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1. INTRODUCTION.

A simple model designed to reflect significant properties of defective crystals was introduced by DAVINI [9]. This continuum model reckons that the state of a crystal is given by prescribing a matrix of lattice vectors L and a positive scalar mass density ρ over a domain Ω and is designed to mimic basic features of the atomistic picture of a crystal as a rather stable collection of identical atoms. To be specific, in real crystals there are generally very many defects, for example 10^6 edge dislocations may cross a square centimetre section of material. Away from any particular defect there is a readily identifiable crystal lattice which extends for many hundred units of lattice spacing, but close to the dislocation (within distances of the order of a few units of lattice spacing) one might say either that there is no well-defined perfect lattice of atoms, or that lattice vectors jump in somewhat ambiguous fashion. The loose assumption of the model is that a process of averaging over distances of a few units of lattice spacing produces a uniquely defined set of three linearly independent lattice vectors, and a mass density ρ, and it is tacit that these averages vary over what we might call "macroscopic" length scales.

In a perfect crystal lattice identical atoms are located at all position vectors

$$x = m_1a_1 + m_2a_2 + m_3a_3$$

with $m_1, m_2, m_3 \in \mathbb{Z}$, $a_1, a_2, a_3 \in \mathbb{R}^3$. The vectors a_1, a_2, a_3 are called the *lattice vectors* and that unique matrix L such that $Le_i = a_i$ for $i = 1, 2, 3$[1] is called henceforward the *lattice matrix*. Lattice matrices L, L' correspond to the same perfect crystal lattice if and only if

$$L' = LH \tag{1.1}$$

for $H \in SL_3(\mathbb{Z}) := \{H \in M^{3\times3} \mid \det H = \pm 1, H_{ij} \in \mathbb{Z}, i, j = 1, 2, 3\}$ (see ERICKSEN [14], FONSECA [15], KINDERLEHRER [21]). Since L is constant, here, any sensible process of averaging lattice vectors gives just the columns of L, in this case. Hence the continuum analogue of the discrete collection of identical atoms has constant L, constant ρ defined over $\Omega \subset \mathbb{R}^3$.

[1]In what follows, $\{e_1, e_2, e_3\}$ is the canonical basis of $\mathbb{R}^3$.

An invertible, orientation preserving mapping $u : \Omega \to \mathbb{R}^3$ is said to induce an *elastic deformation* of the crystal and it leads to a new lattice matrix $L^*(.)$ defined over $u(\Omega)$ via

$$L^*(u(x)) = \nabla u(x)\, L(x), \quad \text{for } x \in \Omega.$$

It is traditional to assert that a crystal is *defective* if, given a lattice matrix $L^*(.)$ over Ω^*, there is no invertible mapping $u^*: \Omega^* \to \mathbb{R}^3$ which leads via an elastic deformation to a lattice matrix constant in $u^*(\Omega^*)$. DAVINI [9] and DAVINI & PARRY [10], [11] discussed subtleties related to this last idea, and in DAVINI & PARRY [11] they showed that any change of state can be factorized into an elastic deformation composed with specific types of non-elastic changes. It is natural to say that all non-elastic changes are plastic, however there are two major classes involved. There is a list of tensors which play a pivotal role in the analysis of DAVINI & PARRY [11], as they remain unchanged when the crystal is deformed elastically (see Theorem 2.3, (2.2)). In this model, the adopted notion of defect is such that deformations that leave these functionals invariant do not change the defects. It turns out that the class of defect-preserving changes of state strictly includes the elastic deformations ; defect-preserving deformations are called *neutral* and generally they involve some kind of rearrangement representing the slip mechanisms of the classic phenomenological plasticity theories (see Theorem 2.9, Corollary 2.10, Examples 2.11) as well as the elastic deformations. Thus, plastic changes of state split into these particular types of rearrangements and into those changes of state which alter the invariants of the crystal lattice.

Here we study equilibria of defective crystals within a variational framework. We factor neutral deformations into components which are exclusively elastic or exclusively slip. Essentially, a neutral change of state of a perfect crystal corresponds to a lattice matrix

$$L(u(x)) = \nabla u(x)\, \{\nabla v(x)\}^{-1},$$

where $u : \Omega \to \mathbb{R}^3$ is the elastic deformation, Ω is the reference configuration and v represents the slip or plastic deformation with $\det \nabla v = 1$ a. e. in Ω. ERICKSEN [13] and DAVINI & PARRY [10] have discussed the likelyhood that crystal equilibria correspond to some kind of variational principle, and offered the opinion that the relevant class of variations should encompass, at the most, the elastic changes and the rearrangements, so excluding any change of state which alters the invariants. In this paper we study the implications of including neutral changes of state in the class of admissible variations while taking the viewpoint that equilibria correspond to minimizers of an energy functional

$$E(u, v) := \int_{\Omega} W(\nabla u(x)\{\nabla v(x)\}^{-1})\, dx \tag{1.2}$$

where W represents the bulk energy density. Precisely, we want to judge whether or not allowing rearrangements leads to physically reasonable predictions in the context of plasticity. Thus, we consider the class of admissible pairs

$$\mathcal{A}(u_0) := \{(u, v) \in W^{1,\infty}(\Omega, \mathbb{R}^3) | \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega,\ \det \nabla v = 1 \text{ a. e. in } \Omega\},$$

which includes the elastic deformations in the case where v is the identity map. Formally, minimizing $E(.,.)$ in $\mathcal{A}$ involves variations of the reference domain ; indeed, setting $\omega := u \circ v^{-1}$ the integral (1.2) becomes

$$\int_{v(\Omega)} W(\nabla\omega(y))dy.$$

Although one occasionally sees field equations and conservation laws in continuum mechanics derived by considering variations of the domain, to our knowledge (1.2) is the first instance where such variations can be seen to correspond to clear, kinematically explicit mechanisms.

In DAVINI & PARRY [10] various properties of smooth minimizers were formally derived and convexity was assumed tacitly. Also, in DACOROGNA & FONSECA [7] existence and smoothness of minimizers for functionals of the type (1.2) were discussed. Here, existence of minimizers is not the issue. In fact, it is well known (see BALL [1]) that certain types of material symmetry are incompatible with the convexity of variational problems arising in the elasticity theory. In particular, for a perfect crystal W is not even quasiconvex (see, ERICKSEN [14], FONSECA [15], KINDERLEHRER [21]) and so, the energy $E(.,.)$ is not sequentially weakly lower semicontinuous. Hence, we are interested in studying the behavior of minimizing sequences and their state functions rather than the macroscopic weak limit.

As in CHIPOT & KINDERLEHRER [3] we assume that solutions may be measure-valued and using the parametrized probability measures of YOUNG [32] and the theory of compensated compactness of MURAT & TARTAR (see TARTAR [26]) we are able to calculate the energy and stresses of the deformed body when the class of variations includes a perfect crystal.

In Section 2 we give a brief description of the model for defective crystals proposed by DAVINI [9] and DAVINI & PARRY [10], [11] and we recall the notion of neutral deformation. We give new characterizations of neutrally related states for defective crystals, and in particular we show that the matrix L of lattice vectors of a state neutrally related to a perfect cubic crystal can be written as

$$L(u(x)) = \nabla u(x) \{\nabla v(x)\}^{-1},$$

with $\det \nabla v = 1$ a. e. in Ω (see Theorem 2.9, Corollary 2.10). This factorization is not unique and in Theorem 2.14 and Corollary 2.15 we characterize the solutions (u^*, v^*) of the equation

$$\nabla u^*(x) \{\nabla v^*(x)\}^{-1} = \nabla u(x) \{\nabla v(x)\}^{-1}.$$

In Section 3 we use the div-curl lemma (see TARTAR [26]) to show that the class of neutral deformations is closed with respect to the weak convergence in $W^{1,\infty}$ (see Theorem 3.2) and also to characterize the Young's probability measure associated to a minimizing sequence $\{L_n\}$. It turns out that the minors of L_n are weakly * continuous (see Proposition 3.7).

In Section 4 we use this result to prove that the relaxation of the energy functional for states neutrally related to a non-defective cubic crystal, inf E(u, v), coincides with

$$\inf \{ \int_\Omega g^{**}(\det \nabla u(x))\, dx \mid u \in W^{1,\infty}(\Omega, \mathbb{R}^3), \det \nabla u > 0 \text{ a. e. in } \Omega, u = u_0 \text{ on } \partial\Omega \}$$

where g^{**} is the convex minorant of the subenergy function of ERICKSEN and FLORY,

$$g(t) := \inf \{W(F) \mid \det F = t\}.$$

This result depends critically upon the material symmetry $SL_3(\mathbb{Z})$ assumed for the function W and proposed by ERICKSEN [14] for elastic crystals (see also FONSECA[15] and KINDERLEHRER [21]). We note that the relevant form of the subenergy is not evident in more general situations, where the symmetry group is not all of $SL_3(\mathbb{Z})$.

Our results lead fairly quickly to the conclusion that the average weak limits of the Cauchy stress stress tensor corresponding to a minimizing sequence must be isotropic (see Theorem 4.1).

Therefore, we deduce that even if one admits neutral deformations in variational principles determining equilibria of the lattice, the crystal is necessarily weak and it may be able to equilibrate only under pressure. ERICKSEN [12] had also remarked that perfect elastic crystals cannot support shear stresses (see FONSECA [15]) and later CHIPOT & KINDERLEHRER [3] showed that the average Cauchy stress for an elastic crystal is also a multiple of the identity. This is not a result that would win unanimous applause from an audience of experimentalists, even though one can find evidence in favour by diligent enquiry. Nevertheless, it makes us reconsider the idealizations that are embedded in the model and it is, perhaps, the friction involved in the slip that is foremost among the effects which have been disregarded. We refer to COTTRELL [5] and READ [23] for assurance that internal friction plays a significant role in the movement of dislocations. It would be appropriate, then, to consider a dynamic model involving the rate of slip (i. e. the rate of change of v), but we choose to consider a simpler alternative which allows us to remain in the variational setting. We modify E(u, v) by introducing a perturbation which depends on the slip v. As showed in Section 2, if $L(u(x)) = \nabla u(x)\{\nabla v(x)\}^{-1}$ is provided then ∇v is not unique and so, if one accepts that the penalization depends just on the lattice L(u(x)), we must confine attention to a class of penalty functionals which remain unchanged according to Theorem 2.14. In FONSECA & PARRY [19] we characterize the integrands g satisfying the following invariance property :

$$\int_\Omega g(\nabla v(x))\, dx = \int_\Omega g(\nabla(v \circ f)(x))\, dx \qquad (1.3)$$

for all Lipschitz functions v and f such that $f(x) = x$ on $\partial\Omega$ and $\det \nabla f(x) = 1$ a. e. in Ω[2]. As it turns out, perturbed problems involving a bulk penalization dictated by (1.3) are reduced, essentially, to the former energy functional (1.2). So we choose to consider here a surface energy penalization as, formally, a change in v corresponds to a variation of the domain. Thus, in Section 5 we study the minimization problem where the total energy becomes

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[2]This class of integrands is larger than the class of null lagrangians.

$$\int_{\Omega} W(\nabla u(x)\{\nabla v(x)\}^{-1})\,dx + \int_{\partial v(\Omega)} \Gamma(v)\,dS$$

and Γ denotes the surface tension. Using results of FONSECA & MÜLLER [18] and showing that two star-shaped domains with the same volume can be transformed into each other by means of an isochoric deformation (see Theorem 5.4), in Theorem 5.2 we prove that the infimum is equal to the sum of the infima, precisely

$$\int_{\Omega} \varphi^{**}(\det \nabla u_0(x))\,dx + \int_{\partial C} \Gamma(v)\,dS$$

where C is the Wulff shape for Γ (see HERRING [20], WULFF [31]). Thus, there is a decoupling of the elastic and plastic parts of the weak limit of the appropriate minimizing sequence. Once more, the weak limit of the corresponding Cauchy stress tensor is isotropic, so that some more subtle modelling or reassessment is required. Nevertheless, even if the results do not quite fit with the physics as yet, the analysis seems to represent a new direction for the calculus of variations which is motivated by mainstream problems in the mechanics of solids.

2. DESCRIPTION OF A MATHEMATICAL MODEL FOR DEFECTIVE CRYSTALS.

We follow the theory for slightly defective crystals proposed by DAVINI [9] and DAVINI & PARRY [10], [11]. In the sequel, Ω is a bounded, open, strongly Lipschitz domain in $\mathbb{R}^3$, M^{3x3} denotes the space of real 3x3 matrices, $M_+^{3x3} := \{ F \in M^{3x3} \mid \det F > 0\}$ and $\{e_1, e_2, e_3\}$ is the canonical basis of $\mathbb{R}^3$.

Definition 2.1.
A *global state of the crystal* is a triple $\Sigma := \{\Omega, L, \rho\}$, where $L : \Omega \to M_+^{3x3}$ and $\rho : \Omega \to [0, +\infty)$ are Lipschitz mappings.

Here Ω represents the macroscopic placement of the body at time t, and at each point $x \in \Omega$, $\rho(x)$ is the *mass density per unit macroscopic volume* (i. e. the number of atoms per unit volume) and L(x) represents averages values over microscopic regions of lattice vectors which define the positions of the atoms.

Consider a change of state from $\Sigma := \{\Omega, L, \rho\}$ to $\Sigma^* := \{\Omega^*, L^*, \rho^*\}$ where $\Omega^* = u(\Omega)$ and $u : \Omega \to \Omega^*$ is the macroscopic deformation. We assume throughout this work that $u : \Omega \to \mathbb{R}^3$ is a Lipschitz mapping with $\det \nabla u > 0$ a. e. in Ω, and that conservation of mass always holds, i. e.

$$\rho^*(u(x)) = \frac{\rho(x)}{\det \nabla u(x)} \quad \text{a. e. in } \Omega. \tag{2.1}$$

Definition 2.2.

