname{dev} E|^2 + 2\mu_\mathbb{D}(\theta) |\operatorname{inc} E|^2\right) dx - \int_\Omega \mathbb{K} \cdot E dx \right\}.$$

As in the continuous time setting, θ is updated according to a principle of maximal dissipation, including a dissipation potential. Here it is formulated globally in space and for a finite time increment as

$$\text{maximize } \mathcal{D}(\theta) - \Phi(\theta) \;\text{ over }\; \{\theta \geq 0\},$$

with

$$\Phi(\theta) = \int_\Omega \phi(\theta) dx,$$

or equivalently

$$\text{minimize} \ -W(\theta) + \Phi(\theta) \ \text{ over } \ \{\theta \geq 0\}. \tag{8.5}$$

Imposing that ϕ is minimized at 0 guarantees the nonnegativity of the global dissipation $\mathcal{D}(\theta)$. Lastly, due to our choice of function $\mu_{\mathbb{D}}(\theta)$, we restrict to $\theta \geq \theta_{\min}$ for a sufficiently small $\theta_{\min} > 0$ that approximates perfect elasticity. We arrive at the joint variational formulation

$$\underset{(\theta,E)\in L^\infty(\Omega,[\theta_{\min},+\infty))\times\mathcal{H}}{\text{minimize}} \int_\Omega \frac{1}{2}\left(\kappa_{\mathbb{A}} \operatorname{tr}^2 E + 2\mu_{\mathbb{A}}(\theta)|\operatorname{dev} E|^2 + 2\mu_{\mathbb{D}}(\theta)|\operatorname{inc} E|^2\right) dx - \int_\Omega \mathbb{K}\cdot E dx + \int_\Omega \phi(\theta) dx. \tag{8.6}$$

It can be solved by alternating minimizations:

- minimization with respect to E is equivalent to solving the governing equation (8.4),
- minimization with respect to θ can be for instance performed by steepest descent or Newton iterations, see also appendix A.

This formulation in terms of a minimum problem of two energetic terms, whose equilibrium balances the dissipation and the energetic cost of some inelastic phenomenon, is reminiscent of the Griffith-Francfort-Marigo model of damage and fracture evolution as introduced in [17] and considered in, e.g., [3, 41]. Here, however, the dissipative term in (8.5) is driven by the compatibility modulus θ, that is a diffuse field.

8.3. **Modeling example.** Since the material response can be viewed as the sum of elastic and plastic phenomena in series we adopt the representation

$$\mu_{\mathbb{A}}(\theta)^{-1} = \mu_0^{-1} + \tilde{\mu}(\theta)^{-1}, \tag{8.7}$$

where μ_0 is the elastic shear modulus and $\tilde{\mu}(\theta)$ is a purely plastic effective shear modulus. It is reasonable to assume that $\lim_{\theta\to 0} \tilde{\mu}(\theta) = +\infty$ and $\tilde{\mu}(\theta)$ is a decreasing function of θ, since in the elastic limit $\theta \to 0$ we expect $\tilde{\mu}$ to be large. Let us write the stationarity condition with respect to θ for (8.6), with E fixed to its optimal value $E = E(\theta)$ by (8.4):

$$-\mu_{\mathbb{A}}'(\theta)|\operatorname{dev} E(\theta)|^2 - \mu_{\mathbb{D}}'(\theta)|\operatorname{inc} E(\theta)|^2 - \phi'(\theta) \in N(\theta),$$

with the normal cone $N(\theta)(x) = (-\infty, 0]$ if $\theta(x) = \theta_{\min}$, $N(\theta)(x) = \{0\}$ if $\theta(x) > \theta_{\min}$. Using (8.7) this is equivalent to

$$-\frac{\tilde{\mu}'(\theta)}{\tilde{\mu}(\theta)^2}|\mu_{\mathbb{A}}(\theta) \operatorname{dev} E(\theta)|^2 + \frac{1}{2\theta^2}|\operatorname{inc} E(\theta)|^2 - \phi'(\theta) \in N(\theta).$$

We suggest the simple laws

$$\tilde{\mu}(\theta) = \frac{k}{\theta}, \qquad \phi(\theta) = \gamma\theta, \qquad k, \gamma > 0. \tag{8.8}$$

The first one implies that $\tilde{\mu}(\theta)$ is proportional to $\mu_{\mathbb{D}}(\theta)$. The second one induces the threshold effect as discussed in section 8.1. We obtain the stationarity condition

$$\frac{1}{k}|\mu_{\mathbb{A}}(\theta) \operatorname{dev} E(\theta)|^2 + 2|\mu_{\mathbb{D}}(\theta) \operatorname{inc} E(\theta)|^2 - \gamma \in N(\theta).$$

In particular for the von Mises stress $\sigma_M = |2\mu_{\mathbb{A}}(\theta) \operatorname{dev} E(\theta)|$ we always have

$$\sigma_M^2 \leq 4\gamma k =: \sigma_Y^2. \tag{8.9}$$

Therefore σ_Y can be identified with the yield stress in perfect plasticity. We recall that hardening could be addressed by the construction of a sequence of increments with adapted modeling choices.

