

DISLOCATION-INDUCED LINEAR-ELASTIC STRAIN DYNAMICS BY A CAHN-HILLIARD-TYPE EQUATION

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ABSTRACT. In a single crystal containing dislocations, the elastic strain defined by a linear constitutive law from the stress tensor can be written as the sum of a symmetric gradient and a solenoidal tensor ϵ^0 , called the dislocation strain. This latter part of the elastic strain is related to dislocations, since its incompatibility equals to the curl of the contortion. The aim of this paper is to derive a time-evolution law for the internal thermodynamic variable ϵ^0 , arising from the Thermodynamics second Law, and to discuss its mathematical setting. This encompasses a discussion on the functional space used and about the equation well-posedness. A fourth-order time-dependent nonlinear PDE involving the incompatibility operator is found, which is similar in form to the Cahn-Hilliard equation, and represents to this respect a tensor generalization for solenoidal fields.

1. INTRODUCTION AND PRELIMINARY RESULTS

Let Ω be a simply-connected smooth and bounded subset of \mathbb{R}^3 . Let \mathcal{L} be a set of dislocation lines in Ω , and the dislocation density $\Lambda_{\mathcal{L}} \in \mathcal{M}(\Omega, \mathbb{M}^3)$ be given by a Radon measure concentrated in \mathcal{L} . As soon as dislocations are present, the strain ϵ can not be a symmetric gradient as the following crucial relation, called Kröner's formula, shows [22]:

$$\text{inc } \epsilon = \text{Curl } \kappa_{\mathcal{L}}, \quad \kappa_{\mathcal{L}} := \Lambda_{\mathcal{L}} - \frac{\mathbb{I}_2}{2} \text{tr} \Lambda_{\mathcal{L}},$$

where \mathbb{I}_2 is the second-rank identity tensor, and $\Lambda_{\mathcal{L}}$ the dislocation density tensor defined as $\Lambda_{\mathcal{L}} = \tau \otimes b \mathcal{H}_{\mathcal{L}}^1$, with τ , the tangent vector to the Lipschitz curve \mathcal{L} , $\mathcal{H}_{\mathcal{L}}^1$ the one-dimensional Hausdorff measure concentrated in \mathcal{L} , and with b the Burgers vector, constant on the line. Moreover, inc is the incompatibility operator, i.e.,

$$\text{inc} F := \text{Curl } \text{Curl}^t F,$$

where the curl of a tensor is taken column-wise. This operator is at the heart of the present work, since it will show to drive the time-evolution of the dislocation-induced strain. Note that the evolution of the dislocations are given by the so-called contortion tensor $\kappa_{\mathcal{L}}$ which cannot be determined from the sole knowledge of its curl, except for particular cases in which it is divergence-free, as for pure edge dislocations. For this reason, this work is not strictly speaking about the dynamics of dislocations.

Classically in linear elasticity, overall equilibrium reads $\text{div} \mathbb{A} \epsilon = 0$ in Ω , with \mathbb{A} the isotropic elasticity tensor. As a consequence, it is shown in [20] that there exists two fields of interest, the displacement u , and F , and auxiliary tensor which is solenoidal and symmetric. These fields satisfy Beltrami decomposition of the elastic strain, viz.,

$$\epsilon = \nabla^S u + \text{inc} F.$$

In this paper, our aim is to derive an evolution law for the internal thermodynamic variable

$$\epsilon^0 := \text{inc} F,$$

which is called the dislocation-induced strain, since it satisfies a regularized Kröner's relation $\text{inc} \epsilon^0 = \text{Curl } \kappa$, i.e. with a smoothed dislocation density (namely, the macroscopic contortion κ) in the right-hand side. Furthermore, ϵ^0 satisfies a time-dependent evolution which turns out to

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be sufficient for the global mechanical dissipation to be positive.

Specifically, in this paper we establish in a first step, study in a second step, and eventually discuss the following nonlinear tensor-valued equation:

$$\alpha \frac{d\epsilon^0}{dt} = \text{inc}(-\mathbb{M} \text{inc}\epsilon^0 - \mathcal{G}(\epsilon^0)) \quad \text{in } \Omega \times [0, T], \quad (1.1)$$

with \mathcal{G} a nonlinear potential, $\alpha > 0$ and \mathbb{M} a positive-definite and symmetric fourth-order material-dependent tensor. For simplicity, and for the sake of physical interpretation, we assume that \mathcal{G} depends only on $e := \text{tr}\epsilon^0$, the trace of the the dislocation-induced strain, which shows to be directly related and hence interpreted as a density of point defects. To achieve this aim, the mathematical nature of the incompatibility operator must be understood, and hence a series of mathematical results must be recalled as preliminary steps.

Observe that evolution law (1.1) shows a form similar to the Cahn-Hilliard equation, but for a tensor-valued unknown ϵ^0 . Indeed, the Laplacian counterpart is precisely the incompatibility operator, since it holds $\text{tr} \text{inc}F = \Delta \text{tr}F$, and hence (1.1) appears as a tensor generalization for solenoidal tensor fields of the classical scalar Cahn-Hilliard equation. From a physical point of view, the scalar version of our equation is related to the dynamics of point defects, which are required for the creation and motion of dislocations, and are related to the variation of matter density. Furthermore, e obeys to the scalar Cahn-Hilliard equation, though with nonstandard boundary conditions. A discussion about this equation, though derived by other means and with a different purpose, can be found in [19]. The purpose of this paper is to show that this equation is well posed in an appropriate functional space, some of its important properties are given. Let us emphasize that particular care is given to justify the equation boundary conditions, which must be sound mathematically, and at the same time have a Physical interpretation.

The notion of Internal Variable of State. We consider F as a mathematical gauge field arising from Beltrami decomposition of symmetric tensors, and without any particular physical meaning. However, its incompatibility, $\epsilon_0 := \text{inc}F$, is the dislocation-induced strain, since it is the only part of the elastic strain which appear in Kröner's formula. It is considered as an Internal Variable of State (IVS), in the sense given here by G. Maugin [14]: "internal variables of state are introduced in thermo-mechanics in addition to the usual observable variables of state (e.g., deformation, temperature, electric and magnetic fields). They are supposed to account in a more or less crude way for the complex internal microscopic processes that occur in the material and manifest themselves at a macroscopic scale in the form of dissipation."

Motivation. In our case, the observable variable of state (OVS) is the stress σ , from which the elastic strain ϵ is deduced by a constitutive law (hence the latter is also an OVS). So far, u and F are vector and tensor fields involved in the decomposition of ϵ . In some sense, u is also observable, measurable, and controlable, depending on its boundary conditions, and on the introduction of a reference configuration, which is an uncomfortable notion in infinitesimal elasticity. As a matter of fact, we prefer to let the identification u as the displacement field as a convenient "vue de l'esprit".

The crucial point is that ϵ^0 is an internal variable which is neither observable, nor measurable or controlable, in the sense of Physicists. Only its existence as a mathematical object and its effect in the form of dissipation is observed. Therefore, the aim of this paper is to show that it naturally obeys a PDE, and thus becomes observable, measurable and controlable in a mathematical sense. It should be emphasized that there exists no consensual procedure in the literature to determine the equation governing an IVS. Our point of view is to derive such equation in the simplest and most natural possible way, while not contradicting (at least), or better, complying (so far as possible) to Thermodynamics principles.

Structure of the work. The main part of this paper is about the derivation of the incompatibility-governed time-dependent model for the dislocation strain. To this aim, considerations about the statics problem, and in particular about the choice of the boundary conditions and their physical meaning are found in Section 3, subsections 3.1 and 3.2, respectively. The evolution law is then found in Section 4, whose mathematical properties, such as existence of solutions and

energetics bounds, are given in Section 5. In the preliminary Section 2, the functional spaces needed to mathematically handle the incompatibility operator are given. Several properties of tensor-valued fields with bounded incompatibility are also recalled, without proofs, to be found in a specifically-dedicated paper [3]. A discussion is proposed in Section 6.

Notations and conventions. Let $E \in \mathbb{S}^3$ and $\beta \in \mathbb{M}^3$, where \mathbb{M}^3 denotes the space of square 3-matrices, and \mathbb{S}^3 of symmetric 3-matrices. Note that subscript t stands for the transpose of a tensor and subscript S for the symmetric part of a tensor. The divergence and curl of a tensor E are defined componentwise as $(\operatorname{div} E)_i := \partial_j E_{ij}$ and $(\operatorname{Curl} E)_{ij} := \epsilon_{jkl} \partial_k E_{il}$, respectively. The incompatibility of a tensor E is the symmetric tensor defined componentwise as follows:

$$(\operatorname{inc} E)_{ij} := (\operatorname{Curl} \operatorname{Curl}^t E)_{ij} = \epsilon_{ikm} \epsilon_{jln} \partial_k \partial_l E_{mn} = (\operatorname{Curl}^t \operatorname{Curl}^t E)_{ij}. \quad (1.2)$$

It also holds $(E \times N)_{ij} = -(N \times E)_{ij} = -\epsilon_{jkm} N_k E_{im}$. Moreover, $\int_{\Omega} \operatorname{Curl} F \cdot E dx = \int_{\Omega} F \cdot \operatorname{Curl} E dx$ and $\int_{\Omega} \operatorname{inc} F \cdot E dx = \int_{\Omega} F \cdot \operatorname{inc} E dx$ for smooth tensor-valued functions E and F with compact support in Ω . It is a key part of this paper (cf. Section 2.1) to determine appropriate boundary conditions in order for this integration by parts to be valid for more general fields. We will also use the short notation

$$a|b := \int_{\Omega} a \cdot b dx.$$

The following theorem is crucial for the developments of this work.

Theorem 1 (Beltrami decomposition [13]). *Let $\Omega \subseteq \mathbb{R}^3$ be a simply-connected domain with smooth boundary, let $p \in (1, +\infty)$ be a real number and let $E \in L^p(\Omega, \mathbb{S}^3)$ be a symmetric tensor. Then, there exist a vector field $u \in W^{1,p}(\Omega, \mathbb{R}^3)$ and a tensor $F \in L^p(\Omega, \mathbb{S}^3)$ with $\operatorname{Curl} F \in L^p(\Omega, \mathbb{S}^3)$, $\operatorname{inc} F \in L^p(\Omega, \mathbb{S}^3)$, $\operatorname{div} F = 0$ in Ω and $FN = 0$ on $\partial\Omega$, where N stands for the unit normal to $\partial\Omega$, satisfying*

$$E = \nabla^S u + \operatorname{inc} F.$$

Moreover u can be taken with vanishing trace on $\partial\Omega$, and such a pair (u, F) is unique.