We say that Σ and Σ^* are *elastically related* if the Cauchy - Born hypothesis is satisfied, namely

$$L^*(u(x)) = \nabla u(x)\, L(x), \quad \text{a. e. } x \in \Omega.$$

Generally, of course, two given states Σ, Σ^* will not be elastically related for any choice of $u : \Omega \to \Omega^*$. That is to say, the set of all states $\Sigma^e = \{\Omega^*, L^e, \rho^e\}$ elastically related to Σ, obtained by choosing $u : \Omega \to \Omega^*$ and setting $L^e(u(x)) = \nabla u(x)\, L(x)$, $\rho^e(u(x)) = \rho(x)/\det \nabla u(x)$, a. e. in Ω, generally does not include Σ^*, i. e. $L^e(.) \neq L^*(.)$, $\rho^e(.) \neq \rho(.)$ for any choice of $u : \Omega \to \Omega^*$. It is the evolution of defects that is said to account for the "discrepancy" $(L^* - L^e)$, $(\rho^* - \rho^e)$, said differently to allow that the behaviour of the lattice matrix (say) is independent of the macroscopic deformation. This is TAYLOR's "conjecture" (see [27]), that there is no change in defectiveness when the change of state is elastic, and really it just hints at what one might consider to be an appropriate definition of defectiveness here.

To be specific, and to begin with, let $\Delta := \{L, \nabla L, \rho, \nabla\rho\}$represent a *local state of the crystal* (later we shall relax the requirement that a local state can depend only on L, ρ and their first derivatives). Then it is natural to search for those integrals of the type

$$\int_c f(\Delta).dx\ ,\ \int_S f(\Delta).\nu(x)\, d\sigma(x),\ \int_V f(\Delta)\ dx \tag{2.2}$$

which will remain invariant under elastic deformations, since elastically related states are not to change the defectiveness. Here c is the boundary of a surface Π and S is the boundary of a volume region V. Clearly, the densities corresponding to these integrals will produce a list of defect measures. As usual an integral

$$\int_\omega f(\Delta)$$

is said to be *elastic invariant* if

$$\int_\omega f(\Delta) = \int_{u(\omega)} f(\Delta^*)$$

for all states Σ* which are elastically related to Σ.

We introduce some notation. The *lattice vectors* are given by

$l_i(x) := L(x)\, e_i,\ i = 1, 2, 3$

and the *dual lattice vectors* are defined by

$d_i(x) := D(x)\, e_i,\ i = 1, 2, 3$

where

$D := L^{-T}.$

Clearly

$l_i(x)\ .\ d_j(x) = \delta_{ij}$ and $l_i(x) = \frac{1}{2}\, \varepsilon_{ijk}\, \frac{d_j \wedge d_k}{\det D}$ with $i, j, k \in \{1, 2, 3\}$.

Also for $i, j \in \{1, 2, 3\}$ we define the following densities :

$b_i := \text{curl}\ d_i$	(*Burger's vectors*)
$\sigma_{ij} := b_i.d_j$	(components of *Bilby's dislocation density tensor*)
$n := 1/\det L = \det D$	(the number of cells per unit volume)
$m := \rho/n$	(atomic mass of an average cell)
$g_i := \nabla m.l_i$	

$\delta_i := \nabla m \wedge d_i.$

Theorem 2.3. (DAVINI [9])

1. (*Invariants associated to line defects*) A line integral

$$\int_c f(\Delta).\, dx$$

is elastic invariant if and only if there exists a function $h : \mathbb{R} \to \mathbb{R}$ such that

$$f = h(m)\, d\,;$$

2. (*Invariants associated to point defects*) A surface integral

$$\int_S f(\Delta).\nu(x)\, dH_2(x)$$

where H_2 is the 2-dimensional Hausdorff measure and $\nu(x)$ is the normal to the surface S at the point x, is elastic invariant if and only if there exists a function $h : \mathbb{R} \to \mathbb{R}$ such that

$$f = h(m)\, d_j \wedge d_k\,;$$

3. A volume integral

$$\int_V f(\Delta)\, dx$$

is elastic invariant if and only if there exists a function $h : \mathbb{R}^3 \to \mathbb{R}$ such that

$$f = h(\sigma/n, m, g)\, n.$$

Therefore, the elastic invariant integrals which have the prescribed form (2.2) are integrals of one of the types

$$\int_c h(m)\, d.dx, \quad \int_S h(m)\, d_i \wedge d_k.\nu\, dH_2 \text{ and } \int_V h(\sigma/n,m,g)n\, dx. \qquad (2.3)$$

It turns out that the class of states Σ for which the elastic invariants remain unchanged is strictly larger than the class of elastically related states (see Examples 2.11)

Remark 2.4. (i) If the curve c is the boundary of a surface Π then the elastic invariants

$$\int_c d_i.dx = \int_\Pi b_i\, .\nu\, dH_2$$

are called the *Burgers numbers* . According to the classical theory of continuous distributions of dislocations, the presence of dislocations is associated to non vanishing Burgers vectors.

(ii) By Stokes's Theorem it follows that the densities associated to the integrals (2.3) are

$$m,\ n,\ \sigma/n,\ g,\ \text{curl}\ d = b,\ \nabla m \wedge d = \delta.$$

Proposition 2.5 (DAVINI & PARRY [10], [11])

If the integrals (2.2) remain invariant under the change of state from Σ to Σ^* then for a. e. $x \in \Omega$

(i) $\det L^*(u(x)) = \det \nabla u(x) \det L(x)$;

(ii) $m^*(u(x)) = m(x)$;

(iii) $g^*(u(x)) = g(x)$;

(iv) $\frac{\sigma^*}{n^*}(u(x)) = \frac{\sigma}{n}(x)$.

Clearly, if $\eta \in \{\sigma/n, g, m\}$ then, by Theorem 2.3 and Proposition 2.5,

$$\int_V \eta n\, dx \quad \text{and} \quad \int_C \eta d_i . dx \tag{2.4}$$

are also elastic invariants with corresponding densities ηn and $\text{curl}(\eta d) = \nabla\eta \wedge d + \eta b$ and so we must add

$$\nabla(\sigma/n) \wedge d,\ \nabla g \wedge d$$

to the list of densities in Remark 2.4 (ii). Also, if $\eta \in \{\sigma/n, g, m\}$, it is easy to show that

$$\int_V (\nabla\eta . d_i)\, n\, dx, \quad \int_C (\nabla\eta . d_i)\, d_j . dx \quad i, j = 1, 2, 3$$

are elastic invariant integrals in the obvious sense, and we note that these invariant integrals are not of the form (2.2). In fact, DAVINI & PARRY [11] show that there is an infinite list of elastic invariant integrals with corresponding densities depending on L, ρ and their derivatives (of arbitrary order). They show, also, that there is a functional basis for this infinite list of densities, and this observation motivates the following definition.

Definition 2.6.

The states Σ and Σ^* are said to be *neutrally related*[3] if the integrals (2.2) and (2.4) remain invariant[4].

As it turns out, in general neutral states involve some kind of slip or rearrangement, representing the slip mechanisms of the classic phenomenological plasticity theories.

Theorem 2.7. (DAVINI [9] and DAVINI & PARRY [10], [11])

The states Σ and Σ^* are neutrally related if and only if for all i, j, k $\in$ {1, 2, 3} and for almost all $x \in \Omega$

1. $\rho^*(u(x)) = \dfrac{\rho(x)}{\det \nabla u(x)}$;
2. $b_i^*(u(x)) = \dfrac{\nabla u(x)}{\det \nabla u(x)} b_i(x)$;
3. $\sigma_{ij}^*(u(x)) = \dfrac{\sigma_{ij}(x)}{\det \nabla u(x)}$;
4. $n^*(u(x)) = \dfrac{n(x)}{\det \nabla u(x)}$;
5. $\delta_i^*(u(x)) = \dfrac{\nabla u(x)}{\det \nabla u(x)} \delta_i(x)$;
6. $\nabla_y(\sigma_{ij}^*/n^*) \wedge d_k^* = \dfrac{\nabla u(x)}{\det \nabla u(x)} \nabla_x(\frac{\sigma_{ij}}{n}) \wedge d_k$ where $y = u(x)$;
7. $\nabla_y(g_i^*) \wedge d_k^* = \dfrac{\nabla u(x)}{\det \nabla u(x)} \nabla_x(g_i) \wedge d_k$.

Remark 2.8. If $\det B \neq 0$, where $Be_i := b_i$, then Σ^* is neutrally related to Σ if and only if Σ^* and Σ are elastically related. In fact, setting $\Sigma' := \{u(\Omega), L', \rho'\}$ with $\rho'(u(x)) := \dfrac{\rho(x)}{\det \nabla u(x)}$

[3] It can be shown that neutrally related states are locally elastically related.

[4] This is slightly different to the notion employed in DAVINI & PARRY [10], [11].

and $L'(u(x)) = \nabla u(x)\, L(u(x))$, then Σ' and Σ are elastically related and by Theorem 2.7 (2) we have

$$b_i^*(u(x)) = \frac{\nabla u(x)}{\det \nabla u(x)}\, b_i(x) = b_i'(u(x))$$

which, together with Theorem 2.7 (3), implies that

$$b_i^*(u(x)).d_j^*(u(x)) = \frac{\sigma_{ij}(x)}{\det \nabla u(x)} = b_i'(u(x)).d_j'(u(x))$$
$$= b_i^*(u(x)).d_j'(u(x)).$$

Finally, as $\det B^* \neq 0$ we conclude that $D^* = D'$ i. e. $L^* = L'$.

Theorem 2.7 suggests taking

$$\rho,\ B,\ \sigma,\ n,\ \delta,\ \nabla\left(\frac{\sigma}{n}\right) \wedge D, \nabla g \wedge D$$

as *local measures of defectiveness.*

We obtain the following characterization for neutral states.

Theorem 2.9.

The states Σ and Σ^* are neutrally related if and only if there exists a Lipschitz function $\varphi : \Omega \to \mathbb{R}^3$ such that for almost all $x \in \Omega$

1. $\rho^*(u(x)) = \dfrac{\rho(x)}{\det \nabla u(x)}$;
2. $L^*(u(x)) = \nabla u(x)\, \{L^{-1}(x) + \nabla\varphi(x)\}^{-1}$;
3. $b_i(x) \,.\, \nabla\varphi_j(x) = 0$ for all $i, j \in \{1, 2, 3\}$;
4. $\det(\mathbb{1} + \nabla\varphi(x)\, L(x)) = 1$;
5. $\nabla m(x) \wedge \nabla\varphi_i(x) = 0$ for all $i = 1, 2, 3$;
6. $\nabla(\sigma_{ij}(x)/n(x)) \wedge \nabla\varphi_k(x) = 0$ for all $i, j, k \in \{1, 2, 3\}$;
7. $\nabla g_i(x) \wedge \nabla\varphi_j(x) = 0$ for all $i, j \in \{1, 2, 3\}$.

Proof. It is easy to show that if $L^*(u(x)) = \nabla u(x)\ \{L^{-1}(x) + \nabla\varphi(x)\}^{-1}$, where φ satisfies equations (3) - (7), then the conditions (1) - (7) of Theorem 2.7 are fullfilled. Conversely, suppose that Σ and Σ^* are neutrally related. Then, using the fact that

$$\mathrm{curl}_x(\phi) = \left(\frac{\nabla u}{\det \nabla u}\right)^{-1} \mathrm{curl}_y(\nabla u^{-T}\phi), \text{ where } y = u(x),$$

by Theorem 2.7 (2) we have

$$\begin{aligned}\mathrm{curl}_x(\nabla u^T L^{*-T} e_i - L^{-T} e_i) &= \left(\frac{\nabla u}{\det \nabla u}\right)^{-1} \mathrm{curl}_y(\nabla u^{-T}\nabla u^T L^{*-T} e_i) - \mathrm{curl}_x(L^{-T} e_i)\\ &= \left(\frac{\nabla u}{\det \nabla u}\right)^{-1} b_i^*(u(x)) - b_i(x)\\ &= 0.\end{aligned}$$

Hence, there exists a Lipschitz function $\varphi : \Omega \to \mathbb{R}^3$, $\varphi = (\varphi_1, \varphi_{,2}, \varphi_3)$, such that for almost all x

$$(\nabla u^T L^{*-T} - L^{-T})\, e_i = \nabla\varphi_i = (\nabla\varphi)^T e_i,$$

i. e.

$$L^{*-1}\nabla u - L^{-1} = \nabla\varphi$$

which proves (2). Therefore, by Theorem 2.7 (2), (3)

$$\begin{aligned}\frac{\sigma_{ij}(x)}{\det \nabla u(x)} &= \sigma^*_{ij}(u(x))\\ &= b_i^* \cdot d_j^* = \frac{\nabla u}{\det \nabla u}\, b_i \cdot (L^{*-T} e_j)\\ &= \frac{\nabla u}{\det \nabla u}\, b_i \cdot \nabla u^{-T}(L^{-T} + \nabla\varphi^T)\, e_j\\ &= \frac{1}{\det \nabla u}\,\sigma_{ij} + \frac{1}{\det \nabla u}\, b_i \cdot \nabla\varphi_j\end{aligned}$$

and so $b_i(x) \cdot \nabla\varphi_j(x) = 0$. Next, by Theorem 2.7 (4)

$$\begin{aligned}\frac{n(x)}{\det \nabla u(x)} &= n^* = (\det L^*)^{-1}\\ &= (\det \nabla u(x))^{-1} \det(L^{-1}(x) + \nabla\varphi(x))\\ &= \frac{n(x)}{\det \nabla u(x)} \det(\mathbb{1} + \nabla\varphi(x)\, L(x))\end{aligned}$$

therefore

$$\det (\mathbb{1} + \nabla\varphi(x)\, L(x)) = 1.$$

In a similar way, (5) - (7) follow from equations (5) - (7) in Theorem 2.7.

According to Definition 2.2, Σ and Σ^* are elastically related if and only if $\varphi = 0$. Next, we analyze the class of states neutrally related to a non-defective cubic crystal.

Corollary 2.10.

$\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$ and $\Sigma = \{u(\Omega), L, \rho\}$ are neutrally related if and only if there exists a Lipschitz mapping $v : \Omega \to \mathbb{R}^3$ such that for almost all $x \in \Omega$

1. $\rho(u(x)) = \dfrac{1}{\det \nabla u(x)}$
2. $L(u(x)) = \nabla u(x)\ \{\nabla v(x)\}^{-1}$;
3. $\det \nabla v(x) = 1$.

Proof. Note that $B_0 = 0$, $m_0 = 1$, $\sigma_0 = 0$ and $g_0 = 0$ a. e. in Ω. Thus Corollary 2.10 follows immediately from Theorem 2.9 setting $v(x) := x + \varphi(x)$.

We give some examples of neutrally related states.

Examples 2.11.

