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A SECOND-ORDER MODEL OF SMALL-STRAIN INCOMPATIBLE ELASTICITY

SAMUEL AMSTUTZ AND NICOLAS VAN GOETHEM

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 achieved on the topic, and with the purpose to eventually settle a firm framework for the macroscopic description of elasto-plastic behaviors based on the incompatibility concept. The starting point for this approach is Kröner's celebrated work [13] on geometric elasticity with defects showing the link between strain incompatibility and the density of dislocations (see also [17, 18]). 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 major 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 [6]. By this choice we intentionally depart from the conventional standpoint of considering the displacement (or the deformation field) 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 [3, 5, 14]). 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 [8] and Maugin [15]), and appropriateness to the mathematical treatment since a variational or weak form is readily obtained. To infer strong forms and prescribe relevant boundary conditions and loads, it is required to carefully study the appropriate function spaces, as we have done in [1, 4], 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. Indeed, we propose interpretations in terms of "micro-hard" and "micro-free" in the spirit of Gurtin and Needleman [9], though our models diverge from the start. Further, we emphasize that we work at the averaged macroscopic scale, i.e., the body is a continuum medium filled with dislocations at a smaller scale, where by dislocations we intend a tensor field called the density of dislocations (in the spirit of Kröner and our previous works). As opposed to other works by the

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second author [16], dislocations here are not geometric field singularities typical of the mesoscopic scale. This is also in contrast to Gurtin and Needleman's crystal plasticity model where local slip systems are prescribed. 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, with isotropic constitutive laws. At the same time, energetic arguments allow to monitor the corresponding tangent moduli that generalize the Lamé coefficients to this second-order model, and this is what we substitute to the flow rules. This approach is not new, since in conventional plasticity, the effective tangent moduli are also byproducts of the flow rules (see [12]).

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. The modeling of external efforts is addressed in Section 5. Mathematical properties of the model for given tangent moduli are established in Section 6, while the evolution of these moduli is discussed in Section 7. Numerical aspects and simulations are reported in Sections 8 through 10.

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 will suffer 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 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 fundamental requirement is the fact that the internal work be an objective quantity, i.e. independent of any reference configuration, boundary condition, or any other arbitrary choice possibly made by the observer. On the contrary, the external work may be non-objective (see [15]). 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

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

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.

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

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

where d/dt stands for the total (or material) derivative. It is immediately recognized that the diagonal components of d_{ij} represent the 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., [10, Section 11.2] and [7, 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 reference configuration nor velocity field. Given a time increment Δt , we will rather work with the strain increment

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

so that (2.2) is retrieved as the limit of $E_{ij}(t)/\Delta t$ when $\Delta t \rightarrow 0$, 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

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

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 assume that E behaves like a second order 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 $\text{Riem}(g)$. Expanding $\text{Riem}(g)$ in terms of E we obtain an expression of form [14]

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

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

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

We use the convention that the Curl of a tensor is computed row-wise, whereby $\text{Curl}^t E$ 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. $\text{inc } \nabla^S u = 0$. Therefore, in the small strain setting encompassing the fact that the remainder $o(\nabla \nabla E)$ can be neglected, we will use $\text{inc } E$ as a representation of the Riemannian curvature.

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 $(\hat{E}, \text{inc } \hat{E})$. 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 $\text{inc } \hat{E}$ 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 $\text{inc } \hat{E}$. We write the internal work as the linear functional

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

Thus the principle of virtual work is expressed as

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

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 $\text{inc } E$ by constitutive laws of form

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

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

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

The model obtained from the first two terms has been studied in [2–4]. It is appealing in that the mixed term in the simplified form $\ell \text{inc } E \cdot \hat{E}$ can be derived by integration by parts from a first gradient (with respect to strain) model including natural assumptions, it leads to well-posed governing equations, and it is consistent with compatible elasticity at the limit $\ell \rightarrow \pm\infty$ under some assumptions. 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 $\mathbb{C}E \cdot \text{inc } \hat{E}$. 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 $\text{inc } E = 0$ or $\text{inc } \hat{E} = 0$. We arrive at the balance law

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

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

2.5. Isotropy. We consider a ball $B \subset \Omega$, and we assume that \mathbb{A} and \mathbb{D} are constant in B . Up to a shift of the coordinate system, we assume for simplicity that B is centered at 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