2. PRELIMINARY RESULTS: FUNCTIONAL SPACES

Define

$$\begin{aligned} H_{\operatorname{curl}}(\Omega; \mathbb{M}^3) &:= \{E \in L^2(\Omega; \mathbb{M}^3) : \operatorname{Curl} E \in L^2(\Omega, \mathbb{M}^3)\}, \\ \mathcal{H}(\Omega) &:= \{E \in H^2(\Omega, \mathbb{S}^3), \operatorname{div} E = 0\}, \\ \mathcal{H}_0(\Omega) &:= \{E \in \mathcal{H}(\Omega) : E = \operatorname{Curl}^t E \times N = 0 \text{ on } \partial\Omega\}. \end{aligned} \quad (2.1)$$

These spaces are naturally endowed with the Hilbertian structure of $H^2(\Omega, \mathbb{S}^3)$.

Some identities in the local basis. Let us consider the local orthonormal basis (τ^A, τ^B, N) on $\partial\Omega$ (for detail on such basis and their extension in Ω , cf. [3]). For a general symmetric tensor T , one has in this basis:

$$\begin{aligned} T &= \begin{pmatrix} T_{AA} & T_{AB} & T_{AN} \\ T_{BA} & T_{BB} & T_{BN} \\ T_{NA} & T_{NB} & T_{NN} \end{pmatrix}, & T \times N &= \begin{pmatrix} T_{AB} & -T_{AA} & 0 \\ T_{BB} & -T_{BA} & 0 \\ T_{NB} & -T_{NA} & 0 \end{pmatrix}, \\ (T \times N)^t \times N &= \begin{pmatrix} T_{BB} & -T_{AB} & 0 \\ -T_{AB} & T_{AA} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (2.2)$$

In the same token,

$$(T \times \tau^A)^t \times \tau^A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & T_{NN} & -T_{BN} \\ 0 & -T_{NB} & T_{BB} \end{pmatrix}, \quad (T \times \tau^B)^t \times \tau^B = \begin{pmatrix} T_{NN} & 0 & -T_{AN} \\ 0 & 0 & 0 \\ -T_{NA} & 0 & T_{AA} \end{pmatrix}, \quad (2.3)$$

and,

$$(T \times \tau^A)^t \times \tau^B = \begin{pmatrix} 0 & 0 & 0 \\ -T_{NN} & 0 & T_{AN} \\ T_{NB} & 0 & -T_{AB} \end{pmatrix}, \quad (T \times \tau^B)^t \times \tau^A = \begin{pmatrix} 0 & -T_{NN} & T_{BN} \\ 0 & 0 & 0 \\ 0 & T_{NA} & -T_{BA} \end{pmatrix}. \quad (2.4)$$

Similarly,

$$(T \times N)^t \times \tau^A = \begin{pmatrix} 0 & T_{NB} & -T_{BB} \\ 0 & -T_{NA} & T_{BA} \\ 0 & 0 & 0 \end{pmatrix}, (T \times N)^t \times \tau^B = \begin{pmatrix} -T_{NB} & 0 & T_{AB} \\ T_{NA} & 0 & -T_{AA} \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.5)$$

2.1. Green formula for the incompatibility operator. Let V be a vector field defined on $\partial\Omega$ and let \tilde{V} be any extension of V in Ω with appropriate regularity. The surface divergence of V is defined on $\partial\Omega$ by

$$\operatorname{div}_S V = \operatorname{div} \tilde{V} - (\partial_N \tilde{V}) \cdot N. \quad (2.6)$$

The following result holding for smooth boundaries is sufficient for our purposes, whereas if the boundary had edges, an additional line-integral term must be supplemented.

Lemma 1 (Surface divergence [10]). *If $V \in W^{1,1}(\partial\Omega, \mathbb{R}^3)$ then*

$$\int_{\partial\Omega} \operatorname{div}_S V dS(x) = \int_{\partial\Omega} \kappa V \cdot N dS(x).$$

Lemma 2 (Amstutz-Van Goethem, 2016 [3]). *For all $U, V \in \mathcal{C}^2(\bar{\Omega}, \mathbb{M}^3)$,*

$$\int_{\Omega} U \cdot \operatorname{Curl} V dx = \int_{\Omega} \operatorname{Curl} U \cdot V dx + \int_{\partial\Omega} (U \times N) \cdot V dS(x).$$

Denote $U^S = (U + U^t)/2$ the symmetric part of a tensor U and recall the definition of incompatibility (1.2). The following results is about integration by parts.

Lemma 3 (Amstutz-Van Goethem, 2016 [3]). *Suppose that $T \in \mathcal{C}^2(\bar{\Omega}, \mathbb{S}^3)$ and $\eta \in H^2(\Omega, \mathbb{S}^3)$. Then*

$$\begin{aligned} \int_{\Omega} T \cdot \operatorname{inc} \eta dx &= \int_{\Omega} \operatorname{inc} T \cdot \eta dx \\ &+ \int_{\partial\Omega} \mathcal{T}_1(T) \cdot \eta dS(x) + \int_{\partial\Omega} \mathcal{T}_0(T) \cdot \partial_N \eta dS(x) \end{aligned} \quad (2.7)$$

with the trace operators defined as

$$\mathcal{T}_0(T) := (T \times N)^t \times N, \quad (2.8)$$

$$\mathcal{T}_1(T) := (\operatorname{Curl} (T \times N)^t)^S + ((\partial_N + \kappa)T \times N)^t \times N + (\operatorname{Curl}^t T \times N)^S. \quad (2.9)$$

Remark 1. *Only $(\partial_N \eta)_T$ matters in the rightmost integral of (2.7), since it equivalently rewrites as $\int_{\partial\Omega} \mathcal{T}_0(T) \cdot \mathcal{T}_0(\partial_N \eta) dS(x)$.*

Remark 2. *Let κ^R the two principal curvatures of $\partial\Omega$. It has been proved in [3] that¹,*

$$\operatorname{Curl} (T \times N)^t = - \sum_R \kappa^R (T \times \tau^R)^t \times \tau^R + (\operatorname{Curl}^t T \times N)^t. \quad (2.10)$$

Taking a η such that $\eta N = 0 = \partial_N \eta$ on $\partial\Omega$, then the boundary terms in (2.7) rewrite as

$$\int_{\partial\Omega} \mathcal{T}_1(T) \cdot \eta dS(x) = \int_{\partial\Omega} \mathcal{T}_1(T)_T \cdot \eta_T dS(x). \quad (2.11)$$

Now, assuming that $(\operatorname{Curl}^t T \times N)^S = 0$ and that $\mathcal{T}_0(T) = \mathcal{T}_0(\partial_N T) = 0$ on $\partial\Omega$, taking into account (2.3), (2.9) and (2.10), the second Neumann boundary conditions writes by (2.11) as

$$\mathcal{T}_1(T)_T = -T_{NN} DN = 0 \text{ in } \partial\Omega, \quad \text{with } DN = \begin{pmatrix} \kappa^A & 0 \\ 0 & \kappa^B \end{pmatrix}, \quad (2.12)$$

with $T_{NN} = TN \cdot N$. In summary we have the following implication:

$$(\operatorname{Curl}^t T \times N)^S = \mathcal{T}_0(T) = \mathcal{T}_0(\partial_N T) = TN \cdot N = 0 \text{ and } \eta N = 0 \text{ on } \partial\Omega \Rightarrow \mathcal{T}_1(T) = 0. \quad (2.13)$$

¹The coefficient ξ in [3] can be taken vanishing.

Remark 3. *The following alternative expression is also established in [3]:*

$$\mathcal{T}_1(T) = - \sum_R \kappa^R (T \times \tau^R)^t \times \tau^R + ((-\partial_N + \kappa)T \times N)^t \times N - \sum_R (\partial_R T \times N)^t \times \tau^R, \quad (2.14)$$

where τ_R stands for the derivative along the R th tangent vector τ^R , for $R = A$ or B . Note that (2.14) is proved in [3, Lemma 3.19], by taking $\xi = 0$ (since we consider smooth surfaces without umbilical points) and noting that each term of (2.14) is symmetric.

2.2. Basic properties. The following lemma is easy to prove from the properties of these functions.

Lemma 4. *Every $E \in \mathcal{H}_0(\Omega)$ satisfies $\operatorname{div} \operatorname{Curl}^t E = 0$ in Ω , $\operatorname{Curl}^t E \times N = \partial_N E \times N = 0$ on $\partial\Omega$. Moreover, $\operatorname{inc} E|_F = E|_{\operatorname{inc} F}$ for every $E, F \in \mathcal{H}_0(\Omega)$.*

Proof. The first statement comes easily from the solenoidal property of E . As for the second, compute componentwise (see [3] for detail)

$$-[\operatorname{Curl}^t E \times N]_{mq} = \left((\partial_N E \times N)^t \times N \right)_{mq} - \left(\left(\sum_R \tau^R \times \partial_R E \right)^t \times N \right)_{mq}, \quad (2.15)$$

where ∂_R means the R th tangential derivative, which here vanishes identically, proving the result. The last statement is a direct consequence of Lemma 3 and Remark 1, and taking into account the density of smooth functions in $\mathcal{H}_0(\Omega)$. \square

Lemma 5. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class C^1 and $F \in H_{\operatorname{curl}}(\Omega; \mathbb{M}^3)$ such that $F \times N = 0$ on $\partial\Omega$. Then $(\operatorname{Curl} F)N = 0$ on $\partial\Omega^2$. Moreover, $(\operatorname{inc} E)N = 0$ on $\partial\Omega$ as soon as $E = (\partial_N E \times N)^t \times N = 0$ on $\partial\Omega$.*

Proof. The first part is proven by taking an arbitrary $\varphi \in H^2(\Omega, \mathbb{R}^3)$, since by integration by parts and Lemma 2, $\langle (\operatorname{Curl} F)N, \varphi \rangle_{\partial\Omega} = \langle \operatorname{Curl} F, D\varphi \rangle = \langle F \times N, D\varphi \rangle_{\partial\Omega} = 0$. The second part follows from the first part, the definition of incompatibility, and identity $0 = \operatorname{Curl}^t F \times N = 0$ from Lemma 4. \square

For a proof of the next Lemma, see, e.g. [5, 11, 24].

Lemma 6 (Kozono-Yanagisawa-von Wahl). *Let $F \in H_{\operatorname{curl}}(\Omega; \mathbb{M}^3)$ such that $\operatorname{div} F = 0$ in Ω and $F \times N = 0$ on $\partial\Omega$. Then $F \in H^1(\Omega, \mathbb{M}^3)$ and it holds*

$$\|\nabla F\|_{L^2(\Omega)} \leq C \|\operatorname{Curl} F\|_{L^2(\Omega)}. \quad (2.16)$$

The next result follows without major difficulty from Lemma 6.