(1) Consider a state $\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$ of a perfect cubic crystal. Set $\Sigma = \{u(\Omega), L, \rho\}$ where $u \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ is invertible, $\det \nabla u(x) > 0$ a. e. in Ω,

$$\rho(u(x)) = \frac{1}{\det \nabla u(x)} \quad \text{a. e. in } \Omega,$$

and

$$L(u(x)) = \nabla u(x)\, (\mathbb{1} + a\otimes b)$$

where $a, b \in \mathbb{R}^3$ are such that $a.b = 0$. By Corollary 2.10 it follows that Σ_0 and Σ are neutrally related.

(2) As in the first example, let $\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$ and $\Sigma = \{u(\Omega), L, \rho\}$, where now

$$L(u(x)) = \nabla u(x) R$$

for some rotation R. Then Σ_0 and Σ are neutrally related.

(3) Let $\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$ and consider a change of state involving no macroscopic deformation, i. e. $u(x) = x$ and $\Sigma = \{\Omega, k\mathbb{1}, 1\}$, $k > 0$. Here $\nabla v = k^{-1}\mathbb{1}$ and, by Corollary 2.10, Σ_0 and Σ are not neutrally related unless $k = 1$. As $D = k^{-1}\mathbb{1}$ is constant, $B = 0$ and so there are no dislocations. However, $m_0 = 1$ while $m = k^3$ which implies that the cell mass was changed and since there is conservation of mass, the interpretation is that if $k < 1$ vacancies are created in passing from Σ_0 to Σ and if $k > 1$ interstitials are created.

(4) Σ and Σ^* are *rearrangements* of one another if there exists $u : \Omega \to \Omega^*$ invertible such that for a. e. $x \in \Omega$

$$\det \nabla u(x) = 1, \ \rho^*(u(x)) = \rho(x), \ L^*(u(x)) = L(x).$$

A *slip* is a rearrangement such that

$$u(x) = x + p(g(x))$$

with $g : \Omega \to \mathbb{R}$, $p : \mathbb{R} \to \mathbb{R}^3$ such that

$$\det(\mathbb{1} + p' \otimes \nabla g) = 1, \text{ i. e. } p'.\nabla g = 0.$$

If $\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$ and $\Sigma^* = \{u(\Omega), \mathbb{1}, 1\}$are rearrangements of one another, then they are neutrally related by application of Corollary 2.10 with $v = u$.

Definition 2.12.

The states $\Sigma = \{\Omega, L, \rho\}$ and $\Sigma^* = \{\Omega^*, L^*, \rho^*\}$ are said to be *equidefective* if they are locally elastically related, i. e. if there exists a Lipschitz mapping $u : \Omega \to u(\Omega) = \Omega^*$ such that

$$\rho^*(u(x)) = \frac{\rho(x)}{\det \nabla u(x)} \quad \text{a. e. in } \Omega$$

and for all $x_0 \in \Omega$ there exist neighborhoods U_1 and U_2 of x_0 in Ω and there exists a Lipschitz function $g : U_1 \to U_2$ such that $g(x_0) = x_0$ and

$$L^*((u \circ v)(x)) = \nabla(u \circ v)(x)\, L(x) \quad \text{for almost all } x \in U_1.$$

Theorem 2.13. (DAVINI & PARRY [10], [11])

If Σ and Σ^* are neutrally related then they are equidefective.

In Theorem 2.9 we proved that if the states Σ and Σ^* are neutrally related then there exists a Lipschitz function $\varphi : \Omega \to \mathbb{R}^3$ such that for almost all $x \in \Omega$

$$L^*(u(x)) = \nabla u(x) \, \{L^{-1}(x) + \nabla\varphi(x)\}^{-1}.$$

In the last results of this section we address the question of characterizing different factorizations of the lattice matrix.

Theorem 2.14.

1. (*Necessary condition*) Let $\Sigma^* = \{u(\Omega), L^*, \rho^*\} = \{\tilde{u}(\Omega), \tilde{L}, \tilde{\rho}\}$ and let $\Sigma = \{\Omega, L, \rho\}$, where $L, L^{-1} \in L^\infty(\Omega, M^{3x3})$, $u, \tilde{u}, \varphi, \tilde{\varphi} \in W^{1,\infty}(\Omega, \mathbb{R}^3)$, $\det \nabla u$, $\det \nabla\tilde{u} > 0$ in Ω, $u = \tilde{u} = u_0$ on $\partial\Omega$, with $u_0 \in C(\overline{\Omega}, \mathbb{R}^3)$ one-to-one in Ω. Suppose, in addition, that

$$L^*(u(x)) = \nabla u(x) \, \{L^{-1}(x) + \nabla\varphi(x)\}^{-1}, \quad \tilde{L}(\tilde{u}(x)) = \nabla\tilde{u}(x) \, \{L^{-1}(x) + \nabla\tilde{\varphi}(x)\}^{-1}.$$

Then there exists $\xi \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that, setting $f := \tilde{u}^{-1} \circ u$, the following hold :

(i) $f(x) = x$ on $\partial\Omega$;

(ii) $\rho(f(x)) = \dfrac{\rho(x)}{\det \nabla f(x)}$ a. e. in Ω ;

(iii) $\nabla\xi(x) = L^{-1}(x) - L^{-1}(f(x))\nabla f(x)$ a. e. in Ω ;

(iv) $\varphi(x) = \tilde{\varphi}(f(x)) - \xi(x) + \text{Const.}$ a. e. in Ω ;

(v) $B(f(x)) = \dfrac{\nabla f(x)}{\det \nabla f(x)} B(x)$ a. e. in Ω .

Moreover, if Σ^* and Σ are neutrally related then for a. e. $x \in \Omega$

(a) $\sigma(f(x)) = \dfrac{\sigma(x)}{\det \nabla f(x)}$;

(b) $n(f(x)) = \dfrac{n(x)}{\det \nabla f(x)}$;

(c) $\delta(f(x)) = \dfrac{\nabla f(x)}{\det \nabla f(x)} \delta(x)$;

(d) $\nabla_y(\frac{\sigma_{ij}}{n}) \wedge d_k = \dfrac{\nabla f(x)}{\det \nabla f(x)} \nabla_x(\frac{\sigma_{ij}}{n}) \wedge d_k$ where $y = f(x)$;

(e) $\nabla_y(g_i) \wedge d_k = \dfrac{\nabla f(x)}{\det \nabla f(x)} \nabla_x(g_i) \wedge d_k$.

2. (*Sufficient condition*) If $\Sigma^* = \{u(\Omega), L^*, \rho^*\}$ corresponds to a change of the state $\Sigma = \{\Omega, L, \rho\}$, where $L, L^{-1} \in L^\infty(\Omega, M^{3x3})$, $u \in W^{1,\infty}(\Omega, \mathbb{R}^3)$, $\det \nabla u > 0$ a. e. in Ω, u is invertible, and if there exist $\xi, f \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that $\det \nabla f > 0$ a. e. in Ω and

(i) $f(x) = x$ on $\partial\Omega$;

(ii) $\rho(f(x)) = \dfrac{\rho(x)}{\det \nabla f(x)}$ a. e. in Ω :

(iii) $\nabla\xi(x) = L^{-1}(x) - L^{-1}(f(x))\nabla f(x)$ a. e. in Ω

then, setting $\tilde{u} := u \circ f^{-1}$, $\tilde{\varphi} := \varphi \circ f^{-1} + \xi \circ f^{-1}$ + Const. and $\tilde{\rho}(\tilde{u}(x)) := \dfrac{\rho(x)}{\det \nabla\tilde{u}(x)}$, we have

$$\Sigma^* = \{u(\Omega), L^*, \rho^*\} = \{\tilde{u}(\Omega), \tilde{L}, \tilde{\rho}\}$$

where $\tilde{L}(\tilde{u}(x)) := \nabla\tilde{u}(x)\ \{L^{-1}(x) + \nabla\tilde{\varphi}(x)\}^{-1}$. Furthermore, if f satisfies the conditions (a) - (e) then Σ^* and Σ are neutrally related.

Proof. 1. As $\tilde{u}$ is invertible (see BALL [2]), set $f := \tilde{u}^{-1} \circ u$. Clearly $f(x) = x$ on $\partial\Omega$ and since

$$\frac{\rho(x)}{\det \nabla u(x)} = \rho^*(u(x)) = \tilde{\rho}(u(x))$$
$$= \tilde{\rho}(\tilde{u}(f(x)))$$
$$= \frac{\rho(f(x))}{\det \nabla\tilde{u}(f(x))}$$
$$= \frac{\rho(f(x)) \det \nabla f(x)}{\det \nabla u(x)}$$

we deduce that

$$\rho(f(x)) = \frac{\rho(x)}{\det \nabla f(x)} \text{ a. e. in } \Omega.$$

Define $\xi(x) := \tilde{\varphi}(f(x)) - \varphi(x)$ + Const. Then

$$
\begin{aligned}
\nabla u(x)\ \{L^{-1}(x) + \nabla\varphi(x)\}^{-1} &= L^*(u(x))\\
&= \tilde{L}(u(x)) = \tilde{L}(\tilde{u}(f(x)))\\
&= \nabla\tilde{u}(f(x))\ \{L^{-1}(f(x)) + \nabla\tilde{\varphi}(f(x))\}^{-1}\\
&= \nabla u(x)\ \{\nabla f(x)\}^{-1}\{L^{-1}(f(x)) + [\nabla\varphi(x) + \nabla\xi(x)](\nabla f(x))^{-1}\}^{-1}\\
&= \nabla u(x)\ \{L^{-1}(f(x))\ \nabla f(x) + \nabla\varphi(x) + \nabla\xi(x)\}^{-1}
\end{aligned}
$$

and so

$$L^{-1}(x) = L^{-1}(f(x))\ \nabla f(x) + \nabla\xi(x) \quad \text{a. e. in } \Omega.$$

This implies that

$$
\begin{aligned}
0 &= \operatorname{curl}\{[L^{-1}(f(x))\ \nabla f(x) - L^{-1}(x)]^T e_i\}\\
&= \operatorname{curl}_x\{(\nabla f(x))^T L^{-T}(f(x))e_i\} - b_i(x)\\
&= \det \nabla f(x)\ \{\nabla f(x)\}^{-1} \operatorname{curl}_{y=f(x)}\{L^{-T}(y)e_i\} - b_i(x)\\
&= \det \nabla f(x)\ \{\nabla f(x)\}^{-1}\ b_i(f(x)) - b_i(x),
\end{aligned}
$$

therefore

$$B(f(x)) = \frac{\nabla f(x)}{\det \nabla f(x)} B(x) \quad \text{a. e. in } \Omega .$$

If Σ and Σ^* are neutrally related, then by Theorem 2.9 (3) and by (iii), (v) we have

$$
\begin{aligned}
\sigma_{ij}(f(x)) &= b_i(f(x)).\ d_j(f(x))\\
&= \frac{\nabla f(x)\ b_i(x).\ L^{-T}(f(x))\ e_j}{\det \nabla f(x)}\\
&= \frac{\nabla f(x)\ b_i(x)\ .\ \nabla f^{-T}(x)(-\nabla\xi^T(x) + L^{-T}(x))e_j}{\det \nabla f(x)}\\
&= \frac{\sigma_{ij}(x)}{\det \nabla f(x)} - \frac{b_i(x).\ [\nabla\tilde{\varphi}(f(x))\ \nabla f(x)]^T\ e_j}{\det \nabla f(x)} + \frac{b_i(x).\nabla\varphi_j(x)}{\det \nabla f(x)}\\
&= \frac{\sigma_{ij}(x)}{\det \nabla f(x)} - b_i(f(x)).\nabla\tilde{\varphi_j}(f(x))\\
&= \frac{\sigma_{ij}(x)}{\det \nabla f(x)}.
\end{aligned}
$$

Equations (b) - (e) follow, in a similar way, from conditions (iii) - (v) and Theorem 2.9 (4) - (7).

2. Suppose that there exist $\xi, f \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that $\det \nabla f > 0$ a. e. in Ω and

(i) $f(x) = x$ on $\partial\Omega$;

(ii) $\rho(f(x)) = \dfrac{\rho(x)}{\det \nabla f(x)}$ a. e. in Ω ;

(iii) $\nabla\xi(x) = L^{-1}(x) - L^{-1}(f(x))\nabla f(x)$ a. e. in Ω.

Setting

$$\tilde{L}(\tilde{u}(x)) := \nabla\tilde{u}(x)\,\{L^{-1}(x) + \nabla\tilde{\varphi}(x)\}^{-1} \text{ and } \tilde{\rho}(\tilde{u}(x)) := \frac{\rho(x)}{\det \nabla\tilde{u}(x)}$$

where

$$\tilde{u} := u\circ f^{-1} \text{ and } \tilde{\varphi} := \varphi\circ f^{-1} + \xi\circ f^{-1} + \text{Const.},$$

we want to show that

$$\tilde{\rho}(u(x)) = \rho^*(u(x)) \text{ and } \tilde{L}(u(x)) = L^*(u(x)).$$

In fact, by (ii)

$$\begin{aligned}\tilde{\rho}(u(x)) &= \tilde{\rho}(\tilde{u}(f(x))) = \\ &= \frac{\rho(f(x))}{\det \nabla\tilde{u}(f(x))} \\ &= \frac{\rho(x)}{\det \nabla f(x) \det \nabla\tilde{u}(f(x))} \\ &= \frac{\rho(x)}{\det \nabla u(x)} \\ &= \rho^*(u(x))\end{aligned}$$

and by (iii)

$$\begin{aligned}\tilde{L}(u(x)) &= \tilde{L}(\tilde{u}(f(x))) \\ &= \nabla\tilde{u}(f(x))\,\{L^{-1}(f(x)) + \nabla\tilde{\varphi}(f(x))\}^{-1} \\ &= \nabla u(x)\,\{\nabla f(x)\}^{-1}\{L^{-1}(f(x)) + [\nabla\varphi(x) + \nabla\xi(x)](\nabla f(x))^{-1}\}^{-1} \\ &= \nabla u(x)\,\{L^{-1}(f(x))\,\nabla f(x) + \nabla\varphi(x) + \nabla\xi(x)\}^{-1} \\ &= \nabla u(x)\,\{L^{-1}(x) + \nabla\varphi(x)\}^{-1} \\ &= L^*(u(x)).\end{aligned}$$

It is easy to check that if (a) - (f) hold then the equations (3) - (8) of Theorem 2.9 are satisfied and so Σ^* and Σ are neutrally related.