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

The series of computations

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

result in

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

Thus, the isotropy condition

$$\mathcal{Q}_E(E) + \mathcal{Q}_I(E) = \mathcal{Q}_E(E^*) + \mathcal{Q}_I(E^*) = \mathcal{Q}_E(Q^t E(Qx) Q) + \mathcal{Q}_I(Q^t \operatorname{inc} E(Qx) Q)$$

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}_E and \mathcal{Q}_I only depend on the scalar invariants of E and $\operatorname{inc} E$. The three invariants of a 3×3 matrix A are $\text{I}(A) := \operatorname{tr} A$, $\text{II}(A) := \frac{1}{2} ((\operatorname{tr} A)^2 - \operatorname{tr}(A^2))$ and $\text{III}(A) := \det A$. Being quadratic we must drop the $\text{III}(E)$ dependence and we get

$$\mathcal{Q}_E(E) = \alpha_E (\text{I}(E))^2 + \beta_E \text{II}(E),$$

for some scalars α_E and β_E , and a similar expression for \mathcal{Q}_I . The 4th order tensor \mathbb{A} is obtained by differentiating twice \mathcal{Q}_E . From $D\text{I}(E) = \mathbb{I}$, $D\text{II}(E) = \text{I}(E)\mathbb{I} - E$, we get

$$D\mathcal{Q}_E(E) = (2\alpha_E + \beta_E)\text{I}(E)\mathbb{I} - \beta_E E,$$

hence

$$\mathbb{A} = D^2 \mathcal{Q}_E(E) = (2\alpha_E + \beta_E)\mathbb{I} \otimes \mathbb{I} - \beta_E \mathbb{I}_4,$$

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

$$\mathbb{A} = 2\mu_E \mathbb{I}_4 + \lambda_E \mathbb{I} \otimes \mathbb{I}, \quad \mathbb{D} = 2\mu_I \mathbb{I}_4 + \lambda_I \mathbb{I} \otimes \mathbb{I}. \quad (2.5)$$

Of course we recognize the standard Hooke's tensor \mathbb{A} , with corresponding Lamé moduli λ_E and μ_E , 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 expression for Σ and Λ :

$$\Sigma = \mathbb{A}E = 2\mu_E \text{dev}(E) + \kappa_E \text{tr}(E)\mathbb{I}, \quad \Lambda = \mathbb{D} \text{inc } E = 2\mu_I \text{dev}(\text{inc } E) + \kappa_I \text{tr}(\text{inc } E)\mathbb{I},$$

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

$$\text{dev}A := A - \frac{1}{3} \text{tr}(A)\mathbb{I}, \quad \kappa_{E/I} = \frac{2}{3}\mu_{E/I} + \lambda_{E/I}.$$

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. [12, 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 depend on E .

3. BURGERS TENSOR, FRANK TENSOR AND MICRO-HARD CONDITION

3.1. Frank and Burgers tensors. In linearized elasticity with line singularities, following the formalism introduced in [19], there are two basic tensors that allow to compute the jump of the rotation and displacement fields, namely the Frank tensor

$$\mathbb{F} = \text{Curl}^t E, \quad \mathbb{F}_{ij} = \epsilon_{ikl} \partial_k E_{jl}, \quad (3.1)$$

and the Burgers tensor¹, given a reference point x_0 ,

$$\mathbb{B} = E + ((x - x_0) \times \text{Curl } E)^t, \quad \mathbb{B}_{ij} = E_{ij} + \epsilon_{ipq} (x_p - x_{0p}) \mathbb{F}_{qj}. \quad (3.2)$$

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

$$E = \nabla^S u, \quad \omega = \frac{1}{2} \text{Curl } u, \quad b = u - \omega \times (x - x_0),$$

we have the relations

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

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

This provides by integration along a path from x_0 to x

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

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

and obviously the above integrals vanish along a closed loop. Turning now to the incompatible case, when E 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, if we consider a loop C which encloses dislocations and / or disclinations, then we can define the Frank and Burgers vectors associated with C as

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

¹Our meaning of the Burgers tensor is different from Gurtin and Needleman's one [9], which for us would be the dislocation density tensor.

We note that, if we place ourselves at the mesoscopic scale (i.e., a continuum scale where the dislocations and disclinations are modeled as singularity lines, namely loops), then 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., [19]).