Lemma 7. *For all $E \in \mathcal{H}_0(\Omega)$ it holds*

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

The following theorem is nonclassical but also easy to prove.

Theorem 2 (Poincaré). *Let $\partial\Omega_0 \subset \partial\Omega$ be non flat with $\mathcal{H}^2(\partial\Omega_0) > 0$. There exists a constant $C > 0$ such that for each $u \in H^1(\Omega; \mathbb{R}^3)$,*

$$\|u\|_{L^2(\Omega)} \leq C \left(\|\nabla u\|_{L^2(\Omega)} + \int_{\partial\Omega_0} |u \times N| dS \right). \quad (2.17)$$

Theorem 3 (Coercivity). *[Amstutz-Van Goethem, 2016 [3]] Let Ω be a bounded and connected domain with C^1 -boundary and let the nowhere flat subset $\partial\Omega_0 \subset \partial\Omega$ with $\mathcal{H}^2(\partial\Omega_0) > 0$. There exists a constant $C > 0$ s.t. for each $E \in \mathcal{H}_0(\Omega)$,*

$$\|E\|_{H^2(\Omega)} \leq C \|\operatorname{inc} E\|_{L^2(\Omega)}. \quad (2.18)$$

²This expression is intended in a classical weak sense, cf. eg. [20]

3. KINEMATICS WITH DISLOCATIONS

First, the complete equations deriving from conservation of momentum are provided. They turn out to be non-classical, since in the presence of dislocations, an auxiliary tensor variable appears as well as a dislocation-induced force in the right-hand side of the Equilibrium equation. Second, we discuss the chosen boundary conditions, from a mathematical and physical standpoint. Let us here emphasize that from now on the forces will be regularized, so that all fields are assumed smooth. This will allow us to perform a thermodynamical study in a classical manner.

3.1. Governing PDEs. The elastic strain is given from the stress tensor σ by $\epsilon := \mathbb{A}^{-1}\sigma$, where \mathbb{A} is the assumed constant elasticity tensor, i.e., $\mathbb{A} = 2\mu\mathbb{I}_4 + \lambda\mathbb{I}_2 \otimes \mathbb{I}_2$, where \mathbb{I}_4 and \mathbb{I}_2 are the fourth- and second-rank identity tensors, respectively³ with μ, λ the Lamé coefficients. Conservation of linear momentum reads

$$\begin{cases} \rho \frac{dv}{dt} - \operatorname{div} \mathbb{A} \epsilon & = f & \text{in } \Omega \\ \sigma N & = g & \text{on } \partial\Omega \end{cases}, \quad (3.1)$$

where ρ is the volumic mass and v the velocity, and with $f \in \mathcal{C}^\infty(\Omega, \mathbb{R}^3)$ and $g \in \mathcal{C}^\infty(\partial\Omega, \mathbb{R}^3)$ the volume and surface forces, respectively. By Beltrami decomposition (cf. Theorem 1), there exists a vector u and a symmetric and solenoidal tensor F such that

$$\epsilon = \nabla^S u + \operatorname{inc} F, \quad (3.2)$$

whereby, recalling the solenoidal property of

$$\epsilon^0 := \operatorname{inc} F,$$

conservation of linear momentum is rewritten as

$$\begin{cases} \rho \frac{dv}{dt} - \operatorname{div}(\mathbb{A} \nabla^S u) & = \mathcal{F}_{\mathcal{L}} := f + \lambda \nabla \operatorname{tr}(\operatorname{inc} F) & \text{in } \Omega \\ (\mathbb{A} \nabla^S u) N & = g - \lambda \operatorname{tr}(\operatorname{inc} F) N & \text{on } \partial\Omega \end{cases}. \quad (3.3)$$

Therefore, u is called the generalized displacement field, since it coincides with the displacement field in the absence of dislocations, i.e. for $\epsilon^0 = \operatorname{inc} F = 0$. Moreover, we set $v := \frac{du}{dt}$, the pointwise velocity.

The right-hand side of (3.3) depends on F , i.e., through $\operatorname{tr} \epsilon^0$, for which an equation must be found. To this aim, we appeal to Kröner's relation, proved in [22], and which reads $\operatorname{inc} \epsilon = \operatorname{inc} \epsilon^0 = \operatorname{Curl} \kappa_{\mathcal{L}}$, where the right-hand side is a concentrated first order distribution. However, in the present work, which deals with thermodynamic consideration, the right-hand side will be regularized by convolution with a certain divergence-free mollifier η_ρ (this amounts to consider a tubular neighbourhood of the line of some fixed radius ρ , which is a common practice in the dislocation literature). Thus, by (3.2), one has

$$\begin{cases} \operatorname{inc} \operatorname{inc} F & = \mathbb{G}_\rho := \operatorname{Curl} \kappa_{\mathcal{L}} \star \eta_\rho & \text{in } \Omega \\ F & = 0 & \text{on } \partial\Omega \\ (\partial_N F \times N)^t \times N & = 0 & \text{on } \partial\Omega \end{cases}, \quad (3.4)$$

where the boundary conditions are chosen in such a way that (3.4) has a unique solution. Indeed, Equations (3.3) and (3.4) are well posed as discussed in [20]. Note that well-posedness in weak form is a direct consequence of coercivity as proved in Section 2. Other boundary conditions of Neumann or mixed type will be discussed below. Furthermore, $\operatorname{div} \mathbb{G}_\rho = 0$ and hence there exist κ called the regularized contortion, such that

$$\mathbb{G}_\rho = \operatorname{Curl} \kappa. \quad (3.5)$$

Note that such model is also discussed in [21].

3.2. Chosen boundary conditions.

³Componentwise, $(\mathbb{I}_4)_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, and $(\mathbb{I}_2)_{ij} = \delta_{ij}$.

Boundary condition for the gauge field F . The boundary conditions of (3.4) are of essential type (i.e. Dirichlet-like). Note that the first boundary condition on F in (3.4) is required to satisfy the boundary conditions of Beltrami decomposition (3.2) of Theorem 1. Furthermore, it has been shown in Lemma 4 that the second boundary condition for F implies that $\text{Curl}^t F \times N = 0$ on $\partial\Omega$, which in turn implies that $(\text{inc}F)N = 0$ by Lemma 5.

On the other hand, in order to determine the natural boundary conditions, a Green formula has been computed in Section 2.1. In particular, the latter shows that the second boundary condition on F may be replaced by a condition on the tangential components of $\text{inc}F$. Specifically, the following equation with pure Neumann boundary conditions has a solution [3]:

$$\begin{cases} \text{inc}(\mathbb{M} \text{inc}F) &= \text{Curl } \kappa \text{ in } \Omega \\ \mathcal{T}_0(\text{inc}F) &= 0 \text{ on } \partial\Omega \\ \mathcal{T}_1(\text{inc}F) &= 0 \text{ on } \partial\Omega \end{cases}, \quad (3.6)$$

with \mathbb{M} positive definite, and where \mathcal{T}_0 and \mathcal{T}_1 are the trace operators as defined in Theorem 3. Note that $\mathcal{T}_0(A) := (A \times N)^t \times N$ stands by (2.2) for the tangential components of tensor A (in a different order). So we will write

$$A_T := \mathcal{T}_0(A),$$

with subscript T standing for *tangential*. To be precise, as a consequence of Green formula, $\mathcal{T}_0(\text{inc}F)$ is the dual of $(\partial_N F)_T$ and $\mathcal{T}_1(\text{inc}F)$ is the dual of F . This and the above remark imply that either $(\text{inc}F)N$, or $(\text{inc}F)_T$ might be prescribed on the boundary, but not both simultaneously.

Remark 4. *Because (3.6) is given with Neumann boundary conditions, uniqueness might only hold in a quotient space. Specifically, the term $\int_{\partial\Omega} \text{Curl}^t F \times N dS(x)$ might not be vanishing in the RHS of the coercivity inequality. Hence, F is fixed up to a gauge field \tilde{F} satisfying $\int_{\partial\Omega} \text{Curl}^t \tilde{F} \times N dS(x) = 0$. This kind of detail is not of interest for the purpose of this work, but the interested reader may read [3].*

With a view to the time-evolution model, we would like to justify the chosen boundary condition for $\epsilon^0 := \text{inc}F$, as derived in the next section. To this aim, we must find a set of mixed essential/natural boundary conditions on F and its derivatives that imply $\mathcal{T}_1(\text{inc}F) = 0$. First let us make a general remark. There are 6 unknowns for a fourth-order operator, and hence 12 complementary conditions must be prescribed on the boundary (for the complete theory we refer to [1, 2]). This is the case if the symmetric F and $(\partial_N F)_T$ are set to zero, for instance, as for the homogeneous Dirichlet boundary condition. For the pure Neumann case, \mathcal{T}_0 provides 3 independent conditions, and \mathcal{T}_1 six, whereby there exists 3 degrees of freedom unprescribed (whence the quotient space).

We assume that $\mathcal{T}_0(\text{inc}F)$ and only the normal components FN are vanishing on the boundary. Then, referring to Green formula expression (2.7) and (2.9) with $T = \epsilon^0 = \text{inc}F$, it is observed that the central term in the right-hand side of $\mathcal{T}_1(\epsilon^0)$ simplifies to $\mathcal{T}_0(\partial_N \epsilon^0)$. By (2.9) and (2.10), it remains to consider the term $((\text{Curl}^t \epsilon^0) \times N)^S$ and the first term of RHS of (2.10). On the one hand, the term $(\text{Curl}^t \epsilon^0) \times N$ is related to the dislocation rotation gradient, since one recognizes $\text{Curl}^t \epsilon$ as the *Frank tensor*, satisfying for a general strain ϵ (by Mitchell-Cesaro-Volterra decomposition and path integrations, see, e.g., [13]),

$$\nabla \omega = \text{Curl}^t \epsilon, \quad (3.7)$$

where ω is the rotation field. Thus, defining the dislocation-induced rotation ω^0 by means of $\nabla \omega^0 := \text{Curl}^t \epsilon^0$, if we impose that ω^0 be constant on $\partial\Omega$ then $\nabla \omega^0 \times N = \text{Curl}^t \epsilon^0 \times N = 0$ on $\partial\Omega$. This is interpreted as a condition of rigid dislocation-induced rotation of the crystal boundary.