Corollary 2.15.

Let $\Sigma = \{u(\Omega), L, \rho\}$ correspond to a change of the state $\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$, where $u \in W^{1,\infty}(\Omega, \mathbb{R}^3)$, $\det \nabla u > 0$ in Ω, $u = u_0$ on $\partial\Omega$, with $u_0 \in C(\overline{\Omega}, \mathbb{R}^3)$ one-to-one in Ω, and

$$L(u(x)) = \nabla u(x) \{\nabla v(x)\}^{-1}$$

for some $v \in W^{1,\infty}(\Omega, \mathbb{R}^3)$, with $\det \nabla v > 0$ in Ω. Then $\Sigma = \{\tilde{u}(\Omega), \tilde{L}, \tilde{\rho}\}$ with

$$\tilde{L}(\tilde{u}(x)) = \nabla\tilde{u}(x) \{\nabla\tilde{v}(x)\}^{-1}$$

if and only if, setting $f := \tilde{u}^{-1} \circ u$, the following hold :

(i) $f(x) = x$ on $\partial\Omega$;

(ii) $\det \nabla f(x) = 1$ a. e. in Ω :

(iii) $v(x) = \tilde{v}(f(x)) + \text{Cont.}$ a. e. in Ω.

Moreover, Σ and Σ_0 are neutrally related if and only if $\det \nabla v = 1$ a. e. in Ω and $\rho(u(x)) = \frac{1}{\det \nabla u(x)}$.

Proof. This result follows immediately from Corollary 2.10 and Theorem 2.14. Indeed, here $B_0 = 0$ and defining $\xi(x) := x - f(x)$, $\varphi(x) := v(x) - x$, we obtain from Theorem 2.14 that

$$\begin{aligned}\tilde{v}(f(x)) &= \tilde{\varphi}(f(x)) + f(x)\\ &= \varphi(x) + \xi(x) + \text{Const.} + f(x)\\ &= \varphi(x) + x + \text{Const.}\\ &= v(x) + \text{Const.}\end{aligned}$$

3. CHARACTERIZATION OF THE YOUNG MEASURE.

Our goal is to study equilibria of crystals within a variational framework when neutrally related states are admissible. As it is well known, the bulk energy density for solid crystals is non quasiconvex and so, in general the energy functional is not lower semicontinuous as minimizing sequences may develop oscillations. In particular, the macroscopic limit is not necessarily a minimizer of E(.,.) and, as it turns out, the sequence itself stores more information on limiting macroscopic state functions of the crystal than the macroscopic configuration itself. This information is given partially by the corresponding Young measure (see YOUNG [32] and TARTAR [26]) as shown in the work of CHIPOT & KINDERLEHRER [3] for elastic crystals. However, before we start the analysis of the Young measures associated to minimizing sequences, we need to make sure that these sequences are "stable" under weak convergence, even if oscillations may occur. We will prove this result using MURAT & TARTAR's div-curl lemma of the theory of compensated compactness (see TARTAR [26]).

3.1 Div-Curl Lemma

Let $\Omega \subset \mathbb{R}^N$ be an open, bounded, strongly Lipschitz domain, and let $u_n, v_n \in L^\infty(\Omega;\mathbb{R}^N)$ be such that $u_n \rightarrow u_\infty$ and $v_n \rightarrow v_\infty$ in L^∞ weak *. If, in addition, $\{\mathrm{div}\ u_n\}$ and $\{\mathrm{curl}\ v_n\}$ are bounded sequences in $H^{-1}_{loc}(\Omega)$ then $u_n . v_n \rightarrow u_\infty . v_\infty$ weakly *.

Theorem 3.2

Let $\Sigma_n = \{u_n(\Omega), L_n, \rho_n\}$ be a sequence of states neutrally related to $\Sigma = \{u(\Omega), L, \rho\}$ and let $\varphi_n : \Omega \rightarrow \mathbb{R}^3$ be such that $L_n(u(x)) = \nabla u_n(x)\ \{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$ for almost all $x \in \Omega$. If $u_n \rightarrow u_\infty$ and $\varphi_n \rightarrow \varphi_\infty$ in $W^{1,\infty}$ weak * then

1. $\det L(x) = \det (\{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1})$ a. e. in Ω ;
2. $\{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1} \rightarrow \{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1}$ in L^∞ weak * ;
3. $L_n(x) \rightarrow L_\infty(x) := \nabla u_\infty(x)\{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1}$ in L^∞ weak *.

Moreover, if $\det \nabla u_\infty > 0$ a. e. in Ω, then the state $\Sigma_\infty := \{u_\infty(\Omega), L_\infty, \rho_\infty\}$ is neutrally related to Σ, where $\rho_\infty(u_\infty(x)) := \dfrac{\rho(x)}{\det \nabla u_\infty(x)}$.

In order to prove this result, we need the following lemmas, the first of which is purely algebraic.

Lemma 3.3.

If A, B $\in M^{3x3}$ and if A is an invertible matrix then

1. $\det(A+B) = \det A + \text{adj } A.B + A.\text{adj } B + \det B$;
2. $\text{adj}(A+B) = \text{adj } A + \frac{\text{adj } A.B}{\det A}\text{adj } A - \frac{\text{adj } A}{\det A} B^T \text{adj } A + \text{adj } B.$

Here, and in what follows, adj A is the matrix of cofactors of A. In particular, if A is invertible then

$$A^{-1} = \frac{(\text{adj } A)^T}{\det A}.$$

Also, the inner product between matrices is defined by

$$A.B := \sum_{i,j=1}^{3} A_{ij} B_{ij} = \text{tr}(A^T B).$$

Lemma 3.4.

If $\Sigma^* = \{u(\Omega), L^*, \rho^*\}$ and $\Sigma = \{\Omega, L, \rho\}$ are neutrally related and if $L^*(u(x)) = \nabla u(x) \{L^{-1}(x) + \nabla\varphi(x)\}^{-1}$ then for almost all $x \in \Omega$ and for i, j, k $\in \{1, 2, 3\}$ the following hold :

1. $\text{curl}\,[\{L^{-1}(x) + \nabla\varphi(x)\}^T e_i] = b_i(x)$;
2. $\text{div}\frac{\{L^{-1}(x) + \nabla\varphi(x)\}^{-1} e_i}{\det L(x)} = \frac{1}{2}\,\varepsilon_{ijk}(\sigma_{jk}(x) - \sigma_{kj}(x)).$

Proof. In fact, by definition of the Burgers' vectors we have

$$\begin{aligned}\text{curl}\,[\{L^{-1}(x) + \nabla\varphi(x)\}^T e_i] &= b_i(x) + \text{curl}\,\nabla\varphi_i(x)\\ &= b_i(x),\end{aligned}$$

and by Theorem 2.9 (4), setting $L'(x) := \{L^{-1}(x) + \nabla\varphi(x)\}^{-1}$, $D' := L'^{-T}$ and $\sigma'_{ij} := \text{curl}\, d'_i \,.\, d'_j$ we have

$$\det L(x) = \det L'(x)$$

which implies that

$$\begin{aligned}\text{div}\frac{\{L^{-1}(x) + \nabla\varphi(x)\}^{-1} e_i}{\det L(x)} &= \text{div}\frac{L'(x) e_i}{\det L'(x)}\\ &= \frac{1}{2}\,\text{div}\frac{\varepsilon_{ijk} \det L'(x)\, d'_j(x) \wedge d'_k(x)}{\det L'(x)}\end{aligned}$$

$$= \frac{1}{2}\, \varepsilon_{ijk}\, (\text{curl } d'_j(x).d'_k(x) - \text{ curl } d'_k(x).d'_j(x))$$
$$= \frac{1}{2}\, \varepsilon_{ijk}\, (\sigma'_{jk}(x) - \sigma'_{kj}(x)). \qquad (3.1)$$

However, by (1)

$$\text{curl } d'_j(x) = \text{curl } [\{L^{-1}(x) + \nabla\varphi(x)\}^T e_i]$$
$$= b_i(x)$$

which, together with Theorem 2.9 (3), yields

$$\sigma'_{ij}(x) = b_i(x).(L^{-T}(x) + \nabla\varphi(x)^T)e_j$$
$$= \sigma_{ij}(x) + b_i(x).\nabla\varphi_j(x)$$
$$= \sigma_{ij}(x). \qquad (3.2)$$

The result follows from (3.1) and (3.2).

Proof of Theorem 3.2 We start by proving (1). By Theorem 2.9 (4) and by Lemma 3.3 (1) we have

$$(\det L(x))^{-1} = \det (L^{-1}(x) + \nabla\varphi_n(x))$$
$$= \det (L^{-1}(x)) + \text{adj } L^{-1}(x)\, .\nabla\varphi_n(x) + L^{-1}(x)\, .\, \text{adj } \nabla\varphi_n(x) + \det \nabla\varphi_n(x)$$

and so, as $\text{adj } \nabla\varphi_n \to \text{adj } \nabla\varphi_\infty$ and $\det \nabla\varphi_n \to \det \nabla\varphi_\infty$ in L^∞ weak * (see BALL [1]), we conclude that

$$(\det L(x))^{-1} = \det (L^{-1}(x) + \nabla\varphi_\infty(x)).$$

Also, by Theorem 2.9 (4) and Lemma 3.3 (2)

$$\{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1} = \det (\{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1})\ \text{ adj } \{L^{-1}(x) + \nabla\varphi_n(x)\}^T$$
$$= \det L(x)\, \{\frac{L(x)}{\det L(x)} + L(x).\nabla\varphi_n{}^T(x)\ \frac{L(x)}{\det L(x)} -$$
$$- \frac{L(x)}{\det L(x)}\, \nabla\varphi_n(x)\, L(x) + \text{adj } \nabla\varphi_n(x)^T \}$$

hence the weak * limit of $\{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$ is equal to

$$\det L(x)\, \{\frac{L(x)}{\det L(x)} + L(x).\nabla\varphi_\infty{}^T(x)\ \frac{L(x)}{\det L(x)} -$$
$$- \frac{L(x)}{\det L(x)}\, \nabla\varphi_\infty(x)\, L(x) + \text{adj } \nabla\varphi_\infty(x)^T \}$$

which by (1) and by Lemma 3.3 (2) reduces to

$$\det(\{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1}) \ \mathrm{adj}\ \{L^{-1}(x) + \nabla\varphi_\infty(x)\}^T = \{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1}.$$

Finally we prove (3). Fix i, j ∈ {1, 2, 3} and set $\omega_n = (\omega_n^1, \omega_n^2, \omega_n^3)$, $v_n = (v_n^1, v_n^2, v_n^3)$ where

$$\omega_n^k := \frac{\partial u_n^i}{\partial x_k}, \quad v_n^k := (L^{-1} + \nabla\varphi_n)^{-1}{}_{kj}.$$

Clearly curl $\omega_n = 0$ and by Lemma 3.4 (2) and Theorem 2.9 (4)

$$\mathrm{div}\ v_n(x) = \mathrm{div}\ [\frac{\{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}e_j}{\det L(x)} \det L(x)]$$

$$= \varepsilon_{jlk}(\sigma_{lk}(x) - \sigma_{kl}(x)) \det L(x) + \nabla(\det L(x)) \,.\, \frac{\{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}e_j}{\det L(x)}$$

$$= \varepsilon_{jlk}(\sigma_{lk}(x) - \sigma_{kl}(x)) \det L(x) + \nabla(\det L(x)) \,.\, \mathrm{adj}\ (L^{-1}(x) + \nabla\varphi_n(x)\}^T e_j$$

which, by Lemma 3.3 (2), belongs to a compact subset of H^{-1}_{loc}. By the Div-Curl Lemma and by (2) we conclude that

$$L_{n_{ij}} = \omega_n \,.\, v_n \to \nabla u^i_\infty \,.\, (L^{-1} + \nabla\varphi_\infty)^{-1}e_j = : L_{\infty_{ij}}.$$

Moreover, if $\det \nabla u_\infty > 0$ a. e. in Ω and if

$$\rho_\infty(u_\infty(x)) := \frac{\rho(x)}{\det \nabla u_\infty(x)},$$

then $\Sigma_\infty := \{u_\infty(\Omega), L_\infty, \rho_\infty\}$ is neutrally related to Σ as, by (1), conditions (1), (2) and (4) of Theorem 2.9 hold and the remaining (3), (5), (6) and (7) are linear in $\nabla\varphi$.

Remark 3.5

(i) In Theorem 3.2, we need the additional information that $\det \nabla u_\infty > 0$ a. e. in order to define the mass density ρ_∞. However, we will see that this condition is automatically fullfilled in the case where the sequence $\{\Sigma_n\}$ minimizes the bulk energy (see Proposition 4.4 (2)).

(ii) We remark that in the proofs of Lemma 3.4 and Theorem 3.2 we only used the conditions (3) and (4) of Theorem 2.9 concerning neutrally related states.

As we mentioned before, we are interested in the characterization of the Young measure associated to a bounded minimizing sequence of lattice matrices. We start by recalling the notion of parametrized probability measures.

Proposition 3.6.

If $\{u_\eta\}$ is a bounded sequence in $L^\infty(\Omega, \mathbb{R}^p)$ then there exists a subsequence $\{u_\varepsilon\}$ and a family of probability measures $\{\mu_x\}_{x\in\Omega}$ (*Young measure*) such that if $f \in C(\mathbb{R}^p)$ then $\{f(u_\varepsilon)\}$ converges in L^∞ weak * to the average function

$$\overline{f}(x) := <\mu_x, f> = \int_{\mathbb{R}^p} f(y)\, d\mu_x(y).$$

As in Theorem 3.2, consider a sequence of states $\Sigma_n = \{u_n(\Omega), L_n, \rho_n\}$ neutrally related to $\Sigma = \{u(\Omega), L, \rho\}$ and let $\varphi_n : \Omega \to \mathbb{R}^3$ be such that $L_n(u(x)) = \nabla u_n(x)\ \{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$ for almost all $x \in \Omega$. Let $u_n \to u_\infty$, $\varphi_n \to \varphi_\infty$ in L^∞ weak *, $L_n(x) \to L_\infty(x) := \nabla u_\infty(x)\{L^{-1}(x) + \nabla \varphi_\infty(x)\}^{-1}$ in L^∞ weak * (see Theorem 3.2 (3)) and let $\{\mu_x\}_{x\in\Omega}$ be the Young's measure corresponding to $\{L_n\}$. If the change is elastic then $\varphi_n = 0$, $L_n = \nabla u_n L$ and as $M \to \det(M)$ and $M \to \operatorname{adj}M$ are null lagrangians, and so weakly * continuous, it follows that

$$\begin{aligned}
\det\Big(\int_{M^{3x3}} M\, d\mu_x(M)\Big) &= \det L_\infty(x) \\
&= \det \nabla u_\infty(x) \det L(x) \\
&= \text{w.*limit} \det \nabla u_n(x) \det L(x) \\
&= \text{w.*limit}\ \det L_n(x) \\
&= \int_{M^{3x3}} \det M\, d\mu_x(M) \qquad (3.3)
\end{aligned}$$

and, in a similar way,

$$\operatorname{adj}\Big(\int_{M^{3x3}} M\, d\mu_x(M)\Big) = \int_{M^{3x3}} \operatorname{adj} M\, d\mu_x(M). \qquad (3.4)$$

The analysis of CHIPOT & KINDERLEHRER [3] relies heavily on (3.3) and (3.4). Next we show that (3.3) and (3.4) still hold for neutrally related states.