It is important to note that 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 . 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 a 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 $u_{S_C} = u_{x_0}$ on $\Omega \setminus S_{\mathcal{L}}$. 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 recall that at the macroscopic scale that we consider, the dislocations are not present in the form of line singularities but modelled 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

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

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

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

which reads

$$\text{Curl } \mathbb{B}N = (x - x_0) \times (\text{inc } EN).$$

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

$$B[C] = \int_S (x - x_0) \times (\text{inc } EN) dS(x). \quad (3.5)$$

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

$$\text{inc } EN = 0 \text{ on } S. \quad (3.6)$$

By (3.5), this is equivalent to saying that, for every $x_0 \in S$, the resultant Burgers vector $B[C']$ of defect lines enclosed in any loop $C' \subset S$ containing x_0 vanishes.

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 [9], thus which is stronger than ours. Similarly, imposing $\text{Curl}^t E \times N = 0$ also yields $\text{inc } EN = 0$.

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 [1]). *Suppose that $E \in \mathcal{C}^2(\bar{\Omega}, \mathbb{S}^3)$ and $\eta \in H^2(\Omega, \mathbb{S}^3)$. Then*

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

with the trace operators defined as

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

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

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

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

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 $u \in L^1(\Omega, \mathbb{R}^3)$ and $\text{div } \text{inc } E = 0$ for all $E \in L^1(\Omega, \mathbb{S}^3)$. The main function space on which we will build our analysis is

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

It is naturally endowed with an Hilbertian structure for the norm

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

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 [1]. Throughout we will denote duality pairings by integrals.

We next define $H_0^{\text{inc}}(\Omega, \mathbb{S}^3)$ as the closure of $\mathcal{C}_c^\infty(\Omega, \mathbb{S}^3)$ in $H^{\text{inc}}(\Omega, \mathbb{S}^3)$. The following properties are proved in [4].

Proposition 2. (1) $H_0^{\text{inc}}(\Omega, \mathbb{S}^3) = \{E \in H^{\text{inc}}(\Omega, \mathbb{S}^3) : \mathcal{T}_0(E) = \mathcal{T}_1(E) = 0 \text{ on } \partial\Omega\}$.
 (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

$$\mathcal{V} = \{E \in L^2(\Omega, \mathbb{S}^3) : \text{inc } E = 0\},$$

$$\mathcal{W} = \{E \in L^2(\Omega, \mathbb{S}^3) : \text{div } E = 0\},$$

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

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

$$\mathcal{V}_{\Gamma_1}^0 = \{E \in \mathcal{V} : \mathcal{T}_0(E) = \mathcal{T}_1(E) = 0 \text{ on } \Gamma_1\},$$

$$\mathcal{V}_{\Gamma_1}^{00} = \{\nabla^S v : v \in H^1(\Omega, \mathbb{R}^3), v = 0 \text{ on } \Gamma_1\},$$

$$\mathcal{W}_{\Gamma_2}^0 = \{E \in \mathcal{W} : EN = 0 \text{ on } \Gamma_2\}.$$

We refer to [4] 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*

$$\mathcal{V} = \{\nabla^S v, v \in H^1(\Omega, \mathbb{R}^3)\}, \quad \mathcal{W} = \{\text{inc } F, F \in \mathcal{Z}\}.$$

- (2) If $E \in L^2(\Omega, \mathbb{S}^3)$ satisfies $\text{inc } E = 0$ in Ω and $\mathcal{T}_0(E) = \mathcal{T}_1(E) = 0$ on $\partial\Omega$ then there exists $v \in H_0^1(\Omega, \mathbb{R}^3)$ 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

$$L^2(\Omega, \mathbb{S}^3) = \mathcal{V}_{\Gamma_1}^{00} \oplus \mathcal{W}_{\Gamma_2}^0, \quad H^{\text{inc}}(\Omega, \mathbb{S}^3) = \mathcal{V} \oplus \mathcal{Z}.$$

- (5) We have the Poincaré inequality

$$\|E\|_{H^1(\Omega, \mathbb{S}^3)} \leq c \|\text{inc } E\|_{L^2(\Omega, \mathbb{S}^3)} \quad \forall E \in \mathcal{Z},$$

for some positive constant c .

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

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 microhard one (3.6).

5. GENERALIZED EXTERNAL FORCES

With the help of the decompositions from Theorem 3 we are going to give alternative representations of the external work (2.1). 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

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

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

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

We recall the following property proved in [4].