9. Numerical resolution

We consider the free boundary problem: find $E \in H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$ such that

$$\int_\Omega \mathbb{A}E \cdot \hat{E} + \mathbb{D} \operatorname{inc} E \cdot \operatorname{inc} \hat{E} = \int_\Omega \mathbb{K} \cdot \hat{E} \qquad \forall \hat{E} \in H^{\mathrm{inc}}(\Omega, \mathbb{S}^3). \tag{9.1}$$

As the space $H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$ does not lend itself to standard discretizations and $\mathbb{K}$ is not directly known, we will work with the decomposition from Theorem 3

$$E = \nabla^S u + E_i \in \mathcal{V} \oplus \mathcal{W}^0_{\partial\Omega}, \qquad \hat{E} = \nabla^S \hat{u} + \hat{E}_i \in \mathcal{V} \oplus \mathcal{W}^0_{\partial\Omega}.$$

Using the representation (6.1) of the external work we arrive at

$$\int_\Omega \Big(\mathbb{A}(\nabla^S u + E_i) \cdot (\nabla^S \hat{u} + \hat{E}_i) + \mathbb{D} \operatorname{inc} E_i \cdot \operatorname{inc} \hat{E}_i \Big)\, dx = \int_\Omega f \cdot \hat{u} dx + \int_{\partial\Omega} g \cdot \hat{u} dS(x). \tag{9.2}$$

Still, the constraints $E_i, \hat{E}_i \in \mathcal{W}^0_{\partial\Omega}$ are not easy to handle through finite element subspaces. For this reason we turn to a mixed formulation. First, specializing (9.2) to the case where $\hat{E}_i = 0$ results in

$$\int_\Omega \mathbb{A}(\nabla^S u + E_i) \cdot \nabla^S \hat{u} dx = \int_\Omega f \cdot \hat{u} dx + \int_{\partial\Omega} g \cdot \hat{u} dS(x) \qquad \forall \hat{u} \in H^1(\Omega, \mathbb{R}^3).$$

Second, since $\mathbb{K} \in \mathcal{V}$ we rewrite (9.1) with $\mathbb{K} = -\nabla^S p$, $p \in H^1(\Omega, \mathbb{R}^3)$, and obtain

$$\int_\Omega \Big(\mathbb{A}(\nabla^S u + E_i) \cdot \hat{E}_i + \mathbb{D} \operatorname{inc} E_i \cdot \operatorname{inc} \hat{E}_i \Big)\, dx = -\int_\Omega \nabla^S p \cdot \hat{E}_i dx \qquad \forall \hat{E}_i \in H^{\mathrm{inc}}(\Omega, \mathbb{S}^3).$$

By summation we arrive at

$$\begin{aligned} &\int_\Omega \Big(\mathbb{A}(\nabla^S u + E_i) \cdot (\nabla^S \hat{u} + \hat{E}_i) + \mathbb{D} \operatorname{inc} E_i \cdot \operatorname{inc} \hat{E}_i + \nabla^S p \cdot \hat{E}_i \Big)\, dx \\ &\qquad = \int_\Omega f \cdot \hat{u} dx + \int_{\partial\Omega} g \cdot \hat{u} dS(x) \qquad \forall (\hat{u}, \hat{E}_i) \in H^1(\Omega, \mathbb{R}^3) \times H^{\mathrm{inc}}(\Omega, \mathbb{S}^3). \end{aligned}$$

This has to be solved by $(u, E_i) \in H^1(\Omega, \mathbb{R}^3) \times H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$ with the additional equation

$$\int_\Omega E_i \cdot \nabla^S \hat{p} dx = 0 \qquad \forall \hat{p} \in H^1(\Omega, \mathbb{R}^3),$$

which represents the condition $E_i \in \mathcal{W}^0_{\partial\Omega} = \mathcal{V}^\perp$. Since u and p are in the present case defined up to rigid body motions, we numerically solve a finite element approximation of

$$\begin{aligned} &\int_\Omega \Big(\mathbb{A}(\nabla^S u + E_i) \cdot (\nabla^S \hat{u} + \hat{E}_i) + \mathbb{D} \operatorname{inc} E_i \cdot \operatorname{inc} \hat{E}_i + \epsilon_u u \cdot \hat{u} + \nabla^S p \cdot \hat{E}_i + E_i \cdot \nabla^S \hat{p} - \epsilon_p p \cdot \hat{p} \Big)\, dx \\ &\quad = \int_\Omega f \cdot \hat{u} dx + \int_{\partial\Omega} g \cdot \hat{u} dS(x) \qquad \forall (\hat{u}, \hat{E}_i, \hat{p}) \in H^1(\Omega, \mathbb{R}^3) \times H^{\mathrm{inc}}(\Omega, \mathbb{S}^3) \times H^1(\Omega, \mathbb{R}^3), \end{aligned} \tag{9.3}$$

with ϵ_u, ϵ_p small positive stabilization parameters. Actually, the unknown p can be eliminated using

$$E_i \cdot \nabla^S \hat{p} - \epsilon_p p \cdot \hat{p} = 0 \ \forall \hat{p} \in H^1(\Omega, \mathbb{R}^3) \Leftrightarrow \begin{cases} p = -\dfrac{1}{\epsilon_p} \operatorname{div} E_i \\ E_i N = 0 \text{ on } \partial\Omega. \end{cases} \tag{9.4}$$