Proposition 3.7.

For almost all $x \in \Omega$ we have

1. $\det \nabla u_\infty(x) \det L(x) = \det L_\infty(x) = \det \Big(\int_{M^{3x3}} M \, d\mu_x(M) \Big)$

$$= \int_{M^{3x3}} \det M \, d\mu_x(M) \; ;$$

2. $\operatorname{adj} L_\infty(x) = \operatorname{adj} \Big(\int_{M^{3x3}} M \, d\mu_x(M) \Big) = \int_{M^{3x3}} \operatorname{adj} M \, d\mu_x(M).$

Proof. By Proposition 3.6

$$L_\infty(x) = \int_{M^{3x3}} M \, d\mu_x(M)$$

and so, by Theorem 3.2 (1), (3)

$$\begin{aligned}
\det \Big(\int_{M^{3x3}} M \, d\mu_x(M) \Big) &= \det L_\infty(x) \\
&= \det (\nabla u_\infty(x) \{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1}) \\
&= \det \nabla u_\infty(x) \det L(x) \\
&= \text{w.*limit} \det \nabla u_n(x) \det L(x) \\
&= \text{w.*limit} \det L_n(x) \\
&= \int_{M^{3x3}} \det M \, d\mu_x(M)
\end{aligned}$$

and in a similar way

$$\begin{aligned}
\operatorname{adj} \Big(\int_{M^{3x3}} M \, d\mu_x(M) \Big) &= \operatorname{adj} L_\infty(x) \\
&= \operatorname{adj} \nabla u_\infty(x) \det L(x) \, \{L^{-1}(x) + \nabla\varphi_\infty(x)\}^T
\end{aligned}$$

with $\operatorname{adj} \nabla u_\infty$ divergence free and, by Lemma 3.4 (1), $\{L^{-1}(x) + \nabla\varphi_\infty(x)\}^T$ has curl b_i. Therefore, by the div-curl lemma we conclude that

$$\begin{aligned}
\operatorname{adj} \Big(\int_{M^{3x3}} M \, d\mu_x(M) \Big) &= \text{w.*limit } \operatorname{adj} \nabla u_n(x) \det L(x) \, \{L^{-1}(x) + \nabla\varphi_n(x)\}^T \\
&= \text{w.*limit} \operatorname{adj} L_n(x) \\
&= \int_{M^{3x3}} \operatorname{adj} M \, d\mu_x(M).
\end{aligned}$$

In the last proposition we proved that $\{\mu_x\}_{x\in\Omega}$ behaves essentially like a Young's measure corresponding to a sequence of gradients. To illustrate this fact, consider the case where $\Sigma = \{\Omega, \mathbb{1}, 1\}$ and $\Sigma_n = \{u_n(\Omega), L_n, \rho_n\}$, with $L_n = \nabla u_n\{\nabla v_n\}^{-1}$ and $\det \nabla v_n = 1$ a. e. in Ω. Suppose further that $\det \nabla u_n \geq \alpha > 0$ a. e. in Ω and $u_n = u_0$ on $\partial\Omega$, with $u_0 \in C(\overline{\Omega}, \mathbb{R}^3)$ one-to-one in Ω. Then (see BALL [2]) u_n are invertible and we define $w_n := v_n \circ u_n^{-1} : u_0(\Omega) \to \mathbb{R}^3$. If $u_n \to u_\infty$ and $v_n \to v_\infty$ in $W^{1,\infty}$ weak * then $\det \nabla u_\infty \geq \alpha$, u_∞ is invertible, $\det \nabla v_\infty = 1$ and $\{w_n\}$ is bounded in $W^{1,\infty}$. Assuming that $w_n \to w_\infty$ in $W^{1,\infty}$ weak * let $\{\lambda_y\}_{y\in u_0(\Omega)}$ be the Young's measure associated to $\{\nabla w_n\}$.

Proposition 3.8

For all $G \in C(M^{3x3}; \mathbb{R})$ and for almost all $x \in \Omega$

$$\int_{M^{3x3}} G(M)\, d\mu_x(M) = \det \nabla u_\infty(x) \int_{M^{3x3}} G(M^{-1}) \det M \;\, d\lambda_{u_\infty(x)}(M).$$

Proof. As $0 < \alpha \leq \det \nabla u_n \leq 1/K < +\infty$ then $\det \nabla w_n = \dfrac{1}{\det \nabla u_n} \geq K > 0$ and we have $\operatorname{supp} \lambda_y \subset \{M \mid \det M \geq K\} \subset M_+^{3x3}$ and $\operatorname{supp} \mu_x \subset \{M \mid \det M \geq \alpha\} \subset M_+^{3x3}$[5].

As $u_n \to u_\infty$ in L^∞ strong, given $\varphi \in \mathcal{D}(u_0(\Omega))$ we have

$$\int_\Omega \varphi(u_n(x))\, G(L_n(x))\, dx \to \int_\Omega \varphi(u_\infty(x)) \left(\int_{M^{3x3}} G(M)\, d\mu_x(M)\right) dx$$

$$= \int_{u_0(\Omega)} \varphi(y) \frac{1}{\det \nabla u_\infty(u_\infty^{-1}(y))} \left(\int_{M^{3x3}} G(M)\, d\mu_{u_\infty^{-1}(y)}(M) \;\, dy\right) \qquad (3.5)$$

and on the other hand

$$\int_\Omega \varphi(u_n(x))\, G(L_n(x))\, dx = \int_{u_0(\Omega)} \varphi(y)\, G(\{\nabla w_n(y)\}^{-1}) \det \nabla w_n(y)\, dy$$

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[5]Here we use the fact that if $\nabla u_n(x) \in K$, where K is a closed set of M^{NxN}, then the Young's measure associated to $\{\nabla u_n\}$ has support contained in K (see TARTAR [26]).

$$\to \int_{u_0(\Omega)} \varphi(y) \left(\int_{M^{3x3}} G(M^{-1}) \det M \, d\lambda_y(M) \right) dy$$

which, together with (3.5) and setting $x = u_\infty^{-1}(y)$ yields

$$\int_{M^{3x3}} G(M) \, d\mu_x(M) = \det \nabla u_\infty(x) \int_{M^{3x3}} G(M^{-1}) \det M \, d\lambda_{u_\infty(x)}(M).$$

Remark 3.9. The conclusions of Proposition 3.7 can be easily obtained using Proposition 3.8. As an example, by Theorem 3.2 (1), (3) with $L = \mathbb{1}$ and setting $G(M) = \det M$ in Proposition 3.8 we deduce that

$$\int_{M^{3x3}} \det M \, d\mu_x(M) = \det \nabla u_\infty(x) \int_{M^{3x3}} \det M^{-1} \det M \, d\lambda_{u_\infty(x)}(M)$$

$$= \det \nabla u_\infty(x) = \det L_\infty(x)$$

$$= \det \left(\int_{M^{3x3}} M \, d\mu_x(M) \right).$$

If $\Sigma_n = \{u_n(\Omega), L_n, \rho_n\}$ are neutrally related to $\Sigma = \{u(\Omega), L, \rho\}$ and if $L_n(u(x)) = \nabla u_n(x) \{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$, where $u_n \to u_\infty$, $\varphi_n \to \varphi_\infty$ in $W^{1,\infty}$ weak * and (see Theorem 3.2 (3)) $L_n(x) \to L_\infty(x) := \nabla u_\infty(x)\{L^{-1}(x) + \nabla\varphi_\infty(x)\}^{-1}$ in L^∞ weak *, we define

$\{\alpha_x\}_{x\in\Omega}$	Young's measure corresponding to $\{\nabla u_n\}$
$\{\beta_x\}_{x\in\Omega}$	Young's measure corresponding to $\{\nabla\varphi_n\}$
$\{\mu_x\}_{x\in\Omega}$	Young's measure corresponding to $\{L_n\}$.

We end this section by showing that the Young measures preserve the structure of the neutral deformations, precisely

Proposition 3.10

1. $\left(\int_{M^{3x3}} M \, d\alpha_x(M) \right) \left(\int_{M^{3x3}} (L^{-1}(x) + M)^{-1} \, d\beta_x(M) \right) = \int_{M^{3x3}} M \, d\mu_x(M)$;
2. $\left(\int_{M^{3x3}} \det M \, d\alpha_x(M) \right) \left(\int_{M^{3x3}} \det (L^{-1}(x) + M)^{-1} \, d\beta_x(M) \right) = \int_{M^{3x3}} \det M \, d\mu_x(M)$;
3. $\left(\int_{M^{3x3}} \operatorname{adj} M \, d\alpha_x(M) \right) \left(\int_{M^{3x3}} \operatorname{adj} (L^{-1}(x) + M)^{-1} \, d\beta_x(M) \right) = \int_{M^{3x3}} \operatorname{adj} M \, d\mu_x(M)$.

Proof. By Theorem 3.2 (2), (3)

$$\left(\int_{M^{3x3}} M \, d\alpha_x(M) \right) \left(\int_{M^{3x3}} (L^{-1}(x) + M)^{-1} \, d\beta_x(M) \right)$$

$$= \nabla u_\infty(x) \text{ w*limit } \{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$$

$$= L_\infty(x)$$

$$= \int_{M^{3x3}} M \, d\mu_x(M),$$

and by Theorem 2.9 (4)

$$\left(\int_{M^{3x3}} \det M \, d\alpha_x(M) \right) \left(\int_{M^{3x3}} \det (L^{-1}(x) + M)^{-1} \, d\beta_x(M) \right)$$

$$= \det \nabla u_\infty(x) \text{ w*limit } \det \{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$$

$$= \det \nabla u_\infty(x) \det L(x)$$

$$= \det L_\infty(x)$$

$$= \int_{M^{3x3}} \det M \, d\mu_x(M).$$

Finally, by Lemma 3.3 (2) we conclude that

$$\left(\int_{M^{3x3}} \text{adj } M \, d\alpha_x(M) \right) \left(\int_{M^{3x3}} \text{adj } (L^{-1}(x) + M)^{-1} \, d\beta_x(M) \right)$$

$$= \text{adj } \nabla u_\infty(x) \text{ w*limit adj } \{L^{-1}(x) + \nabla\varphi_n(x)\}^{-1}$$

$$= \text{adj } \nabla u_\infty(x) \det L(x) \text{ w*limit } \{L^{-1}(x) + \nabla\varphi_n(x)\}^T$$

$$= \text{adj } \nabla u_\infty(x) \det L(x) \{L^{-1}(x) + \nabla\varphi_\infty(x)\}^T$$

$$= \text{adj } L_\infty(x)$$

$$= \int_{M^{3x3}} \text{adj } M \, d\mu_x(M) .$$

4. RELAXATION OF THE BULK ENERGY.

If we are seeking for a mechanical theory asserting that crystal equilibria correspond to extremals of some energy functional then we must impose some constitutive assumptions on the corresponding volume energy density and we must decide if an energy difference can be assigned to pairs of configurations involving continuous distributions of defects. Now, the evolution of defects is commonly associated with plasticity and it should be regarded as an irreversible process in the sense of thermodynamics. In this context, then, there is a fundamental difficulty in prescribing well-defined state variables which have the properties commonly associated with the free energy and entropy densities. One might refer to ERICKSEN [13] for discussion of this, to RICOU [24] or to SERRIN [25] for helpful, relevant ideas. When no irreversible processes enter into consideration, free energy and entropy are well defined.

Recall that changes of state, here, are neutral (i. e. defect-preserving) or such as to alter the elastic invariant integrals (2.2), (2.4). We devote this section to studying the implications of an assertion that neutral deformations provide reversible processes, so that an associated energy density is well-defined (see also DAVINI & PARRY [10]). Assume, in addition that the free energy depends only on the local state $\Delta = \{L, \nabla L, \rho, \nabla\rho\}$ and the absolute temperature θ. Using Galilean invariance and excluding "second-grade" elasticity effects, DAVINI & PARRY [10] deduced that the free energy may be written variously as

$$W(L, \sigma/n, m, g\,;\theta) = \tilde{W}(L^TL, \sigma/n, m, g\,;\theta).$$

Henceforward we focus exclusively on states neutrally related to $\Sigma_0 = \{\Omega, \mathbb{1}, 1\}$ and we recall that such states are characterized explicitly in Corollary 2.10. Thus if $\Sigma = \{u(\Omega), L, \rho\}$ is neutrally related to Σ_0 then

$$L(u(x)) = \nabla u(x)\ \{\nabla v(x)\}^{-1},\ \det \nabla v(x) = 1 \quad \text{a. e. in } \Omega$$

for some Lipschitz mapping $v : \Omega \to \mathbb{R}^3$, and from Proposition 2.5

$$\sigma/n = 0,\ m = 1,\ g = 0 \quad \text{a. e. in } u(\Omega).$$

Under isothermal conditions, i. e. with θ constant, we abbreviate $W(L, 0, 1, 0; \theta)$ as $W(L)$ and we call it the *stored energy density* in state Σ. Then the total stored energy of that state is

$$I(\Sigma) := \int_{u(\Omega)} \rho(y)W(L(y))\,dy = \int_{\Omega} W(\nabla u(x)\{\nabla v(x)\}^{-1})\,dx,$$

the latter equality by conservation of mass and a change of variables.