Lemma 4. If $\mathbb{K} \in \mathcal{V}_{\Gamma_1}^{00}$ and $\text{inc } \hat{F} \in \mathcal{W}_{\Gamma_2}^0$ then

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

Let $f \in L^2(\Omega, \mathbb{R}^3)$ and $g \in H^{-1/2}(\partial\Omega, \mathbb{R}^3)$ be given. Using Lemma 4 we derive the following representation: if $\mathbb{K} = \nabla^S w$, with $w \in H^1(\Omega, \mathbb{R}^3)$ the (weak) solution of

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

then we retrieve the conventional external work

$$W_e(\hat{E}) = \int_{\Omega} f \cdot \hat{v} dx + \int_{\Gamma_2} g \cdot \hat{v} dS(x). \quad (5.1)$$

6. WELL-POSEDNESS AND ELASTIC LIMIT

6.1. 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

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

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

Theorem 5. *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*

$$\int_{\Omega} (\mathbb{A}E \cdot \hat{E} + \mathbb{D} \text{inc } E \cdot \text{inc } \hat{E}) dx = \int_{\Omega} \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{H}. \quad (6.1)$$

6.2. Free boundary condition and strong form. Assuming sufficient regularity for E , integrating the left-hand side of (6.1) 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 $\hat{E} \in \mathcal{C}_c^\infty(\Omega, \mathbb{S}^3)$ 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 encoding the efforts f and g by (5.1).

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

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

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

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

This is our version of the micro-free or microscopically powerless boundary condition, similar in spirit to [9] but different in its expression since the authors of [9] have another kinematical description with prescribed slip systems.

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

Theorem 6. *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*

$$\int_{\Omega} (\mathbb{A}E_k \cdot \hat{E} + \mathbb{D}_k \text{inc } E_k \cdot \text{inc } \hat{E}) dx = \int_{\Omega} \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{H}. \quad (6.2)$$

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

$$\int_{\Omega} \mathbb{A}E_\infty \cdot \hat{E} dx = \int_{\Omega} \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{V}_{\Gamma_1}^0. \quad (6.3)$$

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

$$\|E_k\|_{L^2(\Omega, \mathbb{S}^3)} \leq c, \quad \|\text{inc } E_k\|_{L^2(\Omega, \mathbb{S}^3)} \rightarrow 0, \quad (6.4)$$

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

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

hence $\text{inc } E_\infty = 0$. 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 (6.4),

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

hence $\mathcal{T}_0(E_\infty) = \mathcal{T}_1(E_\infty) = 0$ on Γ_1 . We have shown that $E_\infty \in \mathcal{V}_{\Gamma_1}^0$. Using a test function $\hat{E} \in \mathcal{V}_{\Gamma_1}^0$ in (6.2) 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 (6.3). 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

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

and on the other hand,

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

It follows that

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

from which we infer the strong convergence. \square

In view of Theorem 3, we can rephrase (6.3) in a fully standard form, at least in the following two cases:

- (1) if $\Gamma_1 = \emptyset$ (free boundary condition on $\partial\Omega$) then $\mathcal{V}_{\Gamma_1}^0 = \mathcal{V} = \{\nabla^S v, v \in H^1(\Omega, \mathbb{R}^3)\}$ and the Neumann linear elasticity problem is retrieved;
- (2) if $\Gamma_1 = \partial\Omega$ (hard boundary condition on $\partial\Omega$) then $\mathcal{V}_{\Gamma_1}^0 = \mathcal{V}_{\partial\Omega}^{00} = \{\nabla^S v, v \in H_0^1(\Omega, \mathbb{R}^3)\}$ and the Dirichlet linear elasticity problem is retrieved.

7. DISSIPATION AND EVOLUTION RULES

7.1. General framework. We now address the question of the evolution of the tangent moduli $\kappa_E, \mu_E, \kappa_I, \mu_I$ within an incremental procedure. To do so we study dissipation when changing locally these coefficients. We start with the total work expended during the current increment

$$W = \int_{\Omega} \mathbb{K}_{\text{tot}} \cdot E,$$

where \mathbb{K}_{tot} represents the total external effort. We focus our attention on the first increment, which yields $\mathbb{K}_{\text{tot}} = \mathbb{K}$, hence we have

$$W = \int_{\Omega} (\mathbb{A} E \cdot E + \mathbb{D} \text{inc } E \cdot \text{inc } E) dx.$$

We assume the isotropic constitutive laws (2.5), where we choose $\lambda_I = 0$ for simplicity. This yields

$$W = \int_{\Omega} (\kappa_E (\text{tr } E)^2 + 2\mu_E |\text{dev } E|^2 + 2\mu_I |\text{inc } E|^2) dx.$$

It is convenient to introduce the quantity $\rho = (2\mu_I)^{-1}$, as by Theorem 6, linear elasticity corresponds to the limit $\rho \rightarrow 0$. We call ρ the compatibility modulus. We assume that the elastic shear and compatibility moduli are related by a constitutive law $\mu_E = \mu_E(\rho)$. Moreover, because it is

not expected to play any role in plasticity, the elastic bulk modulus κ_E is assumed constant. For consistence we denote $\mu_I(\rho) = (2\rho)^{-1}$.