We arrive at the variational form

$$\begin{aligned} &\int_\Omega \Big(\mathbb{A}(\nabla^S u + E_i) \cdot (\nabla^S \hat{u} + \hat{E}_i) + \mathbb{D} \operatorname{inc} E_i \cdot \operatorname{inc} \hat{E}_i + \epsilon_u u \cdot \hat{u} + \frac{1}{\epsilon_p} \operatorname{div} E_i \cdot \operatorname{div} \hat{E}_i \Big)\, dx \\ &\qquad = \int_\Omega f \cdot \hat{u} dx + \int_{\partial\Omega} g \cdot \hat{u} dS(x) \qquad \forall (\hat{u}, \hat{E}_i) \in H^1(\Omega, \mathbb{R}^3) \times \mathcal{Y}, \end{aligned} \tag{9.5}$$

with $\mathcal{Y}$ defined in (4.6). Note that the test functions in (9.5) are more constrained than in (9.3), however the two formulations will be proved to be equivalent, which actually is not surprising in view of the density property obtained in Theorem 5.

Theorem 11. *Assume $\mathbb{A},\mathbb{D}$ are uniformly positive definite and Ω is simply-connected.*

1. *The triple $(u,E_i,p)\in H^1(\Omega,\mathbb{R}^3)\times H^{\mathrm{inc}}(\Omega,\mathbb{S}^3)\times H^1(\Omega,\mathbb{R}^3)$ solves (9.3) if and only if $(u,E_i)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Y}$ solves (9.5) and $p=-\epsilon_p^{-1}\operatorname{div} E_i$.*
2. *There exists a unique $(u,E_i)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Y}$ solution of (9.5).*
3. *Moreover, $\nabla^S u+E_i$ converges to the solution of (7.1) (with $\Gamma_1=\emptyset$ and $\mathbb{K}$ defined as in section 6) in $H^{\mathrm{inc}}(\Omega,\mathbb{S}^3)$ when $(\epsilon_u,\epsilon_p)\to 0$.*

Proof. Step 1. Suppose that $(u,E_i,p)\in H^1(\Omega,\mathbb{R}^3)\times H^{\mathrm{inc}}(\Omega,\mathbb{S}^3)\times H^1(\Omega,\mathbb{R}^3)$ solves (9.3). Then we have already shown (9.4), whereby $E_i\in\mathcal{Y}$ and (9.5) is satisfied.
Step 2. Suppose now that $(u,E_i)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Y}$ solves (9.5) and set

$$p=-\frac{1}{\epsilon_p}\operatorname{div} E_i,\qquad E=\nabla^S u+E_i.$$

We have in particular $p\in L^2(\Omega,\mathbb{R}^3)$ and

$$\int_\Omega\left(\mathbb{A}E\cdot\hat{E}_i+\mathbb{D}\operatorname{inc}E\cdot\operatorname{inc}\hat{E}_i-p\cdot\operatorname{div}\hat{E}_i\right)dx=0\qquad\forall\hat{E}_i\in\mathcal{Y}.\tag{9.6}$$

We define the linear form $\Lambda\in H^{\mathrm{inc}}(\Omega,\mathbb{S}^3)'$ by

$$\langle\Lambda,\hat{E}\rangle=\int_\Omega\left(\mathbb{A}E\cdot\hat{E}+\mathbb{D}\operatorname{inc}E\cdot\operatorname{inc}\hat{E}\right)dx\qquad\forall\hat{E}\in H^{\mathrm{inc}}(\Omega,\mathbb{S}^3).\tag{9.7}$$

We infer from (9.6) that $\mathcal{Z}\subset\ker\Lambda$. By Theorem 3 we have $H^{\mathrm{inc}}(\Omega,\mathbb{S}^3)=\mathcal{V}\oplus\mathcal{Z}$, hence denoting by $P:H^{\mathrm{inc}}(\Omega,\mathbb{S}^3)\to\mathcal{V}$ the projection onto $\mathcal{V}$ we have

$$\langle\Lambda,\hat{E}\rangle=\int_\Omega\mathbb{A}E\cdot P(\hat{E})dx\qquad\forall\hat{E}\in H^{\mathrm{inc}}(\Omega,\mathbb{S}^3).$$