We assume further that

i) $W \in C^1(M_+^{3x3}, \mathbb{R})$,

ii) $W(L) \to +\infty$ as $\det L \to 0^+$, $W(L) \geq 0$ and $W(\mathbb{1}) = 0$, (4.1)

iii) $W(L) = W(RLH)$, $R \in O_+(3)$, $H \in SL_3(\mathbb{Z})$. (4.2)

Note that ERICKSEN [14], FONSECA [15] and KINDERLEHRER [21] have based much work on perfect crystals on assumption iii). The motivation for assumption iii) here is a result of DAVINI & PARRY [11], that neutrally related states are locally elastically related.

We shall reckon that equilibria correspond to minimizers of I(.) and use corresponding necessary conditions to assess whether or not the rearrangements should really be allowed to compete in the class of admissible changes by comparison with what are seen as reasonable results in the context of plasticity. Said differently, we use these necessary conditions to judge if the neutral deformations are reversible.

We consider Dirichlet boundary conditions, where Σ is an admissible change if $\Sigma = \{u(\Omega), L, \rho\}$ with $L(u(x)) = \nabla u(x)\{\nabla v(x)\}^{-1}$, $(u, v) \in \mathscr{A}$ and

$$\mathscr{A}(u_0) := \{(u, v) \in W^{1,\infty}(\Omega, \mathbb{R}^3) \mid \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega,\ \det \nabla v = 1 \text{ a. e. in } \Omega\}.$$

This class includes the elastic deformations in the case where v is the identity map. Here $u_0 \in C(\overline{\Omega}, \mathbb{R}^3)$ is one-to-one in Ω. Using Lagrange multipliers, DAVINI & PARRY [10] showed that, independently of the boundary conditions and of the symmetry invariance, at a smooth local minimizer we must have

$$\int_\Omega L^T(x)\, S(L(x))\, dx = \alpha\, \mathbb{1}$$

where the first Piola-Kirchhoff stress tensor S and the Cauchy stress tensor T are given, respectively, by

$$S(F) := \frac{\partial W}{\partial F}(F) \text{ and } T(F) = \frac{1}{\det F} S(F)\, F^T \text{ for all } F \in M_+^{3x3}.$$

Hence, they concluded that there is a weakness in the crystal associated to the presence of slips and rearrangements, as the crystal cannot sustain certain nonzero average stresses. Also, using the material symmetry invariance (4.2), ERICKSEN [12] proved that for elastic crystals at equilibrium the Cauchy stress reduces to a pressure,

$$T = -p\mathbb{1} \qquad (4.3)$$

and later CHIPOT & KINDERLEHRER [3] recovered (4.3) still for elastic changes and when oscillations may develop. Precisely, they showed that if $\{\mu_x\}_{x\in\Omega}$ is the Young's measure corresponding to a minimizing sequence $L_n = \nabla u_n$, where $u_n \to u_\infty$ in $W^{1,\infty}$ weak *, then the average Cauchy stress is still a pressure,

$$\overline{T}(x) = \int_{M^{3x3}} T(M)\, d\mu_x(M)$$

$$= (g^{**})'(\det \nabla u_\infty(x))\, \mathbb{1} \quad \text{a. e. in } \Omega \qquad (4.4)$$

where g^{**} is the convex minorant of the *subenergy function* introduced by ERICKSEN and FLORY,

$$g(t) := \inf \{W(F) \mid \det F = t\}.$$

Here we will show that (4.4) still holds even when neutral changes of state are allowed to compete. Let $\Sigma_n = \{u_n(\Omega), L_n, \rho_n\}$ be a minimizing sequence for I(.). with $(u_n, v_n) \in \mathcal{A}(u_0)$ and

$$L_n(u_n(x)) = \nabla u_n(x)\{\nabla v_n(x)\}^{-1}.$$

Suppose further that $u_n \to u_\infty$ and $v_n \to v_\infty$ in $W^{1,\infty}$ weak *, which, by Theorem 3.2 imply that $L_n \to L_\infty = \nabla u_\infty \{\nabla v_\infty\}^{-1}$ in L^∞ weak *. Let $\{\mu_x\}_{x\in\Omega}$ be the Young's measure associated to $\{L_n\}$.

Theorem 4.1

$$\overline{T}(x) = \int_{M^{3x3}} T(M)\, d\mu_x(M)$$

$$= \frac{1}{\det L_\infty(x)} \overline{S}(x)\, L_\infty^T$$

$$=(g^{**})'(\det \nabla u_\infty(x))\, \mathbb{1} \quad \text{for almost all } x \in \Omega.$$

In order to prove this result we need to obtain the relaxation of the bulk energy functional.

Theorem 4.2.

Let $A \in M_+^{3x3}$ and let $\mathcal{A}(A) := \{(\xi, v) \in W^{1,\infty}(\Omega, \mathbb{R}^3) \times W^{1,\infty}(\Omega, \mathbb{R}^3) \mid \xi(x) = Ax$ on $\partial\Omega$, $\det \nabla v(x) = 1$ a. e. in $\Omega\}$. Then

$$\inf \{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi,v) \in \mathscr{A}(A)\} = \text{meas}\,(\Omega)\; g^{**}(\det A).$$

This result was proven by CHIPOT & KINDERLEHRER [3] and FONSECA [16] in the case where only elastic changes are admissible :

$$\inf \{ \int_\Omega W(\nabla\xi(x))\, dx \mid \xi \in Ax + W_0^{1,\infty}(\Omega, \mathbb{R}^3)\} = \text{meas}\,(\Omega)\, g^{**}(\det A). \qquad (4.5)$$

Proof of Theorem 4.2. Clearly, by (4.5)

$$\inf \{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi, v) \in \mathscr{A}(A)\} \leq$$

$$\inf \{ \int_\Omega W(\nabla\xi(x))\, dx \mid \xi \in Ax+W_0^{1,\infty}(\Omega, \mathbb{R}^3)\} = \text{meas}\,(\Omega)\, g^{**}(\det A)$$

and since det is a null lagrangian, by Jensen's inequality and as $W(F) \geq g^{**}(\det F)$ we have

$$\begin{aligned}\int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx &\geq \int_\Omega g^{**}(\det \nabla\xi(x)\, \det \nabla v(x)^{-1})\, dx \\ &= \int_\Omega g^{**}(\det \nabla\xi(x))\, dx \\ &\geq \text{meas}\,(\Omega)\, g^{**}(\frac{1}{\text{meas}(\Omega)} \int_\Omega \det \nabla\xi(x)\, dx\ ) \\ &= \text{meas}(\Omega)\;\, g^{**}(\det A).\end{aligned}$$

From Theorem 4.2 and using the same argument as in CHIPOT & KINDERLEHRER [3] we obtain the following generalization to the case of inhomogeneous boundary conditions.

Proposition 4.3.

If $u_0 \in C^1(\overline{\Omega}, \mathbb{R}^3)$ is such that either $\det \nabla u_0$ is constant in Ω or

$$\inf \{ \int_\Omega g^{**}(\det \nabla u(x))\, dx \mid u \in W^{1,\infty}(\Omega, \mathbb{R}^3),\ \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega\}$$

$$= \inf \{ \int_\Omega g^{**}(\det \nabla u(x))\, dx \mid u \in C^1(\overline{\Omega}, \mathbb{R}^3),\ \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega \}^6$$

then

$$\inf \{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi, v) \in \mathcal{A}(u_0) \} =$$

$$\inf \{ \int_\Omega g^{**}(\det \nabla u(x))\, dx \mid u \in W^{1,\infty}(\Omega, \mathbb{R}^3),\ \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega \}.$$

Proposition 4.4

Under the hypotheses of Proposition 4.3

1. $$\int_\Omega \overline{W}(x)\, dx = \int_\Omega \left(\int_{M^{3x3}} W(M)\, d\mu_x(M) \right) dx$$
$$\leq \inf \{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi, v) \in \mathcal{A}(u_0) \} ;$$

2. supp $\mu_x \subset M_+^{3x3}$ and $\det \nabla u_\infty > 0$ a. e. in Ω.

Proof. Part (1) is proven exactly as in CHIPOT & KINDERLEHRER [3] and (4.1) and (1) imply that supp $\mu_x \subset M_+^{3x3}$. Finally, by Theorem 3.2

$$\nabla u_\infty(x)\, \{\nabla v_\infty(x)\}^{-1} = L_\infty(x)$$
$$= \int_{M^{3x3}} M\, d\mu_x$$

which, together with Proposition 3.7 (1), yields

$$\det \nabla u_\infty(x) = \int_{M^{3x3}} \det M\, d\mu_x > 0 \quad \text{a. e. in } \Omega.$$

Corollary 4.5

Under the hypotheses of Proposition 4.3

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[6]Using Jensen's inequality, it is easy to check that this hypothesis is satisfied if, as an example, $\det \nabla u_0$ = const. a. e. in Ω.

$$\inf \left\{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi, v) \in \mathcal{A}(u_0) \right\} = \int_\Omega g^{**}(\det \nabla u_\infty(x))\, dx.$$

Proof. Using the same argument as in CHIPOT & KINDERLEHRER [3], by Proposition 4.4 we have $\det \nabla u_\infty > 0$ a. e. in Ω and so, since g is convex and $\det \nabla u_n \rightarrow \det \nabla u_\infty$ weakly *, by Proposition 4.3 we conclude that

$$\begin{aligned} \inf \left\{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi, v) \in \mathcal{A}(u_0) \right\} &\leq \int_\Omega g^{**}(\det \nabla u_\infty(x))\, dx \\ &\leq \liminf \int_\Omega g^{**}(\det \nabla u_n(x))\, dx \\ &\leq \liminf \int_\Omega W(L_n(x))\, dx \\ &= \inf \left\{ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\, dx \mid (\xi, v) \in \mathcal{A}(u_0) \right\}. \end{aligned}$$

Proposition 4.6

Under the hypotheses of Proposition 4.3

1. $\overline{W}(x) = \overline{g}(x) = \overline{g^{**}}(x) = g^{**}(\det \nabla u_\infty(x))$ a. e. in Ω ;
2. $\operatorname{supp} \mu_x \subset \{M \in M_+^{3x3} \mid \alpha(x) \leq \det M \leq \beta(x)\}$ where $[\alpha(x), \beta(x)]$ is the maximal closed interval containing $\det \nabla u_\infty(x)$ on which g^{**} is affine ;
3. $W(M) = g(\det M) = g^{**}(\det M)$ a. e. in $\operatorname{supp} \mu_x$.

Proof. The argument is essentially the same as in CHIPOT & KINDERLEHRER [3], where we must use Proposition 3.7 (1).

Finally, we give the proof of Theorem 4.1.

Proof of Theorem 4.1. By Proposition 4.6 (3), if $M \in \operatorname{supp} \mu_x$ then

$$0 = W(M) - g^{**}(\det M) = \min \{W(.) - g^{**}(\det .)\}$$

and so

$$0 = \frac{\partial W}{\partial M}(M) - (g^{**})'(\det M) \operatorname{adj} M.$$

Also, by Proposition 4.6 (2)

$$(g^{**})'(\det M) = (g^{**})'(\det \nabla u_\infty(x))$$

and we deduce that

$$S(M) = (g^{**})'(\det \nabla u_\infty(x)) \operatorname{adj} M, \tag{4.6}$$

hence, by Proposition 3.7 (2),

$$\begin{aligned} \overline{S}(x) &= \int_{M^{3x3}} (g^{**})'(\det \nabla u_\infty(x)) \operatorname{adj} M \, d\mu_x(M) \\ &= (g^{**})'(\det \nabla u_\infty(x)) \operatorname{adj} L_\infty(x). \end{aligned} \tag{4.7}$$

Finally, by (4.6) and for almost all $x \in \Omega$

$$\begin{aligned} \overline{T}(x) &= \int_{M^{3x3}} T(M) \, d\mu_x(M) = \int_{M^{3x3}} \frac{1}{\det M} S(M) M^T d\mu_x(M) \\ &= (g^{**})'(\det \nabla u_\infty(x)) \int_{M^{3x3}} \frac{1}{\det M} \operatorname{adj}M \, M^T d\mu_x(M) \\ &= (g^{**})'(\det \nabla u_\infty(x)) \, \mathbb{1} \end{aligned}$$

and by (4.7)

$$\begin{aligned} \frac{1}{\det L_\infty(x)} \overline{S}(x) L_\infty^T &= \frac{1}{\det L_\infty(x)} (g^{**})'(\det \nabla u_\infty(x)) \operatorname{adj} L_\infty(x) L_\infty^T \\ &= (g^{**})'(\det \nabla u_\infty(x)) \, \mathbb{1}. \end{aligned}$$

5. PENALIZED VARIATIONAL PROBLEM.

As shown in Theorem 4.1, including neutrally related states as admissible changes seems to render the material weak as it cannot sustain nonzero average shear stresses. We take this as an indication that the neutral deformations are irreversible, indeed this is reasonable since slip along glide planes (which provides neutral deformations by Example $(2.11)_4$) surely involves some kind of dissipation due to friction. So we contemplate problems where the slip, represented by v, is penalised. Now, minimizing E(.,.) corresponds, formally, to a variational problem involving variation of the domain. Indeed, if v was an invertible mapping then

$$I(\Sigma) = \int_{v(\Omega)} W(\nabla\omega(y))\, dy$$

where

$$\omega(y) := u \circ v^{-1}(y).$$

If the solid attained equilibrium at an elastic state then $v(\Omega)$ would be a translation of Ω, i. e. $v(x) = x + \text{Const}$. In this section, we will consider an energy functional were we penalize the boundary $v(\Omega)$ in order to obtain some information regarding the prefered shape for $v(\Omega)$.