Summarizing, by recalling (2.13), if one assumes (i) $FN = 0$ (i.e., 3 conditions), (ii) $\mathcal{T}_0(\text{inc}F) = \mathcal{T}_0(\partial_N \text{inc}F) = 0$ (i.e., 3 + 3 = 6 conditions), and (iii) $\partial_R \omega^0 = 0$, $R = A, B$ on $\partial\Omega$ (i.e., 2 conditions), then the second Neumann boundary condition will be zero for a non-flat boundary if we also assume the additional condition $(\epsilon^0)_{NN} := \epsilon^0 N \cdot N = 0$ (i.e., the 12th and last condition). Remark that as a consequence of $(\epsilon^0)_T = (\epsilon^0)_{NN} = 0$ on $\partial\Omega$, the

trace of ϵ^0 vanishes, i.e.

$$e := \operatorname{tr}\epsilon^0 = 0 \text{ on } \partial\Omega. \quad (3.8)$$

Obvisouly,

$$\partial_R e = \partial_R \operatorname{tr}\epsilon^0 = 0 \text{ for } R = A, B \text{ on } \partial\Omega. \quad (3.9)$$

As resulting from the above considerations, from now on in this work, the following equation for F will be considered:

$$\left\{ \begin{array}{l} \operatorname{inc}(\operatorname{inc}F) = \operatorname{Curl} \kappa \text{ in } \Omega \\ FN = 0 \text{ on } \partial\Omega \\ \mathcal{T}_0(\operatorname{inc}F) = 0 \text{ on } \partial\Omega \\ (\operatorname{inc}F)N \cdot N = 0 \text{ on } \partial\Omega \\ \mathcal{T}_0(\partial_N \operatorname{inc}F) = 0 \text{ on } \partial\Omega \\ \operatorname{Curl}^t(\operatorname{inc}F) \times N = 0 \text{ on } \partial\Omega \end{array} \right. \quad (3.10)$$

Furthermore, by elliptic regularity⁴ and the smoothness of κ , the fields F and $\operatorname{inc}F$ are also smooth.

Note that (3.10)_c entails that

$$\epsilon^0 \times N = -\epsilon_{AA}^0 \tau_A \otimes \tau_B + \epsilon_{BB}^0 \tau_B \otimes \tau_A + \epsilon_{AB}^0 (\tau_A \otimes \tau_A - \tau_B \otimes \tau_B) = 0. \quad (3.11)$$

Boundary condition for the dislocation strain ϵ^0 . We recall the following. The elastic strain writes as $\epsilon = \mathbb{A}^{-1}\sigma = \nabla^S u + \epsilon^0$, where $\operatorname{inc}\epsilon = \operatorname{inc}\epsilon^0 = \operatorname{Curl} \kappa$. The tensor $\epsilon^0 = \operatorname{inc}F$ is called the dislocation strain, since it is the only part of the elastic strain related to the dislocation density.

First note that the Neumann conditions $\mathcal{T}_0(\operatorname{inc}F) = 0$ and $(\operatorname{inc}F)N \cdot N = 0$ in (3.10) exactly mean that $(\epsilon^0)_T = 0$ and $(\epsilon^0)_{NN} = 0$, respectively. Thus, they naturally impose a Dirichlet boundary conditions for ϵ^0 , though incomplete since the components $(\epsilon^0 N) \cdot \tau^R$ remain unprescribed so far (with τ^R , the R th tangent vector to $\partial\Omega$). We also impose $\operatorname{Curl}^t \epsilon^0 \times N = 0$ in (3.10).

In order to chose the remaining boundary conditions for ϵ^0 , we will require that the following integration by parts be valid,

$$\mathbb{M} \operatorname{inc}\epsilon^0 | \operatorname{inc}\epsilon^0 = \operatorname{inc}(\mathbb{M} \operatorname{inc}\epsilon^0) | \epsilon^0. \quad (3.12)$$

As a consequence of (3.10), one already knows that $(\epsilon^0)_T = (\partial_N \epsilon^0)_T = (\epsilon^0)_{NN} = 0$ on $\partial\Omega$. Therefore, recalling that $\mathcal{T}_0(\mathbb{M} \operatorname{inc}\epsilon^0) \cdot \partial_N \epsilon^0 = (\mathbb{M} \operatorname{inc}\epsilon^0) \cdot (\partial_N \epsilon^0)_T = 0$ on $\partial\Omega$, in order for (3.12) to hold it suffices to impose by referring to Green formula (2.7) with $T = \mathbb{M} \operatorname{inc}\epsilon^0$, that the boundary integrand $\mathcal{T}_1(\mathbb{M} \operatorname{inc}\epsilon^0) \cdot \epsilon^0 = 0$ on $\partial\Omega$. Furthermore, by (2.14), only the NR -components (for $R = A, B$) of $\mathcal{T}_1(\mathbb{M} \operatorname{inc}\epsilon^0)$ matter in this product, since $(\epsilon^0)_T = (\epsilon^0)_{NN} = 0$ on $\partial\Omega$. Then only the first and last terms of (2.14) are nonvanishing and (2.14) is equivalently rewritten by virtue of (2.3)-(2.5) as

$$\kappa^{R^*}(\mathbb{M} \operatorname{inc}\epsilon^0)_{RN} + \partial_R(\mathbb{M} \operatorname{inc}\epsilon^0)_{R^*R^*} - \partial_{R^*}(\mathbb{M} \operatorname{inc}\epsilon^0)_{RR^*}, \quad R = A, B, \quad (3.13)$$

where τ_R stands for the derivative along the R th tangent vector τ^R , and κ^R for the R th principal curvature, for $R = A$ or B , and with $A^* = B$ and $B^* = A$. Note that for a cylindrical boundary, the last two terms are recognized as a surface curl.

Let us remark that by Lemma 5, $(\operatorname{inc}\epsilon^0)N = 0$, since $(\operatorname{Curl}^t \epsilon^0) \times N = 0$ on $\partial\Omega$, and hence if one assumes that \mathbb{M} has the same symmetry as the isotropic elasticity tensor, then $(\mathbb{M} \operatorname{inc}\epsilon^0)_{RN} = 0$, and the first term in (3.13) vanishes. In this case, the boundary condition reduces to imposing a vanishing surface curl of $\mathbb{M}\epsilon^0$.

Summarizing, the following boundary conditions will be prescribed for ϵ^0 :

$$\left\{ \begin{array}{l} (\epsilon^0)_T = (\partial_N \epsilon^0)_T = (\epsilon^0)_{NN} = 0 \quad \text{on } \partial\Omega \\ (\operatorname{Curl}^t \epsilon^0) \times N = 0 \quad \text{on } \partial\Omega \\ \kappa^{R^*}(\mathbb{M} \operatorname{inc}\epsilon^0)_{RN} + \partial_R(\mathbb{M} \operatorname{inc}\epsilon^0)_{R^*R^*} - \partial_{R^*}(\mathbb{M} \operatorname{inc}\epsilon^0)_{RR^*} = 0, \quad R = A, B \text{ on } \partial\Omega \end{array} \right. \quad (3.14)$$

⁴The operator $\operatorname{inc} \operatorname{inc}$ reads Δ^2 for symmetric solenoidal fields and equation well posedness is shown in [20]. See also Section 2.

Let us recall that the Dirichlet conditions (i.e. the first 2 lines in (3.14)) follow from the chosen Neumann conditions for F , whereas the Neumann conditions are chosen so as to permit the integration by parts (3.12). About their physical meaning, $\text{Curl}^t \epsilon^0$ is the dislocation Frank tensor, i.e., the rotation gradient generated by the dislocations. Moreover $\mathbb{M} \text{in} \epsilon^0 = \mathbb{M} \text{Curl} \kappa$ is a dislocation flux, as related to the density of dislocation gradients, and the crystal symmetries (i.e., given by the symmetries of tensor \mathbb{M}) and material properties. The Neumann condition is satisfied if for instance the dislocation density on the boundary is prescribed such that $\text{Curl} \kappa$ is purely tangential and constant on the boundary.

4. EVOLUTION LAW FOR THE DISLOCATION STRAIN

The aim of this section is to derive an evolution law for ϵ^0 from the 2nd Principle of Thermodynamics, and by assuming that the evolution of the dislocation density (i.e., Λ , and hence κ) is known (by means of transport-reaction-diffusion type of PDEs⁵). To be precise, the model will be derived from a particular form of the global Clausius-Duhem inequality. Let us stress that the obtained evolution law is too simple to satisfy the Principle in its full generality. In fact, our aim here is to derive a simple model deriving from the Principle, study its mathematical well-posedness, and leave more elaborated models for future works. To this respect, our aim is also to show that the incompatibility operator naturally appears in the model as soon as high-order dislocation density terms are considered in the free energy. Note that evolution laws are often postulated from the static equations, but this procedure is questionable, since it does not necessarily satisfies Thermodynamics principles.

4.1. Model assumptions.

Assumptions on the free energy. Let the Helmholtz free energy be given by

$$\Psi := \hat{\Psi}(\epsilon, \kappa, \text{Curl} \kappa) = \hat{\Psi}_\epsilon(\epsilon) + \Psi_{\text{dislo}}(\epsilon^0, \kappa, \text{Curl} \kappa), \quad (4.1)$$

where a quadratic law in κ and $\text{Curl} \kappa$ is postulated, viz.,

$$\Psi_{\text{dislo}}(\epsilon^0, \kappa, \text{Curl} \kappa) = \frac{1}{2} \mathbb{N} \kappa \cdot \kappa + \frac{1}{2} \mathbb{M} \text{Curl} \kappa \cdot \text{Curl} \kappa + \psi_{\text{dislo}}(\epsilon^0), \quad (4.2)$$

with \mathbb{M} and \mathbb{N} positive-definite fourth-rank tensors. In this work, we will restrict ourselves to symmetric tensors \mathbb{N} of the form

$$\mathbb{N} = 2\beta \mathbb{I}_4, \quad (4.3)$$

where $\beta \geq 0$ is a constant scalar and $(\mathbb{I}_4)_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. Note that \mathbb{N} and hence β has the dimension of a force, since κ , as Λ , has the dimensions of an inverse length, while \mathbb{M} has the dimensions of a force times a surface.

Let us emphasize that high-order dislocation models involving strain derivatives in the form of ϵ and its curl are not new, see e.g., [4].

Assumption of rigid dislocation-induced rotation. We make the assumption that the dislocation-induced rotations are constant along $\partial\Omega$, that is, $\nabla\omega^0 \times N = \text{Curl}^t \epsilon^0 \times N = 0$. Nonetheless, variations of rotation may occur as induced by purely elastic loading, since $\text{Curl}^t \nabla^S u \times N \neq 0$.