The projection P being L^2-orthogonal, defining $R:=P(\mathbb{A}E)\in\mathcal{V}\subset L^2(\Omega,\mathbb{R}^3)$, it follows

$$\langle\Lambda,\hat{E}\rangle=\int_\Omega P(\mathbb{A}E)\cdot\hat{E}dx=\int_\Omega R\cdot\hat{E}dx\qquad\forall\hat{E}\in H^{\mathrm{inc}}(\Omega,\mathbb{S}^3).\tag{9.8}$$

Going back to (9.6) we obtain

$$\int_\Omega\left(R\cdot\hat{E}_i-p\cdot\operatorname{div}\hat{E}_i\right)dx=0\qquad\forall\hat{E}_i\in\mathcal{Y},$$

whereby $R=-\nabla^S p\in L^2(\Omega,\mathbb{S}^3)$. By Korn's inequality, this shows that $p\in H^1(\Omega,\mathbb{R}^3)$. Moreover, combining (9.7) and (9.8) leads to

$$\int_\Omega\left(\mathbb{A}E\cdot\hat{E}_i+\mathbb{D}\operatorname{inc}E\cdot\operatorname{inc}\hat{E}_i\right)dx=-\int_\Omega\nabla^S p\cdot\hat{E}_i dx\qquad\forall\hat{E}_i\in H^{\mathrm{inc}}(\Omega,\mathbb{S}^3).$$

This is exactly (9.3) tested against $\hat{E}_i$. Starting from (9.5), testing (9.3) against $\hat{u}$ is straightforward. Testing (9.3) against $\hat{p}$ is equivalent to (9.4), which is satisfied by construction.
Step 3. We now prove the existence of a constant $c>0$ such that

$$\begin{aligned}&\int_\Omega\left(\mathbb{A}(\nabla^S v+F)\cdot(\nabla^S v+F)+\mathbb{D}\operatorname{inc}F\cdot\operatorname{inc}F+\epsilon_u|v|^2+\frac{1}{\epsilon_p}|\operatorname{div}F|^2\right)dx\\&\geq c\left(\|v\|_{L^2}^2+\|\nabla^S v\|_{L^2}^2+\|F\|^2+\|\operatorname{inc}F\|_{L^2}^2+\|\operatorname{div}F\|_{L^2}^2\right)\qquad\forall(v,F)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Y}.\end{aligned}\tag{9.9}$$

Let assume that (9.9) does not hold true. Then we can construct a sequence $(v_k,F_k)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Y}$ such that

$$\lim_{k\to\infty}\int_\Omega\left(\mathbb{A}(\nabla^S v_k+F_k)\cdot(\nabla^S v_k+F_k)+\mathbb{D}\operatorname{inc}F_k\cdot\operatorname{inc}F_k+\epsilon_u|v_k|^2+\frac{1}{\epsilon_p}|\operatorname{div}F_k|^2\right)dx=0,\tag{9.10}$$

$$\|v_k\|_{L^2}^2 + \|\nabla^S v_k\|_{L^2}^2 + \|F_k\|_{L^2}^2 + \|\operatorname{inc} F_k\|_{L^2}^2 + \|\operatorname{div} F_k\|_{L^2}^2 = 1. \tag{9.11}$$

From (9.10) we immediately see that $\|v_k\|_{L^2} \to 0$. We also infer $\|\operatorname{inc} F_k\|_{L^2} + \|\operatorname{div} F_k\|_{L^2} \to 0$, hence Theorem 4 yields $\|F_k\|_{L^2} \to 0$. Using again (9.10) we find that

$$\|\nabla^S v_k\|_{L^2} \le \|\nabla^S v_k + F_k\|_{L^2} + \|F_k\|_{L^2} \to 0,$$

which contradicts (9.11).

Step 4. The existence and uniqueness of a solution of (9.5) follows from step 3, the Lax-Milgram theorem and Korn's inequality $\|v\|_{L^2}^2 + \|\nabla^S v\|_{L^2}^2 \ge C\|v\|_{H^1}^2$, for some constant C.

Step 5. We turn to the convergence. Consider an infinitesimal sequence $(\epsilon_u^k, \epsilon_p^k)$. We denote by (u^k, E_i^k) the solution of (9.5) obtained with the parameters $\epsilon_u^k > 0$ and $\epsilon_p^k > 0$. We have

$$\int_\Omega \left(\mathbb{A}(\nabla^S u^k + E_i^k)\cdot(\nabla^S \hat{u} + \hat{E}_i) + \mathbb{D}\operatorname{inc} E_i^k \cdot \operatorname{inc} \hat{E}_i + \epsilon_u^k u^k \cdot \hat{u} + \frac{1}{\epsilon_p^k}\operatorname{div} E_i^k \cdot \operatorname{div} \hat{E}_i\right) dx$$
$$= \int_\Omega f\cdot \hat{u} dx + \int_{\partial\Omega} g\cdot \hat{u} dS(x) = \int_\Omega \mathbb{K}\cdot(\nabla^S\hat{u} + \hat{E}_i)dx \qquad \forall(\hat{u},\hat{E}_i)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Y}. \tag{9.12}$$