Suppose that $u_0 \in C^1(\overline{\Omega}\,;\mathbb{R}^3)$ is one-to-one in Ω and $\det \nabla u_0(x) > 0$ in Ω. Suppose further that

$$\int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx \leq \int_{\Omega} g^{**}(\det \nabla u(x))\, dx \tag{5.1}$$

for all $u \in u_0 + W^{1,\infty}(\Omega\,;\mathbb{R}^3)$. Note that, by Jensen's inequality and using the fact that $F \to \det F$ is a null lagrangian, (5.1) is trivially satisfied if $\det \nabla u_0 = \text{constant}$. Consider the energy functional

$$\tilde{I}(\Sigma) = \tilde{E}(u, v) := \int_{\Omega} W(\nabla u(x)\{\nabla v(x)\}^{-1})\, dx + \int_{\partial^* v(\Omega)} \Gamma(\nu(x))\, dH_2(x)$$

where $(u, v) \in \mathscr{A}^*(u_0) := \{(u, v) \in W^{1,\infty}(\Omega, \mathbb{R}^3) \mid \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega,$

$\det \nabla v = 1 \text{ a. e. in } \Omega,\ \text{meas } v(\Omega) = \text{meas } \Omega\}$,

$\partial^* v(\Omega)$ denotes the reduced boundary of $v(\Omega)$, $\nu(x)$ is the outer unit normal to the boundary of $v(\Omega)$, Γ is the Lipschitz anisotropic surface energy density and H_2 is the two-dimensional Hausdorff measure.

Remark 5.1

1. $\tilde{I}(\Sigma)$ does not depend on the representation (u, v) of Σ. Indeed, by Corollary 2.15 if $(\tilde{u}, \tilde{v})$ is another representation of Σ then

$$v(x) = \tilde{v}(f(x)) + \text{Cont. a. e. in } \Omega.$$

where

$f(x) = x$ on $\partial\Omega$ and $\det \nabla f(x) = 1$ a. e. in Ω.

Hence,

$v(\Omega)$ is a translation of $\tilde{v}(\Omega)$

and so

$\tilde{E}(u, v) = \tilde{E}(\tilde{u}, \tilde{v})$.

2. On the definition of $\mathcal{A}^*(u_0)$, v is subject to the constraints $\det \nabla v = 1$ a. e. in Ω and meas $v(\Omega)$ = meas (Ω). These conditions imply that v is invertible a. e. in Ω and $v^{-1} \in W^{1,\infty}(\Omega ; \mathbb{R}^3)$ (see BALL [2]). Without this invertibility assumption on v, it would be possible to find a sequence $\{v_n\}$ of Lipschitz functions with $\det \nabla v_n(x) = 1$ a. e. in Ω and $Per(v_n(\Omega)) \to 0$. In particular, meas $v_n(\Omega) \to 0$ and

$$\int_{\partial^* v_n(\Omega)} \Gamma(v(x))\, dH_2(x) \to 0.$$

Indeed, by a result of MARCUS & MIZEL [22], if $\det \nabla v = 1$ a. e. in Ω then vol $(\Omega) \leq$ meas (Ω) and it is possible to have strict inequality. In fact, let $\Omega = B(0, R) \subset \mathbb{R}^2$, define in polar coordinates

$$v(r,\theta) := \left(\frac{r}{\sqrt{2}}, 2\theta\right)$$

and assume that v_n is obtained by composing v with itself n times,

$$v_n := v \circ v \ldots v \circ v : B(0, R) \to B\left(0, \left(\frac{R}{\sqrt{2}}\right)^n\right).$$

It is easy to verify that $v_n \to 0$ in $W^{1,\infty}$ weak *, $\det \nabla v_n = 1$ a. e. and, clearly,

$$Per\left(B\left(0, \left(\frac{R}{\sqrt{2}}\right)^n\right)\right) \to 0.$$

It is well known (see HERRING [20], FONSECA [17], FONSECA & MÜLLER [18], TAYLOR [28], [29], [30], WULFF [31]) that the shape that minimizes the surface energy

$$\int_{\partial^* A} \Gamma(v)\, dH_2$$

among all sets A of finite perimeter with constant volume, meas A = meas Ω, is the dilation λC of the Wulff set C, where

$$\lambda := \sqrt[3]{\frac{\text{meas } \Omega}{\text{meas } C}}$$

and

$C := \{x \in \mathbb{R}^3 | \, x.n \le \Gamma(n)$ for all unit vector $n\}$.

In what follows, we assume that

(H) Ω is a bounded, open, star-shaped domain[7] with respect to $x_0 \in \text{int}\, \Omega$, $B(x_0, \varepsilon) \subset \Omega$ for some $\varepsilon > 0$, there exists a finite partition of Ω, $\Omega = \Omega_1 \cup \Omega_2 \cup .... \cup \Omega_p$, such that Ω_i is a cone with vertex at x_0, $\partial(\Omega_i) \cap \partial\Omega \in C^1$, $B(x_0, \varepsilon) \cap \Omega_i$ is convex for all $i = 1, ..., p$. Further, we assume that there exist $\alpha > 0$ such that $\nu(x).x \ge \alpha$ for all $x \in \partial\Omega$, where $\nu(x)$ denotes the outward unit normal to $\partial\Omega$ at x.

Also, without loss of generality we can suppose that $\text{meas}(\Omega) = \text{meas}(C)$.

Theorem 5.2.

Let $u_0 \in C^1(\overline{\Omega}\, ; \mathbb{R}^3)$, be such that $\det \nabla u_0(x) > 0$ in Ω and u_0 satisfies (5.1). If C and Ω satisfy the condition (H)[8] then

$$\inf \{\tilde{E}(u, v) \mid (u, v) \in \mathcal{A}^*(u_0)\} = \int_\Omega g^{**}(\det \nabla u_0(x))\, dx + \int_{\partial^* C} \Gamma(\nu(x))\, dH_2(x).$$

The proof of Theorem 5.2 relies on the following two results.

Proposition 5.3.

If $y_0 \in C^1(\overline{\Omega}\, ; \mathbb{R}^3)$ is such that $\det \nabla y_0(x) > 0$ in Ω and if $y \in C^1(\overline{\Omega}\, ; \mathbb{R}^3)$ verifies $y = y_0$ on $\partial\Omega$ then

$$\inf\{ \int_\Omega W(\nabla u(x))\, dx \mid u \in y_0 + W^{1,\infty}(\Omega\, ; \mathbb{R}^3)\} \le \int_\Omega g^{**}(\det \nabla y(x))\, dx.$$

Proof. It is included in the proof of Theorem 4.1 in CHIPOT & KINDERLEHRER [3].

---

[7]We say that Ω is *star-shaped* with respect to an interior point $x_0 \in \Omega$ if any ray with origin at x_0 has a unique common point with the boundary $\partial\Omega$.

[8]In general, the Wulff set C for solid crystals is a polyhedron.

Theorem 5.4

If Ω and Ω' satisfy (H) and if meas(Ω) = meas(Ω') then there exists $v \in W^{1,\infty}(\Omega,\Omega')$ such that $v(\Omega) = \Omega'$, det $\nabla v = 1$ a. e. in Ω, v is invertible and $v \in C^1(\overline{U}_i)$ for some finite partition of Ω into strongly Lipschitz domains $\{U_i\}$.

Using these results we prove Theorem 5.2, and then devote the rest of this section to proving Theorem 5.4.

Proof of Theorem 5.2. By (5.1) and Proposition 4.3 we have

$$\tilde{E}(u, v) := \int_\Omega W(\nabla u(x)\{\nabla v(x)\}^{-1})\, dx + \int_{\partial^* v(\Omega)} \Gamma(v(x))\, dH_2(x)$$

$$\geq \int_\Omega g^{**}(\det \nabla u_0(x))\, dx + \int_{\partial^* C} \Gamma(v(x))\, dH_2(x). \tag{5.2}$$

On the other hand, using Theorem 5.4 let $v \in W^{1,\infty}(\Omega,C)$ be such that $v(\Omega) = C$, det $\nabla v = 1$ a. e. in Ω, v is invertible and $v \in C^1(\overline{\Omega}_i)$ for some finite partition of Ω into strongly Lipschitz domains $\{\Omega_i\}_{i=1,\dots p}$. Clearly, $u_0 \circ v^{-1} \in C^1(\overline{v(\Omega_i)})$ and so, by Proposition 5.3 and changing variables

$$\inf \{ \int_{v(\Omega_i)} W(\nabla w(z))\, dz \mid w \in W^{1,\infty}(v(\Omega_i)),\ \det \nabla w > 0 \text{ a. e.},\ w = u_0 \circ v^{-1} \text{ on } \partial v(\Omega_i)\}$$

$$\leq \int_{v(\Omega_i)} g^{**}(\det\nabla(u_0 \circ v^{-1})(z))\, dz$$

$$= \int_{\Omega_i} g^{**}(\det \nabla u_0(x))\, dx.$$

Fix $\varepsilon > 0$ and let $w_i \in W^{1,\infty}(v(\Omega_i))$, be such that det $\nabla w > 0$ a. e., $w = u_0 \circ v^{-1}$ on $\partial v(\Omega_i)$ and

$$\int_{v(\Omega_i)} W(\nabla w_i(z))\, dz \leq \int_{\Omega_i} g^{**}(\det \nabla u_0(x))\, dx + \varepsilon. \tag{5.3}$$

Let $w(z) = \sum_{i=1}^{p} \chi_{v(\Omega_i)}(z)\, w_i(z)$ if $z \in C$, where χ_A denotes the characteristic function of the set A. Clearly $w \in W^{1,\infty}(C)$, det $\nabla w > 0$ a. e. in Ω, $w = u_0 \circ v^{-1}$ on ∂C and by (5.3)

$$\int_C W(\nabla w(z))\, dz = \sum_{i=1}^{p} \int_{v(\Omega_i)} W(\nabla w_i(z))\, dz$$

$$\leq \sum_{i=1}^{p} \int_{\Omega_i} g^{**}(\det \nabla u_0(x))\, dx + p\varepsilon$$

$$= \int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx + p\varepsilon.$$

Thus, letting $\varepsilon \to 0^+$ we deduce that

$$\inf \{ \int_{v(\Omega)} W(\nabla w(z))\, dz \mid w \in W^{1,\infty}(v(\Omega)),\ \det \nabla w > 0 \text{ a. e. and } w = u_0 \circ v^{-1} \text{ on } \partial v(\Omega)\}$$

$$\leq \int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx \qquad (5.4)$$

and, by (5.2) and changing variables we have with $u = w \circ v$

$$\int_{v(\Omega)} W(\nabla w(z))\, dz = \int_{\Omega} W(\nabla w(v(x)))\, dx$$

$$= \int_{\Omega} W(\nabla u(x)\{\nabla v(x)\}^{-1})\, dx$$

$$\geq \int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx$$

which, together with (5.4) yields

$$\inf \{ \int_{v(\Omega)} W(\nabla w(z))\, dz \mid w \in W^{1,\infty}(v(\Omega)),\ \det \nabla w > 0 \text{ a. e. and } w = u_0 \circ v^{-1} \text{ on } \partial v(\Omega)\}$$

$$= \int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx.$$

Let $w_k \in W^{1,\infty}(v(\Omega))$ be such that $\det \nabla w_k > 0$ a. e., $w_k = u_0 \circ v^{-1}$ on $\partial v(\Omega)$ and

$$\int_{v(\Omega)} W(\nabla w_k(z))\, dz \to \int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx$$

and set $u_k := w_k \circ v$. We conclude that

$$\tilde{E}(u_k, v) := \int_{\Omega} W(\nabla u_k(x)\{\nabla v(x)\}^{-1})\, dx + \int_{\partial^* v(\Omega)} \Gamma(\nu(x))\, dH_2(x)$$

$$= \int_{v(\Omega)} W(\nabla w_k(z))\, dz + \int_{\partial^* C} \Gamma(\nu(x))\, dH_2(x)$$

$$\to \int_{\Omega} g^{**}(\det \nabla u_0(x))\, dx + \int_{\partial^* C} \Gamma(\nu(x))\, dH_2(x)$$

and by (5.2) the result is proven.

Next, assume that Ω satisfies (H) and we suppose without loss of generality that $x_0 = 0$, $\overline{B}(0, \varepsilon) \subset\subset \Omega \subset\subset \overline{B}(0, 1/\varepsilon)$ for some $\varepsilon < 1$. Let

$$\mu(x) := \inf \{t > 0 \mid x \in t\Omega\}$$

be the Minkowski functional of Ω.

Lemma 5.5

1. μ is homogeneous of degree one, i. e. $\mu(tx) = t\,\mu(x)$ if $t > 0$;

2. μ is continuous.

Proof. 1. is trivial.

2.Since $\overline{B}(0, \varepsilon) \subset\subset \Omega \subset\subset \overline{B}(0, 1/\varepsilon)$ we have

$$\varepsilon\|x\| \leq \mu(x) \leq 1/\varepsilon\, \|x\| \tag{5.5}$$

for all $x \in \mathbb{R}^N$. Then, if $x_n \to 0$ it follows from (5.5) that $\mu(x_n) \to 0 = \mu(0)$. Suppose that $x_n \to x^* \neq 0$. By (5.5), $\{\mu(x_n)\}$ is a bounded sequence and we can assume that $\mu(x_n) \to \alpha > 0$. Since

$$\frac{x_n}{\mu(x_n)} \in \partial\Omega$$

we have

$$\frac{x^*}{\alpha} \in \partial\Omega.$$

So

$$\frac{x^*}{\mu(x^*)}, \frac{x^*}{\alpha} \in \partial\Omega \text{ and they lie on the same ray through the origin}$$

hence

$$\alpha = \mu(x^*).$$

Lemma 5.6

$\mu \in W^{1,\infty}(\mathbb{R}^N)$.