Additional remark. The relation $\text{in} \epsilon^0 = \text{Curl} \kappa$ yields

$$\kappa = \text{Curl}^t \epsilon^0 + \nabla\varphi, \quad (4.4)$$

for some vector φ satisfying by the identity $\text{div} \epsilon^0 = 0$,

$$\mathcal{L}_{0,1}(\varphi) = \text{div} \nabla^S \varphi = \text{div} \kappa^S \quad (4.5)$$

where we have chosen $\varphi = 0$ on $\partial\Omega$. Remark that this latter choice yields that $\text{Curl}^t \epsilon^0 \times N = 0$ on $\partial\Omega$ implies that $\kappa \times N = 0$ and hence $\text{Curl} \kappa N = \text{in} \epsilon^0 N = 0$ on $\partial\Omega$, by Lemma 5.

⁵For point defects such a law was studied in [23]

4.2. Thermodynamics considerations. The notions invoqued in this section are classical in Thermodynamics. References can be found in e.g. [12, 15]. The idea is to derive an evolution law which would at least satisfy the 2nd Principle of Thermodynamics, *globally in Ω* .

The pointwise (otherwise termed *local*) isothermal Clausius-Duhem inequality reads

$$\begin{aligned} 0 \leq D &= \sigma \cdot \nabla \dot{u} - \dot{\Psi} \\ &= \sigma \cdot (\dot{\epsilon} - \text{inc} \dot{F}) - \delta_\epsilon \Psi \cdot \dot{\epsilon} - \delta_\kappa \Psi \cdot \dot{\kappa} - \delta_{\text{Curl} \kappa} \Psi \cdot \text{Curl} \dot{\kappa} - \delta_{\epsilon^0} \Psi \cdot \dot{\epsilon}^0 \\ &= -\sigma \cdot \text{inc} \dot{F} + \dot{\epsilon}(\sigma - \delta_\epsilon \hat{\Psi}_e) - \delta_\kappa \Psi_{\text{dislo}} \cdot \dot{\kappa} - \delta_{\text{Curl} \kappa} \Psi_{\text{dislo}} \cdot \text{Curl} \dot{\kappa} - \delta_{\epsilon^0} \psi_{\text{dislo}} \cdot \dot{\epsilon}^0. \end{aligned}$$

Hence it is classically deduced that $\sigma = \delta_\epsilon \hat{\Psi}_e$ and hence one has

$$0 \leq D = -\sigma \cdot \text{inc} \dot{F} - (\mathbb{N} \kappa \cdot \dot{\kappa} + \mathbb{M} \text{Curl} \kappa \cdot \text{Curl} \dot{\kappa}) - \delta_{\epsilon^0} \psi_{\text{dislo}} \cdot \dot{\epsilon}^0. \quad (4.6)$$

Introduce the global mechanical dissipation as

$$\mathcal{D} := \int_{\Omega} D dx.$$

The isothermal global form of the second Law of Thermodynamics (or global Clausius-Duhem inequality) in Ω reads⁶

$$\mathcal{D} \geq 0. \quad (4.7)$$

Inequality (4.7) will allow us to derive the sought evolution equation for the dislocation strain. Recall the notation

$$a|b := \int_{\Omega} a \cdot b dx.$$

By the symmetry of σ , Theorem 1 yields a unique (Ψ, G) satisfying $\sigma = \nabla^S \Psi + \text{inc} \mathbb{S}$ with $\Psi = 0, \mathbb{S} = 0, (\text{Curl}^t \mathbb{S}) \times N = 0$ on $\partial\Omega$ (the same remark as for (3.4) holds for \mathbb{S}). In particular, one has $\text{inc} \text{inc} \mathbb{S} = \text{inc} \sigma$, where it is remarked that the dependence of \mathbb{S} upon ϵ^0 must not be linear. Furthermore

$$\sigma \cdot \text{inc} \dot{F} = \nabla^S \Psi \cdot \text{inc} \dot{F} + \text{inc} \mathbb{S} \cdot \text{inc} \dot{F}, \quad (4.8)$$

which by integrations by parts (justified by Lemma 4) yields

$$\sigma | \text{inc} \dot{F} = \text{inc} \mathbb{S} | \text{inc} \dot{F} = \mathbb{S} | \text{inc} \text{inc} \dot{F} = \mathbb{S} | \text{inc} \dot{\epsilon} = \mathbb{S} | \text{inc} \dot{\epsilon}^0 = \text{inc} \mathbb{S} | \dot{\epsilon}^0. \quad (4.9)$$

Moreover, by Beltrami decomposition again, the symmetric tensor $\delta_{\epsilon^0} \psi_{\text{dislo}}$ can be decomposed as

$$\delta_{\epsilon^0} \psi_{\text{dislo}} = \nabla^S \eta + \text{inc} \mathbb{K}_{\epsilon^0}, \quad (4.10)$$

for some vector-valued η (here taken with $\eta = 0$ on $\partial\Omega$), and where \mathbb{K}_{ϵ^0} is a symmetric divergence-free tensor, whose dependence upon ϵ^0 must not be linear, too. Hence, recalling the solenoidal property of ϵ^0 , $\delta_{\epsilon^0} \psi_{\text{dislo}} | \dot{\epsilon}^0 = \text{inc} \mathbb{K}_{\epsilon^0} | \dot{\epsilon}^0$. Thus, by (4.4), Eqs. (4.6) and (4.7) rewrite as

$$\begin{aligned} 0 \leq \mathcal{D} &= - \text{inc} \mathbb{S}_{\epsilon^0} | \dot{\epsilon}^0 \\ &\quad - (\mathbb{N}(\text{Curl}^t \epsilon^0 + \nabla \varphi) | (\text{Curl}^t \dot{\epsilon}^0 + \nabla \dot{\varphi}) + \mathbb{M} \text{inc} \epsilon^0 | \text{inc} \dot{\epsilon}^0 + \text{inc} \mathbb{K}_{\epsilon^0} | \dot{\epsilon}^0), \end{aligned} \quad (4.11)$$

where the dependence of \mathbb{S} upon ϵ^0 is emphasized.

Let us now consider the second term of the right-hand side. By the symmetry property of \mathbb{N} and since $\varphi = \dot{\varphi} = 0$ on the boundary, it holds

$$\mathbb{N} \text{Curl}^t \epsilon^0 | (\text{Curl}^t \dot{\epsilon}^0 + \nabla \dot{\varphi}) = \mathbb{N} \text{Curl}^t \epsilon^0 | \text{Curl} \dot{\epsilon}^0 - \text{div}(\mathbb{N} \text{Curl}^t \epsilon^0) | \dot{\varphi}. \quad (4.12)$$

Obviously $\text{div} \text{Curl}^t \epsilon^0 = \text{div} \text{Curl} \epsilon^0 = 0$, and hence, integrating by parts $\mathbb{N} \text{Curl}^t \epsilon^0 | \text{Curl} \dot{\epsilon}^0$ by recalling (4.3) and Lemma 2, allows one to rewrite (4.12) as

$$\beta \text{inc} \epsilon^0 | \dot{\epsilon}^0 + \beta \text{Curl} \epsilon^0 | \text{Curl} \dot{\epsilon}^0 + 2\beta \int_{\partial\Omega} (\text{Curl}^t \epsilon^0)^S \times N \cdot \dot{\epsilon}^0 dS, \quad (4.13)$$

⁶The global form expressed in its full generality would require a positive integral in any time-dependent control volume in Ω .

where the integrand in boundary term of (4.13) rewrites as $-(\text{Curl}^t \epsilon^0)^S \cdot (\epsilon^0 \times N)$ and hence vanishes by (3.11). Now, by definition of the Frank tensor (3.7), it holds

$$\beta \text{Curl} \epsilon^0 | \text{Curl} \epsilon^0 = \beta \text{Curl}^t \epsilon^0 | \text{Curl}^t \epsilon^0 = \beta \nabla \omega^0 | \nabla \dot{\omega}^0.$$

Therefore, (4.13) rewrites as

$$\beta \text{inc} \epsilon^0 | \dot{\epsilon}^0 + \beta \nabla \omega^0 | \nabla \dot{\omega}^0. \quad (4.14)$$

From the right-hand side of (4.11), and by $\text{div} \text{Curl}^t \epsilon^0 = \text{div} \text{Curl} \epsilon^0 = 0$, one is left with

$$\mathbb{N} \nabla \varphi | (\text{Curl}^t \dot{\epsilon}^0 + \nabla \dot{\varphi}) = \mathbb{N} \nabla^S \varphi | \nabla^S \dot{\varphi} = 2\beta \nabla^S \varphi | \nabla^S \dot{\varphi}, \quad (4.15)$$

with φ the unique solution to (4.5)⁷.

Summarizing, (4.11) is rewritten as

$$\begin{aligned} 0 \leq \mathcal{D} &= -\beta \nabla \omega^0 | \nabla \dot{\omega}^0 - 2\beta \nabla^S \varphi | \nabla^S \dot{\varphi} - \beta \text{inc} \epsilon^0 | \dot{\epsilon}^0 - \text{inc}(\mathbb{M} \text{inc} \epsilon^0 + \mathbb{H}_{\epsilon^0}) | \dot{\epsilon}^0 \\ &= -\frac{d}{dt} \mathcal{E}_\beta(\epsilon^0, \kappa) - \text{inc}(\mathbb{M} \text{inc} \epsilon^0 + \beta \epsilon^0 + \mathbb{H}_{\epsilon^0}) | \dot{\epsilon}^0, \end{aligned} \quad (4.16)$$

where the nonlinear term with respect to ϵ^0 is the following symmetric and solenoidal tensor:

$$\mathbb{H}_{\epsilon^0} := \mathbb{K}_{\epsilon^0} + \mathbb{S}_{\epsilon^0},$$

and with a stored quadratic dislocation energy \mathcal{E}_β defined as

$$\mathcal{E}_\beta(\epsilon^0, \kappa) := \frac{\beta}{2} (\nabla \omega^0 | \nabla \omega^0 + 2\nabla^S \varphi | \nabla^S \varphi). \quad (4.17)$$

Let us remark that if the free-energy is independent of κ , that is, if $\beta = 0$ then $\mathcal{E}_\beta = 0$ and (4.16) immediately yields

$$-\text{inc}(M \text{inc} \epsilon^0 + \beta \epsilon^0 + \mathbb{H}_{\epsilon^0}) | \dot{\epsilon}^0 = \mathcal{D} \geq 0.$$

4.3. Time-evolution the dislocation strain. Let us now consider a certain time scale, which is lower than that of dissipative phenomena associated to the evolution of dislocations (the law for κ), but high enough not to invalidate the hypothesis of local state (see [12]). We will consider a thought experiment with a certain number of pure edge dislocations in such a way that $\varphi = 0$, whereas the norm of $\nabla \omega^0$ can reach arbitrarily high values. Thus one can render $-\frac{d}{dt} \mathcal{E}(\epsilon, \kappa)$ arbitrarily negative, and in order for the global dissipation \mathcal{D} to remain positive in (4.16), the term $\text{inc}(\mathbb{M} \text{inc} \epsilon^0 + \beta \epsilon^0 + \mathbb{H}_{\epsilon^0}) | \dot{\epsilon}^0$ must be non positive. For this reason the following evolution law for ϵ^0 is postulated:

$$0 = \alpha \dot{\epsilon}^0(t) + \text{inc}(\mathbb{M} \text{inc} \epsilon^0(t) + \mathcal{G}(\epsilon^0(t))), \quad (4.18)$$

for some material-dependent coefficient $\alpha \geq 0$ and with the solenoidal tensor-valued nonlinear term

$$\mathcal{G}(\epsilon^0) := \mathbb{H}_{\epsilon^0} + \beta \epsilon^0 = \mathcal{G}(\epsilon^0) - \mathbb{L},$$

where \mathbb{L} stands for a symmetric (not necessarily divergence-free) tensor independent of ϵ^0 . We introduce the generalized dislocation force as the following symmetric and solenoidal tensor:

$$\mathbb{G} := \text{inc} \mathbb{L}.$$

Moreover, the boundary conditions (4.19) and the initial condition $\epsilon^0(0) = \epsilon_0^0$ at $t = 0$ are prescribed.