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

$$\int_{\Omega} \left(\kappa_E \operatorname{tr} E(\rho) \operatorname{tr} \hat{E} + 2\mu_E(\rho) \operatorname{dev} E(\rho) \cdot \operatorname{dev} \hat{E} + 2\mu_I(\rho) \operatorname{inc} E(\rho) \cdot \operatorname{inc} \hat{E} \right) dx = \int_{\Omega} \mathbb{K} \cdot \hat{E} dx \quad \forall \hat{E} \in \mathcal{H}, \quad (7.1)$$

and $W(\rho)$ the work

$$W(\rho) = \int_{\Omega} \mathbb{K} \cdot E(\rho) dx.$$

The dissipation for the increment under consideration is the difference between the actual work and the corresponding elastic work for the same loading, i.e.,

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

Obviously we have the variational formulation

$$-W(\rho) = \inf_{E \in \mathcal{H}} \left\{ \int_{\Omega} (\kappa_E \operatorname{tr}^2 E + 2\mu_E(\rho) |\operatorname{dev} E|^2 + 2\mu_I(\rho) |\operatorname{inc} E|^2) dx - 2 \int_{\Omega} \mathbb{K} \cdot E dx \right\}.$$

We assume that the increment consists of an evolution process for ρ which reaches equilibrium when

$$d\mathcal{D} \leq \delta\Phi,$$

where $d\mathcal{D}$ is the infinitesimal dissipation and $\delta\Phi$ is the energetic cost of defects activation. This condition basically means that creation and/or motion of dislocations has an energetic cost, and that the energy required for such processes is entirely dissipated inside the body. Furthermore, we postulate that this energetic expense derives from a potential, namely $\delta\Phi = d\Phi$. This leads to the stationarity condition

$$\frac{d\mathcal{D}}{d\rho}(\hat{\rho} - \rho) \leq \frac{d\Phi}{d\rho}(\hat{\rho} - \rho) \quad \forall \hat{\rho} \geq 0.$$

We recognize the first order optimality condition of the problem

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

itself equivalent to

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

We further assume the existence of a specific energy $\phi(\rho)$ such that

$$\Phi(\rho) = \int_{\Omega} \phi(\rho) dx.$$

Lastly, due to our choice of function $\mu_I(\rho)$, we restrict to $\rho \geq \rho_{\min}$ for a sufficiently small ρ_{\min} that approximates perfect elasticity. We arrive at the joint variational formulation

$$\underset{(\rho, E) \in L^\infty(\Omega, [\rho_{\min}, +\infty)) \times \mathcal{H}}{\text{minimize}} \int_{\Omega} (\kappa_E \operatorname{tr}^2 E + 2\mu_E(\rho) |\operatorname{dev} E|^2 + 2\mu_I(\rho) |\operatorname{inc} E|^2) dx - 2 \int_{\Omega} \mathbb{K} \cdot E dx + \int_{\Omega} \phi(\rho) dx. \quad (7.2)$$

It can be solved by alternating minimizations:

- minimization with respect to E is equivalent to solving the governing equation (7.1),
- minimization with respect to ρ can be for instance performed by steepest descent or Newton iterations, see also appendix A.

7.2. Example. Since the material response can be viewed as the sum of elastic and plastic phenomena in series we adopt the representation

$$\mu_E(\rho)^{-1} = \mu_0^{-1} + \tilde{\mu}(\rho)^{-1}, \quad (7.3)$$

where μ_0 is the elastic shear modulus and $\tilde{\mu}(\rho)$ is a purely plastic effective shear modulus. It is reasonable to assume that $\lim_{\rho \rightarrow 0} \tilde{\mu}(\rho) = +\infty$ and $\tilde{\mu}(\rho)$ is a decreasing function of ρ . Let us write the stationarity condition for (7.2):

$$-2\mu'_E(\rho)|\operatorname{dev}E(\rho)|^2 - 2\mu'_I(\rho)|\operatorname{inc}E(\rho)|^2 - \phi'(\rho) \in N(\rho),$$

with the normal cone $N(\rho)(x) = (-\infty, 0]$ if $\rho(x) = \rho_{\min}$, $N(\rho)(x) = \{0\}$ if $\rho(x) > \rho_{\min}$. Using (7.3) this is equivalent to