Choosing $(\hat{u}, \hat{E}_i) = (u, E_i)$ in (9.12), we infer

$$\|\nabla^S u^k + E_i^k\|_{L^2}^2 + \|\operatorname{inc} E_i^k\|_{L^2}^2 + \epsilon_u^k\|u^k\|_{L^2}^2 + \frac{1}{\epsilon_p^k}\|\operatorname{div} E_i^k\|_{L^2}^2 = O(1). \tag{9.13}$$

Therefore there exists $E \in L^2(\Omega, \mathbb{S}^3$ and $T \in L^2(\Omega, \mathbb{S}^3)$ such that $\nabla^S u^k + E_i^k \rightharpoonup E$ and $\operatorname{inc} E_i^k \rightharpoonup T$ weakly in $L^2(\Omega, \mathbb{S}^3)$, for a non-relabelled subsequence. It is immediately recognized that $T = \operatorname{inc} E$, since for all $\Phi \in \mathcal{C}_c^\infty(\Omega, \mathbb{S}^3)$ we have

$$\int_\Omega T\cdot\Phi dx = \lim_{k\to\infty}\int_\Omega \operatorname{inc} E_i^k\cdot\Phi dx = \lim_{k\to\infty}\int_\Omega \operatorname{inc}(\nabla^S u^k + E_i^k)\cdot\Phi dx$$
$$= \lim_{k\to\infty}\int_\Omega (\nabla^S u^k + E_i^k)\cdot\operatorname{inc}\Phi dx = \int_\Omega E\cdot\operatorname{inc}\Phi dx = \int_\Omega \operatorname{inc} E\cdot\Phi dx.$$

Passing to the limit in (9.12) choosing $\hat{E}_i$ as divergence-free, using $\|\epsilon_u^k u^k\|_{L^2} = O(\sqrt{\epsilon_u^k})$ by (9.13) and the Cauchy-Schwarz inequality, we arrive at

$$\int_\Omega \left(\mathbb{A}E\cdot(\nabla^S\hat{u} + \hat{E}_i) + \mathbb{D}\operatorname{inc} E\cdot\operatorname{inc}\hat{E}_i\right)dx$$
$$= \int_\Omega \mathbb{K}\cdot(\nabla^S\hat{u} + \hat{E}_i)dx \qquad \forall(\hat{u},\hat{E}_i)\in H^1(\Omega,\mathbb{R}^3)\times\mathcal{Z}. \tag{9.14}$$

Using the Beltrami decomposition from Theorem 3 we infer that E solves (7.1). The uniqueness of the cluster point guarantees the convergence of the full sequence.

Step 6. Lastly we prove the strong convergence. We use

$$\int_\Omega \left(\mathbb{A}(\nabla^S u^k + E_i^k - E)\cdot(\nabla^S u^k + E_i^k - E) + \mathbb{D}\operatorname{inc}(E_i^k - E)\cdot\operatorname{inc}(E_i^k - E)\right)dx$$
$$= \int_\Omega \left(\mathbb{A}(\nabla^S u^k + E_i^k)\cdot(\nabla^S u^k + E_i^k) + \mathbb{D}\operatorname{inc} E_i^k\cdot\operatorname{inc} E_i^k\right)dx$$
$$-2\int_\Omega \left(\mathbb{A}(\nabla^S u^k + E_i^k)\cdot E + \mathbb{D}\operatorname{inc} E_i^k\cdot\operatorname{inc} E\right)dx + \int_\Omega \left(\mathbb{A}E\cdot E + \mathbb{D}\operatorname{inc} E\cdot\operatorname{inc} E\right)dx.$$

By (9.12) the first integral in the above right hand side is bounded above by $\int_\Omega \mathbb{K}\cdot(\nabla^S u^k + E_i^k)dx$. Using the weak convergence and (7.1) we obtain

$$\limsup_{k\to\infty}\int_\Omega \left(\mathbb{A}(\nabla^S u^k + E_i^k - E)\cdot(\nabla^S u^k + E_i^k - E) + \mathbb{D}\operatorname{inc}(E_i^k - E)\cdot\operatorname{inc}(E_i^k - E)\right)dx$$
$$\le \int_\Omega \mathbb{K}\cdot E dx - \int_\Omega \left(\mathbb{A}E\cdot E + \mathbb{D}\operatorname{inc} E\cdot\operatorname{inc} E\right)dx = 0.$$

This proves the strong convergence $\nabla^S u^k + E_i^k \to E$ in $H^{\mathrm{inc}}(\Omega, \mathbb{S}^3)$. $\square$