Specifically, the sought time-dependent boundary value problem for the dislocation strain reads, by recalling (3.14),

$$\left\{ \begin{array}{ll} \alpha \partial_t \epsilon^0 + \text{inc}(\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)) - \mathbb{G} = 0 & \text{in } \Omega \times [0, T] \\ (\epsilon^0)_T = (\partial_N \epsilon^0)_T = (\epsilon^0)_{NN} = 0 & \text{on } \partial\Omega \times [0, T] \\ (\text{Curl}^t \epsilon^0) \times N = 0 & \text{on } \partial\Omega \times [0, T] \\ \kappa^{R^*} (\mathbb{M} \text{inc} \epsilon^0)_{RN} + \partial_R (\mathbb{M} \text{inc} \epsilon^0)_{R^*R^*} - \partial_{R^*} (\mathbb{M} \text{inc} \epsilon^0)_{RR^*} = 0 & R = A, B \text{ on } \partial\Omega \times [0, T] \end{array} \right. \quad (4.19)$$

⁷Thus linearly depending on $\text{div} \kappa^S$.

Furthermore, the following energy relation also holds:

$$\frac{d}{dt} \mathcal{E}_\beta(\epsilon, \kappa) \leq \alpha |\dot{\epsilon}^0|^2. \quad (4.20)$$

In particular, the energy \mathcal{E}_β decreases in time as soon as the dislocation strain is stationary.

5. WELL POSEDNESS OF THE EVOLUTION

5.1. Weak forms. Recall first the notation $a|b = (a, b)_2$, where the right-hand side stands for the scalar product in L^2 (of scalars, vectors, tensors, etc.). The weak form associated to (4.19) reads: for all $t \in [0, T]$, find $E(t) \in \mathcal{H}_0(\Omega)$ such that

$$(i) \quad \alpha \frac{dE}{dt}(t) | F + \mathbb{M} \text{inc} E(t) | \text{inc} F + \mathcal{G}(E(t)) | \text{inc} F - \mathbb{G} | F = 0 \quad \text{for all } F \in \mathcal{H}_0(\Omega), \quad (5.1)$$

with \mathbb{M} a fourth-rank symmetric and positive-definite tensor, where \mathcal{G} is a symmetric tensor-valued nonlinear term (not necessarily divergence-free), \mathbb{G} represents a tensor-valued generalized force, and with $\alpha > 0$.

$$(ii) \quad E(0) = E_0 \in L^2(\Omega; \mathbb{S}^3).$$

By integration by parts, and recalling Lemma 2, (5.1) writes as: find $E \in \mathcal{H}_0(\Omega)$ such that

$$\alpha \frac{dE}{dt} | F + \mathbb{M} \text{inc} E | \text{inc} F + \text{Curl} \mathcal{G}(E) | \text{Curl}^t F - \mathbb{G} | F = 0 \quad \text{for all } F \in \mathcal{H}_0(\Omega). \quad (5.2)$$

The bilinear form associated to the linear part of the PDE reads

$$a(E, F) = \mathbb{M} \text{inc} E | \text{inc} F. \quad (5.3)$$

Its coercivity in $H^2(\Omega)$ is an immediate consequence of Theorem 3.

Remark that in the case of the dislocation model of Section 4.3, $\mathcal{G}(\epsilon^0) = \mathbb{H}_{\epsilon^0} + \beta \epsilon^0$. Recalling (4.18) and assuming for simplicity that $\mathbb{H}_{\epsilon^0} = \mathbb{H}(x)$ is independent of ϵ^0 , the weak form associated to this linear model writes as: find $E \in \mathcal{H}_0(\Omega)$ s.t.

$$\alpha \frac{dE}{dt} | F + (\mathbb{M} \text{inc} E + \beta E) | \text{inc} F - \tilde{\mathbb{G}} | F = 0 \quad \text{for all } F \in \mathcal{H}_0(\Omega), \quad (5.4)$$

with $\tilde{\mathbb{G}} := \mathbb{G} + \text{inc} \mathbb{H}$. In this case the equation is a linearization of the general Cahn-Hilliard system.

Now, if \mathcal{G} is assumed to be an objective tensor, it will write in terms of its invariant, the first of which is the trace of E .

Assumption on the nonlinearity. The nonlinear term is assumed to write as a polynomial in the trace of E plus an affine term in E .

Assumption 1 (Nonlinear term). *Let $E \in \mathbb{S}^3$. It is assumed that*

$$\mathcal{G}(E) = \beta E - \frac{1}{3} \varphi(\text{tr} E) \mathbb{I}_2, \quad (5.5)$$

with $\beta > 0$ a constant scalar and φ a scalar-valued polynomial defined as

$$\varphi(v) = \sum_{i=1}^{2p-1} \rho_i v^i, \quad p \geq 2, \quad (5.6)$$

where $\rho_{2p-1} > 0$. In particular, $\mathcal{G}(E)$ is a symmetric second-rank tensor.

Remark 5. *The divergence of the nonlinear in (5.5) term must not be zero, since $\text{div} \mathcal{G}(E) = -\frac{1}{3} \varphi'(e) \nabla e \neq 0$ unless φ is trivially independent of e . However, as referring to the dislocation model of Section 4.3, one has $\text{div} \mathcal{G}(E) = \text{div} \mathcal{G}(E) - \text{div} \mathbb{L} = 0$ and hence $\text{div} \mathbb{L} = \frac{1}{3} \varphi'(e) \nabla e$. Without going into details (see, e.g., [8, 17]), \mathbb{L} then plays the role of a constraint reaction to ensure the condition $\text{div} \mathcal{G}(E) = 0$, and one could take \mathbb{L} of the form $\mathbb{L} = \mathbb{C} \nabla^S w$ for a certain elasticity-kind-of-tensor \mathbb{C} , and w an associated vector field.*

Furthermore, one has $(\text{Curl} \mathcal{G}(E))_{ij} = \beta (\text{Curl} E)_{ij} - \frac{1}{3} \epsilon_{ijk} \varphi'(\text{tr} E) \partial_k \text{tr} E$. It follows that

$$\text{Curl} \mathcal{G}(E) | \text{Curl}^t E = \beta \text{Curl} E | \text{Curl}^t E + \varphi'(\text{tr} E) | (\nabla \text{tr} E)^2. \quad (5.7)$$

5.2. Energy estimates. For simplicity the estimates will be done taking $\alpha = 1$.

Theorem 4. *Under Assumption 1, let E be a solution of (5.1). Then*

$$\frac{d}{dt} \|E(t)\|_{L^2}^2 \leq C \|E(t)\|_{L^2}^2 \quad (5.8)$$

for some $C > 0$. Moreover it holds,

$$\|E\|_{L^\infty(0,T;L^2)} + \|E\|_{L^2(0,T;H^2)}^2 + \left\| \frac{dE}{dt} \right\|_{L^2(0,T;H^{-2})} \leq C \|E_0\|_{L^2}^2 \quad (5.9)$$

These estimates also hold for E solution of (5.4).

Proof. By (5.6), the polynomial $\sum_{i=1}^{2p-2} \rho_i v^i$ is bounded from below by a constant. Hence by (5.7), there exists $\tilde{c} \geq 0$ such that

$$\text{Curl } \mathcal{G}(E(t)) | \text{Curl}^t E(t) \geq -\beta \| \text{Curl } E(t) \|_{L^2}^2 - \tilde{c} \| \nabla \text{tr} E(t) \|_{L^2}^2.$$

Denoting $\mathcal{C}(E(t)) := \beta \| \text{Curl } E(t) \|_{L^2}^2 + \tilde{c} \| \nabla \text{tr} E(t) \|_{L^2}^2 \geq 0$ and letting $F = E$ in (5.2), one has

$$\begin{aligned} & \frac{d}{dt} \frac{1}{2} \|E(t)\|_{L^2}^2 + \mathbb{M} \text{inc } E(t) | \text{inc } E - \mathcal{C}(E(t)) - \mathbb{G} | E(t) \\ & \leq \frac{d}{dt} \frac{1}{2} \|E(t)\|_{L^2}^2 + \mathbb{M} \text{inc } E(t) | \text{inc } E(t) + \text{Curl } \mathcal{G}(E(t)) | \text{Curl}^t E(t) - \mathbb{G} | E(t) = 0, \end{aligned}$$

and hence there exists $C_{\mathbb{G}} > 0$, a constant independent of E s.t.

$$\frac{d}{dt} \frac{1}{2} \|E(t)\|_{L^2}^2 + \mathbb{M} \text{inc } E(t) | \text{inc } E(t) \leq \mathcal{C}(E(t)) + \mathbb{G} | E(t) \leq C_{\mathbb{G}} (\| \nabla E(t) \|_{L^2}^2 + \|E(t)\|_{L^2}).$$