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

We suggest the simple laws

$$\tilde{\mu}(\rho) = \frac{k}{\rho}, \quad \phi(\rho) = \gamma\rho, \quad k, \gamma > 0. \quad (7.4)$$

We obtain the stationarity condition

$$\frac{2}{k}|\mu_E(\rho)\operatorname{dev}E(\rho)|^2 + |\mu_I(\rho)\operatorname{inc}E(\rho)|^2 - \gamma \in N(\rho).$$

In particular for the von Mises stress $\sigma_M = |2\mu_E(\rho)\operatorname{dev}E(\rho)|$ we always have

$$\sigma_M^2 \leq 2\gamma k =: \sigma_Y^2. \quad (7.5)$$

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

8. NUMERICAL RESOLUTION

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

$$\int_{\Omega} \mathbb{A}E \cdot \hat{E} + \mathbb{D}\operatorname{inc}E \cdot \operatorname{inc}\hat{E} = \int_{\Omega} \mathbb{K} \cdot \hat{E} \quad \forall \hat{E} \in H^{\operatorname{inc}}(\Omega, \mathbb{S}^3). \quad (8.1)$$

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

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

Using the representation (5.1) of the external work we arrive at

$$\int_{\Omega} \left(\mathbb{A}(\nabla^S u + E_i) \cdot (\nabla^S \hat{u} + \hat{E}_i) + \mathbb{D}\operatorname{inc}E_i \cdot \operatorname{inc}\hat{E}_i \right) dx = \int_{\Omega} f \cdot \hat{u} dx + \int_{\partial\Omega} g \cdot \hat{u} dS(x). \quad (8.2)$$

Still, the constraints $E_i, \hat{E}_i \in \mathcal{W}_{\partial\Omega}^0$ are not easy to handle through finite element subspaces. For this reason we turn to a mixed formulation. First, specializing (8.2) to the case where $\hat{E}_i = 0$ results in

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

Second, since $\mathbb{K} \in \mathcal{V}$ we rewrite (8.1) with $\mathbb{K} = -\nabla^S p$, $p \in H^1(\Omega, \mathbb{R}^3)$, and obtain

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

By summation we arrive at

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

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

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

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

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

with ϵ_u, ϵ_p small stabilization parameters.

9. 2D MODEL

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

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

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

$$\operatorname{inc} E = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \partial_{xx} E_{yy} + \partial_{yy} E_{xx} - 2\partial_{xy} E_{xy} \end{pmatrix}, \quad (9.1)$$

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

$$\mathbb{D} \operatorname{inc} E \cdot \operatorname{inc} \hat{E} = (\lambda_I + 2\mu_I) \operatorname{inc} E \cdot \operatorname{inc} \hat{E}.$$

The 2D model reads

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

for all kinematically admissible plane virtual strain \hat{E} . Of course, \mathbb{K} has to be constructed in the form (9.1).

Remark 1. *Let us consider the particular case in which λ_E, μ_E are constant, $\operatorname{inc} \mathbb{K} = 0$ and $\operatorname{div} K = 0$. Set*

$$\begin{cases} E_{xx} = \frac{1}{4\mu_E(\lambda_E + \mu_E)} ((\lambda_E + 2\mu_E)\mathbb{K}_{xx} - \lambda_E\mathbb{K}_{yy}) \\ E_{yy} = \frac{1}{4\mu_E(\lambda_E + \mu_E)} ((\lambda_E + 2\mu_E)\mathbb{K}_{yy} - \lambda_E\mathbb{K}_{xx}) \\ E_{xy} = \frac{1}{2\mu_E} \mathbb{K}_{xy}. \end{cases}$$

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

10. NUMERICAL EXAMPLES

The computations are performed using the finite element software FreeFem++ [11]. The codes are available at <https://github.com/samuel-amstutz/incompatibility.git>. We use the built-in Hsieh-Clough-Tocher elements (of class C^1) for the approximation of E_i and P2 elements for the approximation of u and p . We use dual Newton iterations as explained in appendix A to solve the minimization problem in the independent variable ρ .