Proof. We want to show that

$$|\mu(x) - \mu(y)| \le K \|x - y\| \quad \text{for all } x, y \in \mathbb{R}^N, \text{ and for some } K > 0. \tag{5.6}$$

(i) Using hypothesis (H) we start by proving that

$$\mu \in C^1(\Omega_i \setminus \{0\}) \text{ for all } i = 1, ..., p.$$

As $\partial(\Omega_i) \cap \partial\Omega \in C^1$, there exists $\varphi_i \in C^1$(closure of the convex envelope of Ω_i) such that if $x \in \partial(\Omega_i) \cap \partial\Omega$ then $\varphi_i(x) = 0$ and $0 \neq \nabla\varphi_i(x)$ is parallel to the normal to $\partial\Omega$ at x. Thus, as Ω is star-shaped,

$$\nabla\varphi_i(x) \,.\, x \neq 0 \text{ if } x \in \partial\Omega_i \cap \partial\Omega. \tag{5.7}$$

Let $x_0 \in \Omega_i \setminus \{0\}$, with $B(x_0, \delta) \subset \Omega_i \setminus \{0\}$. For t small enough,

$$\frac{x_0 + te_k}{\mu(x_0+te_k)} \in \partial\Omega_i \cap \partial\Omega$$

and so, by the mean-value theorem

$$\begin{aligned} 0 &= \frac{1}{t} \left[\varphi_i\left(\frac{x_0 + te_k}{\mu(x_0+te_k)}\right) - \varphi_i\left(\frac{x_0}{\mu(x_0)}\right) \right] \\ &= \frac{1}{t} \nabla\varphi_i(y_t). \left[\frac{x_0 + te_k}{\mu(x_0+te_k)} - \frac{x_0}{\mu(x_0)} \right] \\ &= \frac{1}{t\, \mu(x_0+te_k)\, \mu(x_0)} \nabla\varphi_i(y_t). \left[te_k\, \mu(x_0) - (\mu(x_0 + te_k) - \mu(x_0))\, x_0\right] \\ &= \frac{\nabla\varphi_i(y_t).e_k}{\mu(x_0+te_k)} - \frac{\nabla\varphi_i(y_t).x_0}{\mu(x_0+te_k)\mu(x_0)} \frac{\mu(x_0 + te_k) - \mu(x_0)}{t}, \end{aligned} \tag{5.8}$$

where $y_t \to \dfrac{x_0}{\mu(x_0)}$ as $t \to 0$. Hence, as by (5.7) and by the continuity of $\nabla\varphi_i$ we have

$$\nabla\varphi_i(y_t).x_0 \neq 0,$$

by (5.8) we deduce that

$$\frac{\mu(x_0 + te_k) - \mu(x_0)}{t} = \frac{\nabla\varphi_i(y_t).e_k}{\nabla\varphi_i(y_t).x_0/\mu(x_0)}.$$

Therefore μ is differentiable at x_0 and

$$\nabla\mu(x_0) = \frac{\nabla\varphi_i\left(\frac{x_0}{\mu(x_0)}\right)}{\nabla\varphi_i\left(\frac{x_0}{\mu(x_0)}\right).\frac{x_0}{\mu(x_0)}}.$$

Finally, by (H)

$$\|\nabla\mu(x_0)\| = \frac{1}{\nu\left(\frac{x_0}{\mu(x_0)}\right) . \frac{x_0}{\mu(x_0)}} \le \frac{1}{\alpha}. \tag{5.9}$$

(ii) If x = 0 then by (5.5) we have

$$|\mu(x) - \mu(y)| = \mu(y) \leq 1/\varepsilon \|y\| = 1/\varepsilon \|x - y\|.$$

(iii) If $x, y \in \Omega_i \cap B(0, \varepsilon)$ and $x \neq 0 \neq y$ then (5.6) follows from the mean value theorem and (5.9),

$$|\mu(x) - \mu(y)| \leq K_i \|x - y\|.$$

By the continuity of μ (see Lemma 5.5 (2)) and by (ii), this result still holds if $x, y \in \overline{\Omega}_i \cap \overline{B}(0, \varepsilon)$.

(iv) Suppose now that $x, y \in \overline{B}(0, \varepsilon) \subset\subset \Omega$ and $x \in \overline{\Omega}_i$, $y \in \overline{\Omega}_j$ where Ω_i and Ω_j are adjacent. The segment determined by x and y intersects $\partial\Omega_i \cap \partial\Omega_j$ at a point z and so by (iii) we deduce that

$$|\mu(x) - \mu(y)| \leq |\mu(x) - \mu(z)| + |\mu(z) - \mu(y)|$$

$$\leq (K_i + K_j) [\|x - z\| + \|z - y\|]$$

$$= (K_i + K_j) \|x - y\|.$$

We conclude that if $x, y \in \overline{B}(0, \varepsilon)$ then

$$|\mu(x) - \mu(y)| \leq (K_1 + ... + K_p) \|x - y\|.$$

(v) Finally, if $x, y \in \mathbb{R}^N$ choose R large enough so that

$$\|x\|, \|y\| \leq R.$$

Then by Lemma 5.5 (1) and by (iv)

$$\frac{\varepsilon}{R} |\mu(x) - \mu(y)| = |\mu(\frac{\varepsilon x}{R}) - \mu(\frac{\varepsilon y}{R})|$$

$$\leq (K_1 + ... + K_p) \| \frac{\varepsilon x}{R} - \frac{\varepsilon y}{R} \|,$$

i. e.

$$|\mu(x) - \mu(y)| \leq K \|x - y\|.$$

Lemma 5.7

If Ω satisfies (H) and if meas (Ω) = meas B(0, 1) then there exists $\omega : B(0, 1) \to \Omega$ such that

1. $\omega \in W^{1,\infty} (B(0, 1); \Omega)$;

2. $\omega(B(0, 1)) = \Omega$;

3. det $\nabla\omega \in W^{1,\infty}(B(0, 1))$, det $\nabla\omega \geq \alpha$ a. e. in $B(0, 1)$, for some $\alpha > 0$;

4. ω is invertible, $\omega^{-1} \in W^{1,\infty}$ and $\nabla\omega^{-1}(y) = (\nabla\omega(\omega^{-1}(y)))^{-1}$ a. e. $y \in \Omega$.

Proof. Choose M large enough so that

$$B(0, 1) \subset\subset M\Omega.$$

Consider a cut-off function $\eta \in C([0, \infty))$ such that $0 \leq \eta \leq 1$, $\eta(t) = 1$ if $0 \leq t \leq 1/4$, $\eta(t) = 0$ if $t \geq 1/2$, $\eta'(t) < 0$ if $1/4 < t < 1/2$, define

$$\phi(x) := \eta(\|x\|)$$

and set

$$\bar{\omega}(x) := \phi(x)x + (1 - \phi(x))\frac{\|x\| \, x}{\mu(x)}$$

where

$$\mu(x) := \inf \{t > 0 \mid x \in tM\Omega\}$$

is the Minkowski functional of $M\Omega$ (note that $M\Omega$ still satisfies (H)). By (5.5) there exists $\beta > 0$ such that

$$\beta \leq \frac{\|x\|}{\mu(x)} \leq 1/\beta \quad \text{if } x \neq 0 \tag{5.10}$$

and define

$$F(x) := \frac{\|x\| \, x}{\mu(x)} \quad \text{if } x \neq 0, \ F(0) = 0.$$

We claim that

$$F : B(0, 1) \to M\Omega.$$

Indeed, if $\|x\| \leq 1$ then $\mu(F(x)) = \|x\| \leq 1$, i. e. $F(x) \in M\Omega$. Therefore, if $1 \geq \|x\| > 1/2$ then $\bar{\omega}(x) = F(x) \in M\Omega$ and if $\|x\| \leq 1/2$ then $x \in B(0, 1) \subset M\Omega$, $F(x) \in M\Omega$ and so, as $M\Omega$ is star-shaped with respect to the origin, $\bar{\omega}(x) \in M\Omega$. We conclude that

$$\bar{\omega} : B(0, 1) \to M\Omega.$$

Moreover, F is a bijection with inverse function given by

$$F^{-1}(y) = \frac{\mu(y)y}{\|y\|} \text{ if } y \neq 0, \ F^{-1}(y) = 0 \text{ if } y = 0$$

and F is a Lipschitz function, where by Lemma 5.6

$$\nabla F(x) = \frac{\|x\|}{\mu(x)}\left[\mathbb{1} + x\otimes\left(\frac{x}{\|x\|^2} - \frac{\nabla\mu(x)}{\mu(x)}\right)\right] \quad \text{if } x \neq 0. \tag{5.11}$$

By Lemma 5.5 (1), μ is homogeneous of degree one and so

$$\nabla\mu(x).x = \mu(x) \text{ a. e. in } \mathbb{R}^N \tag{5.12}$$

which implies that

$$\det \nabla F(x) = \left(\frac{\|x\|}{\mu(x)}\right)^N. \tag{5.13}$$

Hence

$$\bar{\omega} \in W^{1,\infty}(B(0, 1); M\Omega). \tag{5.14}$$

Also, if $x \neq 0$ then

$$\nabla\bar{\omega}(x) = G(x)[\mathbb{1} + G^{-1}(x)(x - F(x))\otimes\nabla\phi(x)]$$

where

$$G(x) := \phi(x)\,\mathbb{1} + (1 - \phi(x))\nabla F(x).$$

From (5.11), (5.12) and (5.13) it follows that

$$\det G(x) = \left[\phi(x) + (1 - \phi(x))\frac{\|x\|}{\mu(x)}\right]^N$$

and so

$$\begin{aligned}\det \nabla\bar{\omega}(x) &= \left[\phi(x) + (1 - \phi(x))\frac{\|x\|}{\mu(x)}\right]^N.\left[1 + G^{-1}(x)(x - F(x)).\eta'(\|x\|)\frac{x}{\|x\|}\right]\\ &= \left[\phi(x) + (1 - \phi(x))\frac{\|x\|}{\mu(x)}\right]^N.\left[1 + \frac{\|x\|}{\phi(x)\mu(x)+(1-\phi(x))\|x\|}\,\eta'(\|x\|)(\mu(x) - \|x\|)\right]\\ &\geq \left[\phi(x) + (1 - \phi(x))\frac{\|x\|}{\mu(x)}\right]^N\end{aligned}$$

because $\eta' \leq 0$ and, as $x/\|x\| \in \bar{B}(0, 1) \subset M\Omega$, $\mu(x/\|x\|) \leq 1$, i. e. $\mu(x) - \|x\| \leq 0$. By Lemma 5.6 and by (5.10) we conclude that

$$\det \nabla\bar{\omega}(x) \in W^{1,\infty}(B(0, 1)) \text{ and } \det \nabla\bar{\omega}(x) \geq \bar{\alpha} := \min\{1, \beta\}^N. \tag{5.15}$$

Next, we show that

$$\bar{\omega} \text{ is invertible, } \bar{\omega}^{-1} \in W^{1,\infty} \text{ and } \nabla\bar{\omega}^{-1}(y) = (\nabla\bar{\omega}(\bar{\omega}^{-1}(y)))^{-1} \text{ a. e. } y \in M\Omega. \tag{5.16}$$

Indeed, if ω^* denotes the restriction of $\bar{\omega}$ to $B(0, 1/2)$ then ω^* is a Lipschitz function with Jacobian bounded away from zero and $\omega^*(x) = F(x)$ if $x \in \partial B(0, 1/2)$, where $F(.)$ is a one-to-one and continuous function. Thus (see BALL [2]), ω^* admits an inverse function $g \in W^{1,p}(F(B(0,1/2), B(0,1/2)), p > N$, with

$$\nabla g(y) = (\nabla\bar{\omega}(\bar{\omega}^{-1}(y)))^{-1}$$
$$= \frac{1}{\det \nabla\bar{\omega}(x)} \operatorname{adj}\nabla\bar{\omega}\,(x)^T \qquad \text{for } x = g(y),$$

which, by (5.15), implies that $g \in W^{1,\infty}(F(B(0,1/2), B(0,1/2))$. We deduce that (5.16) holds, where

$$\bar{\omega}^{-1}(y) := \begin{cases} F^{-1}(y) & \text{if } y \notin F(B(0,\ 1/2)) \\ g(y) & \text{if } y \in F(B(0,\ 1/2)) \end{cases} .$$

Note that if $\|x\| = 1/2$, $y = F(x)$ then

$$g(y) = g(\bar{\omega}(x)) = x = F^{-1}(y).$$

The result now follows from (5.14), (5.15) and (5.16) setting $\omega(x) : = \frac{\bar{\omega}(x)}{M}$.

Remark 5.8

It follows immediately from Lemmas 5.5 and 5.6 that $\omega \in C(\bar{B}_i)$ where $B_i := M\Omega_i \cap B(0,1)$.

Proof of Theorem 5.4. Let Ω and Ω' satisfy (H), $\text{meas}(\Omega) = \text{meas}(\Omega') = \text{meas}(B(0,1))$. Choose $\omega : B(0,\ 1) \to \Omega$ as in Lemma 5.7 and define

$$f(x) := \det \nabla\omega(x).$$

Then f is a Lipschitz function bounded away from zero and as ω is invertible we have

$$\int_{B(0,1)} f(x)\,dx = \int_{B(0,1)} \det \nabla\omega(x)\,dx$$
$$= \text{meas}\,(\omega(B(0,\ 1))$$
$$= \text{meas}\,\Omega$$
$$= \text{meas}\,(B(0,\ 1)).$$

Therefore (see DACOROGNA & MOSER [8]), there exists $u \in \text{Diff}^{1,\alpha}(\bar{B}(0,\ 1)), \bar{B}(0,\ 1)))$, with $0 < \alpha < 1$, such that

$$\begin{cases} \det \nabla u(x) = f(x) & \text{in } B(0, 1) \\ u(x) = x & \text{on } \partial B(0, 1) \end{cases}.$$

Set

$$\xi(x) := u \circ \omega^{-1}(x) \quad \text{for } x \in \Omega.$$

By Lemma 5.7 the function ξ is invertible, $\xi \in W^{1,\infty}(\Omega, B(0, 1))$ and

$$\nabla\xi(x) = \nabla u(\omega^{-1}(x)) \{\nabla\omega(\omega^{-1}(x))\}^{-1}.$$

Thus for a. e. $x \in \Omega$

$$\det \nabla\xi(x) = f(\omega^{-1}(x)) \frac{1}{f(\omega^{-1}(x))}$$

$$= 1.$$

Note also that ξ^{-1} is a Lipschitz mapping with $\nabla\xi^{-1}(y) = \{\nabla\xi(\xi^{-1}(y))\}^{-1}$ for almost all y.

In a similar way, construct $\xi' \in W^{1,\infty}(\Omega', B(0, 1))$, bijection, such that

$$\det \nabla\xi'(x) = 1 \quad \text{a. e. } x \in \Omega'.$$

Setting

$$v := \xi'^{-1} \circ \xi \in W^{1,\infty}(\Omega, \Omega'),$$

it follows that $v(\Omega) = \Omega'$, $\det \nabla v = 1$ a. e. in Ω and v is invertible. Finally, by Remark 5.8 we deduce that $v \in C^1(\overline{U}_i)$ for some finite partition of Ω into strongly Lipschitz domains $\{U_i\}$.

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A special class of defect preserving deformations in solid crystals, the neutral deformations, is studied. Using the theory of compensated compactness it is shown that neutral deformations are closed with respect to weak convergence and a variational analysis of such states is undertaken. In particular, by means of the div-curl lemma minimizing sequences and their respective Young's probability measures are characterized.

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