10. 2D model

With numerical investigations in mind we now briefly discuss the 2D version of the model under the plane strain assumption

$$E = \begin{pmatrix} E_{xx} & E_{xy} & 0 \\ E_{xy} & E_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{10.1}$$

where E_{xx}, E_{xy} and E_{yy} are functions of the space variables (x, y). We find

$$\mathrm{inc}\, E = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \partial_{xx} E_{yy} + \partial_{yy} E_{xx} - 2\partial_{xy} E_{xy} \end{pmatrix},$$

and with the same form for $\hat{E}$, we have

$$\mathbb{D}\, \mathrm{inc}\, E \cdot \mathrm{inc}\, \hat{E} = (\lambda_{\mathbb{D}} + 2\mu_{\mathbb{D}})\, \mathrm{inc}\, E \cdot \mathrm{inc}\, \hat{E}.$$

The 2D linearized model reads

$$\int_\Omega \left(\mathbb{A}E \cdot \hat{E} + \mathbb{D}\, \mathrm{inc}\, E \cdot \mathrm{inc}\, \hat{E} \right) dx = \int_\Omega \mathbb{K} \cdot \hat{E} dx$$

for all kinematically admissible plane virtual strain $\hat{E}$. Of course, $\mathbb{K}$ has to be constructed in the form (10.1).

Remark 3. *Let us consider the particular case in which $\lambda_{\mathbb{A}}, \mu_{\mathbb{A}}$ are constant,* $\mathrm{inc}\, \mathbb{K} = 0$ *and* $\mathrm{div}\, \mathbb{K}$ *is constant (constant body force). Set*

$$\begin{cases} E_{xx} = \dfrac{1}{4\mu_{\mathbb{A}}(\lambda_{\mathbb{A}} + \mu_{\mathbb{A}})} \left((\lambda_{\mathbb{A}} + 2\mu_{\mathbb{A}}) \mathbb{K}_{xx} - \lambda_{\mathbb{A}} \mathbb{K}_{yy} \right) \\ E_{yy} = \dfrac{1}{4\mu_{\mathbb{A}}(\lambda_{\mathbb{A}} + \mu_{\mathbb{A}})} \left((\lambda_{\mathbb{A}} + 2\mu_{\mathbb{A}}) \mathbb{K}_{yy} - \lambda_{\mathbb{A}} \mathbb{K}_{xx} \right) \\ E_{xy} = \dfrac{1}{2\mu_{\mathbb{A}}} \mathbb{K}_{xy}. \end{cases}$$

We easily check that the planar components of $\mathbb{A}E$ coincide with those of $\mathbb{K}$ and $\mathrm{inc}\, E = 0$*, thus E is indeed the solution. There is no incompatibility in this case.*

11. Numerical examples

The computations are performed using the finite element software FreeFem++ [21]. The codes are available at `https://github.com/samuel-amstutz/incompatibility.git`. We use the built-in Hsieh-Clough-Tocher elements (of class $\mathcal{C}^1$) for the approximation of E_i and P2 elements for the approximation of u and p in the mixed formulation (9.3). We use dual Newton iterations as explained in appendix A to solve the minimization problem in the independent variable θ, see (8.6).

11.1. **Perforated plate under uniaxial traction.** We consider a square plate of unit size perforated with a disc of radius 0.1 in its middle. A unit uniform traction is applied on the left and right borders. We perform 20 iterations of alternating minimizations, and within each iteration 10 dual Newton steps. The material parameters are $\kappa_{\mathbb{A}} = 83$, $\mu_0 = 38.46$, $k = 10^4$, $\sigma_Y = 1$, whereby γ is derived by (8.9). Other parameters are $\theta_{\min} = 10^{-3}$, $\epsilon_u = \epsilon_p = 10^{-6}$. We use an unstructured mesh with 4704 triangular elements. Our findings are displayed in Figure 1. The incompatibility field reveals that, as expected, the inelastic deformations concentrate in the regions of high shear, while a large region remains compatible, thus purely elastic. Moreover, the inequality in (8.9) is satisfied.