10.1. 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 $\kappa_E = 0.83$, $\mu_0 = 0.3846$, $k = 10^4$, $\sigma_Y = 1$, whereby γ is derived by (7.5). Other parameters are $\rho_{\min} = 10^{-3}$, $\epsilon_u = \epsilon_p = 10^{-6}$. 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. Moreover, the inequality in (7.5) is satisfied.

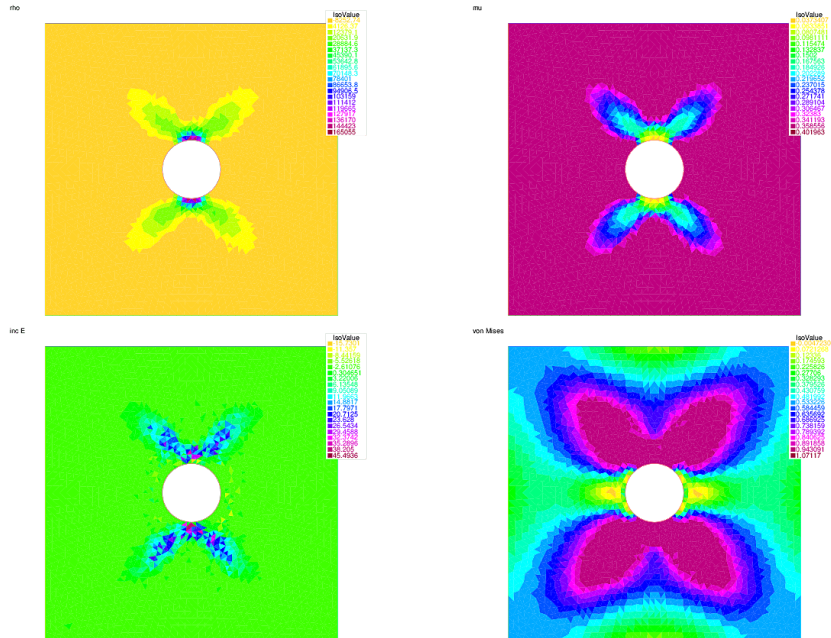


FIGURE 1. Perforated plate under uniaxial traction. Top: ρ and μ_E . Bottom: $\text{inc } E$ and σ_M^2 .

10.2. Plate with inclusion under shear. We investigate further the role of the coefficient μ_I 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. The material coefficients are taken piecewise constant as $\mu_E = 10^{-3}$ and $2\mu_I = 10^{-5}$ in the inclusion, $\mu_E = 0.3$ and $2\mu_I = 10^3$ outside. The mesh consists of 15046 elements. We show our results in Figure 2. The incompatibility profile is consistent with the motion of dislocations within the inclusion, which accumulate nearby the interface because they cannot penetrate in the almost elastic medium.

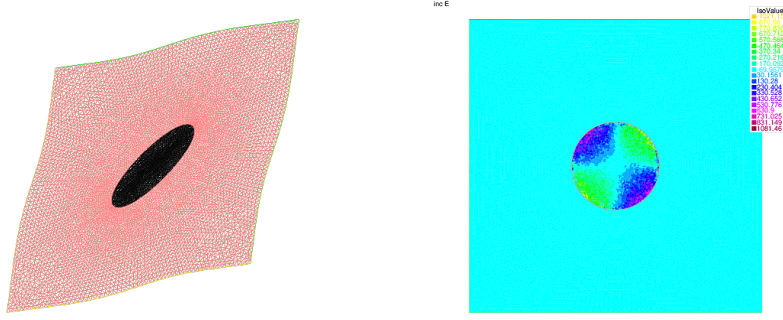


FIGURE 2. Plate with inclusion under shear: enhanced displacement and incompatibility.

11. CONCLUDING REMARKS

This paper contributes to the theme of incompatible elasticity, with a view to devise a model of elasto-plasticity grounded on intrinsic considerations. Compared with our previous work on the topic, the main novelties are the following: (i) the model is of higher 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) evolution rules for the tangent moduli are discussed; (iv) numerical 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 further address the complete time incremental evolution problem as well as 3d numerical simulations, with the ultimate goal of modeling real macroscopic material behaviors.

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APPENDIX A. DUAL NEWTON METHOD

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

$$F(\rho) = a\mu_E(\rho) + \frac{b}{\rho} + \rho,$$

given $a, b \geq 0$. Recall that $\mu_E(\rho)$ is defined by (7.3) and (7.4). Therefore F is convex. Here we consider the non-trivial case where $a, b > 0$, and we study the minimization over $\{\rho > 0\}$, as it suffices then to threshold the solution. As ρ 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 since it tends to increase the range of attained values. We propose the following dual formulation.