The interpolation inequality and general Cauchy inequality [7] yield

$$\begin{aligned} \frac{d}{dt} \frac{1}{2} \|E(t)\|_{L^2}^2 + \mathbb{M} \text{inc } E(t) | \text{inc } E(t) & \leq c (\|E(t)\|_{L^2} \|E(t)\|_{H^2} + \|E(t)\|_{L^2}) \\ & \leq c\varepsilon \|E(t)\|_{H^2}^2 + \frac{4\varepsilon + c}{4\varepsilon} \|E(t)\|_{L^2}^2, \end{aligned} \quad (5.10)$$

for some constant $c := c_{\mathbb{G}} > 0$, a constant independent on E . Furthermore, positive-definiteness and coercivity (cf. Theorem 3) of \mathbb{M} yield $C_{\mathbb{M}} \|E\|_{H^2} \leq \mathbb{M} \text{inc } E | \text{inc } E$ for some constant $C_{\mathbb{M}} > 0$. Thus, it follows from Theorem 3 and by choosing ε small enough, that

$$\frac{d}{dt} \frac{1}{2} \|E(t)\|_{L^2}^2 \leq \frac{d}{dt} \frac{1}{2} \|E(t)\|_{L^2}^2 + \bar{C} \|E(t)\|_{H^2}^2 \leq \frac{4\varepsilon + c}{2\varepsilon} \frac{1}{2} \|E(t)\|_{L^2}^2, \quad (5.11)$$

for some $\bar{C}(t) \geq 0$ (in the sequel, the dependences of the constants on \mathbb{G} and \mathbb{M} are omitted for conciseness). As a consequence of the differential form of Gronwall Lemma [7, B.2.j.], (5.11) we deduce that

$$\max_{t \in [0, T]} \|E(t)\|_{L^2} \leq C \|E_0\|_{L^2}, \quad (5.12)$$

for some constant $C > 0$. Moreover, by (5.10) and time integration in $[0, T]$, one has

$$\int_0^t \frac{d}{ds} \frac{1}{2} \|E(s)\|_{L^2}^2 ds + \bar{C} \int_0^t \|E(s)\|_{H^2}^2 ds \leq \hat{C} \int_0^t \|E(s)\|_{L^2}^2 ds, \quad (5.13)$$

for some $\hat{C} \geq 0$. Hence by (5.12),

$$\frac{1}{2} \|E(t)\|_{L^2}^2 - \frac{1}{2} \|E(0)\|_{L^2}^2 + \bar{C} \int_0^t \|E(s)\|_{H^2}^2 \leq C \hat{C} T \|E_0\|_{L^2} \quad (5.14)$$

and thus

$$\|E\|_{L^2(0,T;H^2)}^2 := \int_0^T \|E(t)\|_{H^2}^2 dt \leq \frac{2\hat{C}CT + 1}{2\bar{C}} \|E_0\|_{L^2}^2. \quad (5.15)$$

To conclude, take any $V \in H_0^2(\Omega; \mathbb{M}^3)$ and let $F = V$ in (5.2). Set $V = V^S + V^A$, the symmetric-skewsymmetric decomposition of V , and $V^S = \nabla^S v + V^0$, the Beltrami decomposition of its symmetric part, with $V^0 \in \mathcal{H}_0(\Omega)$. Then, by means of some integrations by parts, it

holds

$$\begin{aligned} \frac{dE}{dt}|V + \mathbb{M} \operatorname{inc} E| \operatorname{inc} V + \mathcal{G}(E)| \operatorname{inc} V - \mathbb{G}|V &= \frac{dE}{dt}|V^0 + M \operatorname{inc} E| \operatorname{inc} V^0 + \mathcal{G}(E)| \operatorname{inc} V^0 - \mathbb{G}|V^0 \\ &= 0. \end{aligned}$$

Thus, we have for some constants $C_1, C_2^i > 0$,

$$\left| \frac{dE}{dt}|V \right| \leq C_1 \|E\|_{H^2} \|V\|_{H^2} + \sum_{i=0}^{2p-1} C_2^i \|E\|_{L^2}^i \|V\|_{H^2},$$

and hence by (5.12) and (5.15), and with a nonrelabeled constant $C > 0$,

$$\left\| \frac{dE}{dt} \right\|_{L^2(0,T;H^{-2})} := \int_0^T \left\| \frac{dE}{dt} \right\|_{H^{-2}} dt \leq C \left(\|E_0\|_{L^2}^2 + \sum_{i=0}^{2p-1} \|E_0\|_{L^2}^i \right), \quad (5.16)$$

where $H^{-2}(\Omega) := (H_0^2(\Omega; \mathbb{M}^3))'$. The proof is achieved by (5.12), (5.14) and (5.16), since for the second statement, it suffices to take $\varphi \equiv 0$. \square

5.3. Existence and uniqueness of the weak solution. It is now well-known that the energy estimates of Theorem 4 and classical decomposition in discrete subspaces of H^2 , the so-called Galerkin approximation (see, e.g., [7, 16, 18]), yield the following theorem. Note that compactness is recovered in $H^2(\Omega; \mathbb{S}^3)$ while the divergence-free properties also pass to the limit. Therefore the solution belongs to $\mathcal{H}_0(\Omega)$ by the second statement of Lemma 4.

Theorem 5. *There exists a unique weak solution E of (5.1) and (5.4) in $\mathcal{H}_0(\Omega)$. Moreover $E \in \mathcal{C}(0, T; H^{-2})$.*

Note that continuity in time is an immediate consequence of (5.9).

6. DISCUSSION

6.1. Tensor version of Cahn-Hilliard. The derived equations are similar in form to the well-known Cahn-Hilliard equations, but here the variable is a divergence-free tensor E . Recall the strong form of (5.1) in Ω :

$$\alpha \frac{dE}{dt}(t) + \operatorname{inc}(\mathbb{M} \operatorname{inc} E(t) + \mathcal{G}(E(t))) = 0. \quad (6.1)$$

Recall the identity $\operatorname{tr} \operatorname{inc} A = \Delta \operatorname{tr} A - \operatorname{div} \operatorname{div} A$. Then, Assumption 1 yields

$$\operatorname{tr} \operatorname{inc} \mathcal{G}(E) = \Delta \operatorname{tr}(\mathcal{G}(E) - \mathbb{L}) = -\Delta \operatorname{tr} \mathbb{L} + \beta \operatorname{tr} E - \varphi(\operatorname{tr} E), \quad (6.2)$$

since $\operatorname{tr} \operatorname{inc} A = \Delta \operatorname{tr} A$ for solenoidal fields A . Assume also that $\mathbb{M} = 2\tilde{\mu} \mathbb{I}_4 + \tilde{\lambda} \mathbb{I}_2 \otimes \mathbb{I}_2$ for some $\tilde{\mu} > 0$ and set $\tilde{\beta} := 2(\tilde{\mu} + \tilde{\lambda})$.

Let us introduce

$$e := \operatorname{tr} E,$$

and compute the trace of (6.1). By (6.2), one has

$$\alpha \frac{d}{dt} e(t) = \operatorname{tr} \operatorname{inc}(-\mathbb{M} \operatorname{inc} E(t) - \mathcal{G}(E(t))) = \Delta \left(-\tilde{\beta} \Delta e(t) - \beta e(t) + \varphi(e(t)) + \operatorname{tr} \mathbb{L} \right), \quad (6.3)$$

or, more simply,

$$\alpha \frac{d}{dt} e(t) = \Delta \left(-\tilde{\beta} \Delta e(t) + \psi(e(t)) \right), \quad \psi(e) := \varphi(e) - \beta e + \operatorname{tr} \mathbb{L} \quad (6.4)$$

which is recognized as the classical scalar version of Cahn-Hilliard equation for e with the nonlinear term ψ . Note that in the classical derivation of Cahn-Hilliard equation, $\tilde{\beta}$ should depend on a small parameter related to a scaling in the free-energy. In terms of our model, the part of the strain which is relevant for the variations of dislocation density, i.e., $E = \epsilon^0$ (by the relation $\operatorname{Curl} \kappa = \operatorname{inc} \epsilon^0$) has a trace e , and therefore is interpreted as dislocation-induced variation of matter density. It is remarkable that e obeys the law (6.4).

About its boundary conditions, it is already known by (3.8) that $e = 0$ on $\partial\Omega$. We also assume that $\Delta e = 0$ on $\partial\Omega$ and the initial condition $e(0) = \operatorname{tr} E_0$. It is well known that (6.3) is well posed (cf. [6] for this particular choice of boundary conditions), though the solution might only be unique up to some gauges, since $\partial_N e$ is not fixed.

Moreover, it is easy to see that $\frac{d}{dt} \int_{\Omega} edx = - \int_{\partial\Omega} \tilde{\beta} \partial_N \Delta edS(x) + \int_{\partial\Omega} (\varphi'(e) - \beta) \partial_N edS(x)$. From a physical viewpoint, this property simply reflects the inflow of point defects. In fact, any variation of e is due to the change in interstitial and vacancy densities. In some sense e might be viewed as a point-defect density: positive in the case of an excess of interstitials, and negative if vacancies exceed interstitials. Furthermore, assuming that e depends on the temperature T , one has a leading boundary inflow proportional to the normal temperature gradient, i.e., given by $(\varphi'(e) - \beta)e'(T)\partial_N T$. Hence the point defects will be conserved, $\frac{d}{dt} \int_{\Omega} edx = 0$ as soon as the normal temperature gradient vanishes at the boundary. Otherwise, point defect will be introduced or removed from the boundary. Furthermore, the fact that $e = 0$ on $\partial\Omega$ means that point defects are only present inside Ω . Remark that point defects on the boundary is a kind of non sense, since an excess/lack of atom indeed changes the boundary location. Recall also that dislocations are nucleated by the collapse of point-defect clusters. Hence determining their density is crucial for dislocation modelling.

Note also that e is the potential yielding the bulk dislocation force ∇e in (3.3). Therefore, the work done by this force only depends on the variation of point-defect density at the path endpoints. Specifically, the displacement is solution to

$$\begin{cases} \rho \frac{d^2}{dt^2} u - \operatorname{div}(\mathbb{A} \nabla^S u) &= f + \lambda \nabla e \quad \text{in } \Omega \times [0, T] \\ (\mathbb{A} \nabla^S u) N &= g - \lambda e N \quad \text{on } \partial\Omega \times [0, T] \end{cases}, \quad (6.5)$$

as coupled with the point-defect density

$$\begin{cases} \partial_t e(t) + \Delta \left(\tilde{\beta} \Delta e(t) + \psi(e(t)) \right) = 0 & \text{in } \Omega \times [0, T] \\ e = \Delta e = 0 & \text{on } \partial\Omega \times [0, T] \\ e(0) = e_0 & \text{in } \Omega \times [0, T] \end{cases}, \quad (6.6)$$

where the bulk force term in the right-hand side will be explained in the next comment. It represents a dissipative force related to point-defects, as a source of sink.

6.2. Comment about the forcing term. Note that $\operatorname{tr} \mathbb{L}$ in (6.3) stands for an external time-dependent field in Gurtin's formalism of microforce balance [9].