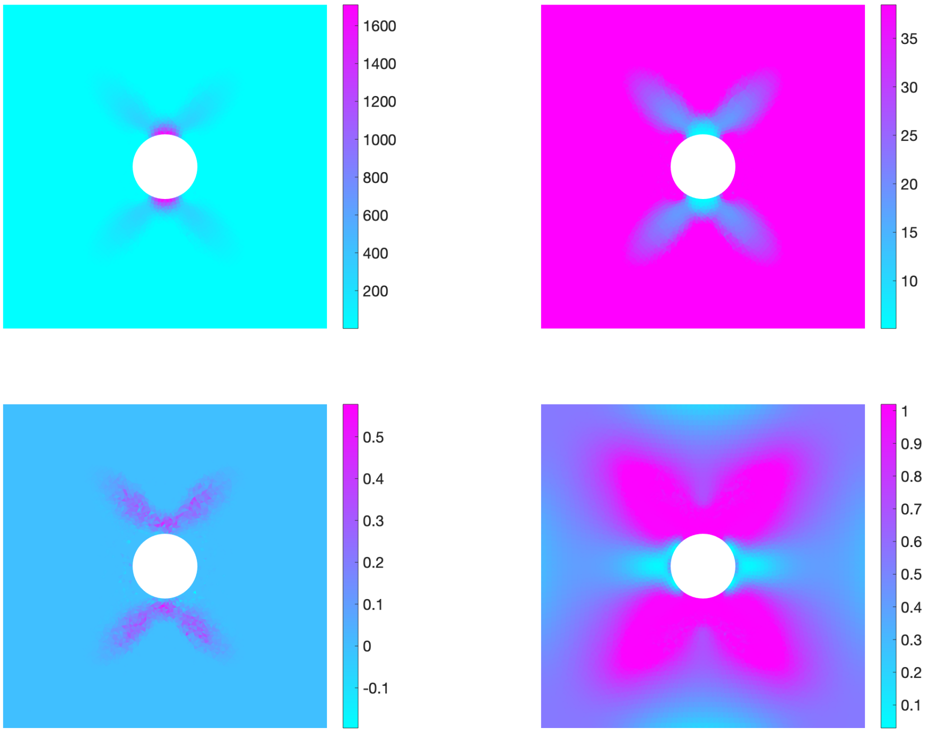

FIGURE 1. Perforated plate under uniaxial traction. Top: θ and $\mu_{\mathbb{A}}$. Bottom: inc E and σ_M^2.

11.2. **Traction with necking.** We now consider a plate of size 1×0.5 with two half-circular perforations at the middle of the bottom and top edges. The mesh consists of 3806 elements. In order to highlight the necking effect we have set $\sigma_Y^2 = 0.9$ and performed 50 iterations to reach convergence. The other parameters are the same as in the previous case. Outputs are displayed in Figure 2. In Figure 3 we show similar results obtained with a refined mesh of 6750 elements, to illustrate the convergence of the finite element method.

11.3. **Plate with inclusion under shear.** We investigate further the role of the tangent material coefficients through the following numerical experiment. The domain at hand is a unit square subjected to a shear load applied on the edges. A circular inclusion of radius 0.15 is located in the middle. We prescribe the piecewise constant coefficients $\mu_{\mathbb{A}} = 10^{-3}$ and $2\mu_{\mathbb{D}} = 10^{-5}$ in the inclusion, $\mu_{\mathbb{A}} = 0.3$ and $2\mu_{\mathbb{D}} = 10^3$ outside. The mesh consists of 15046 elements. We show our results in Figure 4. The incompatibility profile is coherent with the accumulation of dislocations nearby the boundary of the inelastic inclusion due to the variation of their mobilities. Indeed, dislocations are transported inside the inclusion under the shear efforts, but they cannot escape because $\mu_{\mathbb{D}}$ is very large outside.

12. Concluding remarks: plasticity without plastic strain?

This paper contributes to the theme of incompatible elasticity, with a view to devise a model of elasto-plasticity grounded on intrinsic considerations. Indeed, plastic effects in a deformable solid are here driven by the incompatibility of the total macroscopic strain, to be understood in a specific sense, and not by a plastic strain as in conventional approaches. Compared with our previous work on the topic, the main novelties are the following: (i) the model is of higher

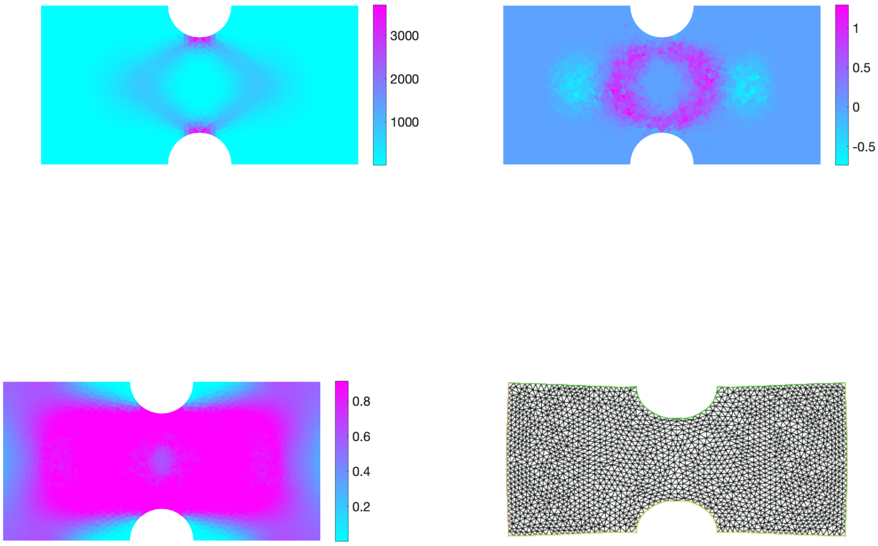

Figure 2. Second example of plate under uniaxial traction. Top: θ and inc E. Bottom: σ_M^2 and enhanced deformed configuration (displacements with a factor 5).