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

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

we arrive at

$$F(\rho) = \sup_{r \geq 0} a\mu_E(\rho) + \rho(1-r) + 2\sqrt{br}.$$

This yields

$$\inf_{\rho>0} F(\rho) = \inf_{\rho \geq \rho_{\min}} \sup_{r \geq 0} L(\rho, r) = a\mu_E(\rho) + \rho(1-r) + 2\sqrt{br}.$$

As, F is strictly convex and goes to infinity at 0 and $+\infty$, it admits a unique minimizer $\bar{\rho}$. A short calculation reveals that the pair

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

is a saddle point of L , whereby

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

The inner minimization is realized by

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

which entails

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

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 ρ by (A.1). We can check that the result is also valid when $b = 0$ for the minimization over $\{\rho \geq 0\}$.

REFERENCES

- [1] S. Amstutz and N. Van Goethem. Analysis of the incompatibility operator and application in intrinsic elasticity with dislocations. *SIAM J. Math. Anal.*, 48(1):320–348, 2016.
- [2] S. Amstutz and N. Van Goethem. Incompatibility-governed elasto-plasticity for continua with dislocations. *Proc. R. Soc. A*, 473(2199), 2017.
- [3] S. Amstutz and N. Van Goethem. The incompatibility operator: from Riemann’s intrinsic view of geometry to a new model of elasto-plasticity. *CIM Series in Mathematical Sciences (Hal report 01789190)*, 2018.
- [4] S. Amstutz and N. Van Goethem. Existence and asymptotic results for an intrinsic model of small-strain incompatible elasticity. *Discrete Contin. Dyn. Syst., Ser. B*, 25(10):3769–3805, 2020.
- [5] Ph. G. Ciarlet. *An Introduction to Differential Geometry with Applications to Elasticity*. Springer, 2006.
- [6] Ph. G. Ciarlet and C. Mardare. Intrinsic formulation of the displacement-traction problem in linearized elasticity. *Math. Models Methods Appl. Sci.*, 24(6):1197–1216, 2014.
- [7] G. Duvaut. *Mécanique des milieux continus*. Collection Mathématiques appliquées pour la maîtrise. Masson, 1990.
- [8] P. Germain. The method of virtual power in continuum mechanics. part 2: Microstructure. *SIAM Journal on Applied Mathematics*, 25(3):556–575, 1973.
- [9] M. E. Gurtin and A. Needleman. Boundary conditions in small-deformation, single-crystal plasticity that account for the Burgers vector. *J. Mech. Phys. Solids*, 53(1):1–31, 2005.
- [10] Morton E. Gurtin, Eliot Fried, and Lallit Anand. *The mechanics and thermodynamics of continua*. Cambridge University Press, Cambridge, 2010.
- [11] F. Hecht. New development in freefem++. *J. Numer. Math.*, 20(3-4):251–265, 2012.
- [12] K. Krabbenhöft. *Basic computational plasticity*. Lecture notes, Department of Civil Engineering, Technical University of Denmark, 2002.
- [13] E. Kröner. Continuum theory of defects. In R. Balian, editor, *Physiques des défauts, Les Houches session XXXV (Course 3)*. North-Holland, Amsterdam, 1980.
- [14] G. Maggiani, R. Scala, and N. Van Goethem. A compatible-incompatible decomposition of symmetric tensors in L^p with application to elasticity. *Math. Meth. Appl. Sci.*, 38(18):5217–5230, 2015.

- [15] G. A. Maugin. The method of virtual power in continuum mechanics: Application to coupled fields. *Acta Mechanica*, 35:1–70, 1980.
- [16] R. Scala and N. van Goethem. A variational approach to single crystals with dislocations. *SIAM J. Math. Anal.*, 51(1):489–531, 2019.
- [17] N. Van Goethem. The non-Riemannian dislocated crystal: a tribute to Ekkehart Kröner’s (1919-2000). *J. Geom. Mech.*, 2(3):303–320, 2010.
- [18] N. Van Goethem. Strain incompatibility in single crystals: Kröner’s formula revisited. *J. Elast.*, 103(1):95–111, 2011.
- [19] N. Van Goethem and F. Dupret. A distributional approach to the geometry of 2D dislocations at the continuum scale. *Ann. Univ. Ferrara*, 58(2):407–434, 2012.

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