Let us rewrite (4.10) as $\delta_{\epsilon^0} \psi_{\text{dislo}} = \mathbb{P}^C + \mathbb{P}^D$, where the symmetric gradient \mathbb{P}^C is impactless on the mechanical dissipation. Accordingly, let $\psi_{\text{dislo}} = \psi_{\text{dislo}}^C + \psi_{\text{dislo}}^D$, where the first term is a conservative contribution, whereas the latter is dissipative. One has $\operatorname{div} \mathbb{P}^D = \operatorname{div} \delta_{\epsilon^0} \psi_{\text{dislo}}^D = \delta_{\epsilon^0}^2 \psi_{\text{dislo}}^D \nabla \epsilon^0 = 0$, which entails that ψ_{dislo}^D must be affine in ϵ^0 . Hence,

$$\psi_{\text{dislo}}^D(\epsilon^0) = \operatorname{inc} \mathbb{K}_0 \cdot \epsilon^0 + \mathbb{C}_0,$$

for some constant tensor \mathbb{C}_0 . Now, from the expression of the dissipation term of (4.11), $\operatorname{inc} \mathbb{K}_0 | \dot{\epsilon}^0 = \mathbb{K}_0 | \operatorname{inc} \epsilon^0 = \mathbb{K}_0 | \operatorname{Curl} \dot{\kappa}$, one recognizes \mathbb{K}_0 as a thermodynamic force.

Now, letting

$$\psi_{\text{dislo}}^C(\epsilon^0) = \psi^C(\operatorname{tr} \epsilon^0) + \tilde{\psi}^C(\nabla \operatorname{tr} \epsilon^0),$$

with $\psi^C(e) = \int_0^e \varphi(v) dv - \frac{1}{2} \beta e^2 + \operatorname{tr} L e$ and $\tilde{\psi}^C(\nabla e) = \frac{1}{2} \tilde{\beta} \nabla e \cdot \nabla e$, (6.6) rewrites as the classical parabolic diffusion equation of the form

$$\begin{cases} \partial_t e(t) + \operatorname{div} j =, \quad j := -\nabla \mu, \quad \mu = \delta_e \left(\psi^C(e) + \tilde{\psi}^C(\nabla e) \right), & \text{in } \Omega \times [0, T] \\ e = \Delta e = 0 & \text{on } \partial\Omega \times [0, T] \\ e(0) = e_0 & \text{in } \Omega \times [0, T] \end{cases}. \quad (6.7)$$

6.3. Gradient flow. Let us assume the existence of a scalar \mathcal{H} such that

$$\langle \operatorname{inc} \mathcal{G}(\epsilon^0), F \rangle = \lim_{\epsilon \rightarrow 0} \frac{\mathcal{H}(\epsilon^0 + \epsilon F) - \mathcal{H}(\epsilon^0)}{\epsilon},$$

for every $F \in \mathcal{H}_0(\Omega)$. Note that for a nonlinear term of the form (5.5), one has $\mathcal{H}(\epsilon^0) = -(\mathbb{G}, \epsilon^0) + \frac{\beta}{2} (\operatorname{Curl}^t \epsilon^0, \operatorname{Curl} \epsilon^0) - \frac{1}{3} \phi(\operatorname{tr} \epsilon^0) \mathbb{I}_2$, where $\varphi = \phi'$. By defining the incompatibility energy as

$$\Phi(\epsilon^0) := \int_{\Omega} \left(\frac{1}{2} \mathbb{M} \operatorname{inc} \epsilon^0 \cdot \operatorname{inc} \epsilon^0 + \mathcal{H}(\epsilon^0) \right) dx,$$

it is obvious by integration by parts that the Gâteaux derivative of Φ at $\epsilon^0 \in \mathcal{C}^\infty(\Omega)$ in the direction $F \in \mathcal{H}_0(\Omega)$ reads

$$\langle \text{grad}_{L^2}^{\mathcal{H}_0} \Phi(\epsilon^0), F \rangle = \int_{\Omega} \text{inc} (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)) \cdot F dx = \int_{\Omega} (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)) \cdot \text{inc} F dx$$

For a general $\epsilon^0 \in \mathcal{H}(\Omega)$, one has

$$\langle \text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi(\epsilon^0), F \rangle := \int_{\Omega} (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)) \cdot \text{inc} F dx,$$

where $\mathcal{H}^{-1} := (\mathcal{H}_0(\Omega))'$. By Riesz theorem, the linear and continuous map $\text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi(\epsilon^0)$ is associated to a unique $F^0 \in \mathcal{H}_0$ such that $\text{inc} \text{inc} F^0 = \text{inc} (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0))$ and $\langle \text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi(\epsilon^0), F \rangle := \int_{\Omega} \text{inc} F^0 \cdot \text{inc} F dx$. By analogy with the scalar Cahn-Hilliard system, let us call $\text{inc} F^0$ the “chemical potential”. Furthermore, one has $\|\text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi(\epsilon^0)\|_{\mathcal{H}^{-1}}^2 = \|\text{inc} F^0\|_{L^2}^2 = (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0), \text{inc} F^0)_{L^2}$, and hence our model evolution equation writes as the following \mathcal{H}^{-1} -gradient flow:

$$\dot{\epsilon}^0 = \partial_t \epsilon^0 = -\frac{1}{\alpha} \text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi := -\frac{1}{\alpha} \text{inc} (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)). \quad (6.8)$$

Now, (6.8) implies that $\frac{d}{dt} \Phi = \langle \text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi, \dot{\epsilon}^0 \rangle = \langle \text{inc} (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)), \dot{\epsilon}^0 \rangle = (\mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0), \text{inc} \dot{\epsilon}^0)_{L^2} = -\frac{1}{2} \left(\alpha |\dot{\epsilon}^0|^2 + \frac{1}{\alpha} \|\text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi\|_{\mathcal{H}^{-1}(\Omega)}^2 \right)$ and (4.16) writes as

$$0 \leq \mathcal{D} = -\frac{d}{dt} (\mathcal{E}_\beta(\epsilon^0, \kappa) + \Phi(\epsilon^0)) = \mathcal{D}_{\text{dislo}} + \mathcal{D}_{\text{incomp}},$$

with the dislocation-induced dissipation term $\mathcal{D}_{\text{dislo}} := -\frac{d}{dt} \mathcal{E}_\beta(\epsilon^0, \kappa)$, vanishing as soon as the free energy is independent of κ , and the incompatibility-induced dissipation term $\mathcal{D}_{\text{incomp}} := \frac{1}{\alpha} \|\text{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi\|_{\mathcal{H}^{-1}(\Omega)}^2 = -\frac{d}{dt} \Phi$, due to the dependence of the free energy on $\text{Curl} \kappa = \text{inc} \epsilon^0$. Thus the incompatibility-induced dissipated energy in $[0, T]$ is decreasing, since

$$\mathcal{E}_{\text{incomp}} = \int_0^T \mathcal{D}_{\text{incomp}} dt = \Phi(0) - \Phi(T) \geq 0,$$

and hence stationnarity means that minimization is reached. Therefore, the system should progress toward a stable equilibrium state, a global minimizer of Φ . This is the basic justification for minimization schemes in a quasi-static setting. Note that maximizing the incompatibility-induced dissipated energy is equivalent to minimizing the incompatibility energy $\Phi(T)$. Set $\beta = \phi = 0$. Then, for long time-behaviour, one can simply consider the variational problem

$$\inf_{E \in \mathcal{H}^* \subset \mathcal{H}(\Omega)} \int_{\Omega} \left(\frac{1}{2} \mathbb{M} \text{inc} E \cdot \text{inc} E - \mathbb{G} \cdot E \right) dx,$$

as done in [3].

6.4. Concluding remark. This work represents the first step towards a deep understanding of time-evolution of dislocation networks at the mesoscale. Its principal aim was to put light on the importance of the incompatibility operator in the study of dislocations, and to propose an evolution in time of the dislocation-induced strain. This required to first introduce and/or recall some properties of this operator as well as its appropriate functional space. The evolution law is based on thermodynamical principles and on the postulate of maximal dissipation adopted for the model internal variables. It turns out that as a consequence of the second Law of Thermodynamics, the evolution takes the form of the following tensor formulation of Cahn-Hilliard system:

$$\alpha \partial_t \epsilon^0 = -\text{inc} \mu \quad (6.9)$$

where $\mu := \mathbb{M} \text{inc} \epsilon^0 + \mathcal{G}(\epsilon^0)$ is called the tensor “chemical potential”, with \mathbb{M} a positive-definite fourth-rank tensor with the dimensions of a force times a square distance, and \mathcal{G} a potential.

Moreover, the classical scalar Cahn-Hilliard system is recovered for the trace of the dislocation strain, called e , which is interpreted as the density of point defects, since it allows one to change the solid density by adding or removing single atoms. Remark that this fourth-order equation

for e is non classical at all, since point defects are classically modeled by second-order reaction-diffusion equations [23]. Furthermore, ∇e also appears to play the role of a conservative bulk force in the displacement equation. Note also that the Thermodynamics derivation of the model equations lead to a nonlinear term whose explicit expression is not known. For simplicity we have considered a general polynomial term in the trace of ϵ^0 , i.e. in e . Of course more elaborate choice can be made with a view to a general model, but note that the physical sense of the other two invariants of the dislocation strain is not clear.

A crucial quantity we have introduced is the incompatibility energy

$$\Phi(E) := \int_{\Omega} \left(\frac{1}{2} \mathbb{M} \operatorname{inc} E \cdot \operatorname{inc} E + \frac{\beta}{2} \operatorname{inc} E \cdot E - \frac{1}{3} \phi(\operatorname{tr} E) - \mathbb{G} \cdot E \right) dx,$$

with $\beta > 0$ a scalar with the dimensions of a force, and the scalar Φ and solenoidal tensor \mathbb{G} with the dimensions of a surface force density. Furthermore, Φ is a nonlinear potential depending on $e = \operatorname{tr} E$, and related to point defects. We have shown that the time-evolution of the incompatible strain ϵ^0 is given by (6.9), which in turns yields the following energy equation:

$$\alpha \frac{d}{dt} \Phi(\epsilon^0) + \|\operatorname{grad}_{\mathcal{H}^{-1}}^{\mathcal{H}_0} \Phi\|_{\mathcal{H}^{-1}(\Omega)}^2 = 0,$$

for some $\alpha > 0$. Therefore, solutions for large times, ϵ_{∞}^0 , should approach the minima of the incompatibility energy, viz.,

$$\Phi(\epsilon_{\infty}^0) = \inf_{E \in \mathcal{H}^* \subset \mathcal{H}(\Omega)} \Phi(E),$$

which may therefore be considered as the associated quasi-static variational problem.

This work and the formalism introduced are expected to open the way for more involved, complete and realistic models for the evolution of dislocation networks at the mesoscale.

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