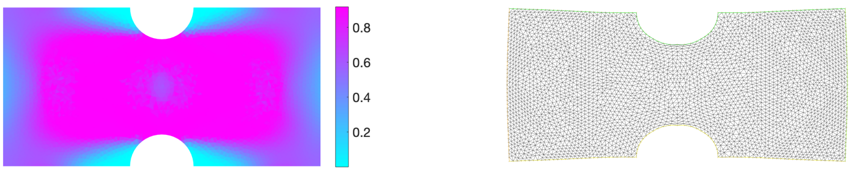

Figure 3. Second example with refined mesh (σ_M^2 and deformation).

order, but shows a variational structure; (ii) the two classical types of boundary conditions are incorporated and given a clear and coherent physical meaning; (iii) the strain is given a multiscale interpretation; (iv) evolution rules for the tangent moduli are discussed; (v) numerical aspects are addressed and simulations on simple academic examples illustrate the relevance of the model. In addition, as in our previous work, pure linearized elasticity is recovered as a limit case. Future research may deal with the complete time incremental evolution problem as well as 3d numerical simulations, with the ultimate goal of modeling real macroscopic material behaviors.

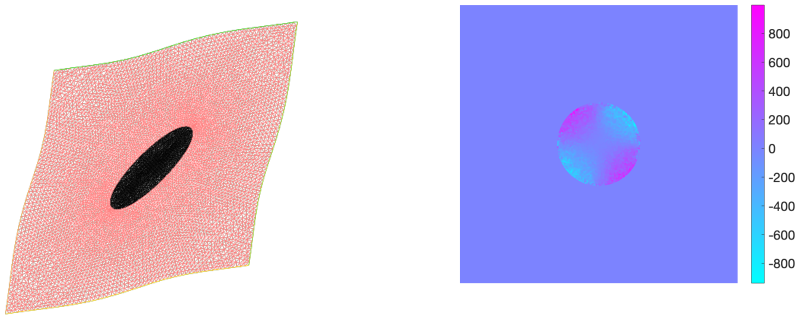

FIGURE 4. Plate with inclusion under shear: enhanced deformation and incompatibility field.

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Appendix A. Dual Newton method

The goal of this section is to minimize over $\{\theta \geq \theta_{\min}\}$ the function

$$F(\theta) = a\mu_{\mathbb{A}}(\theta) + \frac{b}{\theta} + \theta,$$

given $a, b \geq 0$. Recall that $\mu_{\mathbb{A}}(\theta)$ is defined by (8.7) and (8.8). Therefore F is convex. Here we consider the non-trivial case where $a, b > 0$, and we study the minimization over $\{\theta > 0\}$, as it suffices then to threshold the solution. As θ potentially covers the whole positive half-line, it is sometimes delicate to find a good initialization for the direct Newton method, especially when k is large. We propose the following dual formulation.

After Legendre-Fenchel conjugacy of the convex lower-semicontinuous function

$$\mathbb{R} \ni \theta \mapsto \begin{cases} \dfrac{b}{\theta} + \theta & \text{if } \theta > 0 \\ +\infty & \text{if } \theta \leq 0, \end{cases}$$

we arrive at

$$F(\theta) = \sup_{r \geq 0} \; a\mu_{\mathbb{A}}(\theta) + \theta(1-r) + 2\sqrt{br} \qquad \forall \theta > 0.$$

This yields

$$\inf_{\theta > 0} F(\theta) = \inf_{\theta > 0} \sup_{r \geq 0} \; L(\theta, r), \qquad L(\theta, r) = a\mu_{\mathbb{A}}(\theta) + \theta(1-r) + 2\sqrt{br}.$$

As, F is strictly convex and goes to infinity at 0 and $+\infty$, it admits a unique minimizer $\bar{\theta}$, and since the function F is decreasing on the interval $(0, \sqrt{b}]$ we have $\bar{\theta} > \sqrt{b}$. A short calculation reveals that the pair

$$(\bar{\theta}, \bar{r} = \frac{b}{\bar{\theta}^2})$$

is a saddle point of L, and since $\bar{r} < 1$ we have

$$\inf_{\theta > 0} F(\theta) = \sup_{0 \leq r < 1} \inf_{\theta \geq 0} \; L(\theta, r).$$

The inner minimization is realized by

$$\theta = \max\left(0, \sqrt{\frac{ak}{1-r}} - \frac{k}{\mu_0}\right), \tag{A.1}$$

which entails after some algebra

$$\inf_{\theta>0} F(\theta) = a\mu_0 + \sup_{0\le r<1} g(r), \qquad g(r) = 2\sqrt{br} - \max\left(0, \sqrt{a\mu_0} - \sqrt{\frac{k(1-r)}{\mu_0}}\right)^2.$$

Set

$$r^* = \max\left(0, 1 - \frac{a\mu_0^2}{k}\right).$$

Clearly, g is maximized over $[r^*, 1)$. Hence we define

$$h(r) = 2\sqrt{br} - \left(\sqrt{a\mu_0} - \sqrt{\frac{k(1-r)}{\mu_0}}\right)^2.$$

We apply the Newton method for the maximization of h over the interval $[r^*, 1]$. Then we infer θ by (A.1).

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