REMARKS ON VARIATIONAL PROBLEMS
FOR DEFECTIVE CRYSTALS

by

Irene Fonseca
Department of Mathematics
Carnegie Mellon University
Pittsburgh, PA 15213

and

Gareth Parry
University of Bath
School of Mathematical Sciences
Bath, Avon, BA2 7AY, U.K.

WORKSHOP ON CALCULUS OF VARIATIONS AND
NONLINEAR MATERIAL BEHAVIOR
November 1-4, 1990

REMARKS ON VARIATIONAL PROBLEMS FOR DEFECTIVE CRYSTALS

IRENE FONSECA

Department of Mathematics, Carnegie Mellon University

Pittsburgh, Pennsylvania 15213, U. S. A.

and

GARETH PARRY

University of Bath, School of Mathematical Sciences

Claverton Down

Bath, Avon, BA2 7AY, U. K.

Table of Contents :

1. INTRODUCTION.

In this work we assume that we are dealing with slightly defective crystals, i. e. crystals exhibiting so few defects that a lattice is distinguishable at the microscopic scale. A (perfect) *crystal* is a discrete array of identical atoms arranged in a periodic way and filling the space $\mathbb{R}^3$, precisely there exist lattice vectors a_1, a_2, a_3 with corresponding lattice matrix L such that $Le_i = a_i$ for i = 1, 2, 3[1] and the position vector of any atom is given by

$$x = m_1 a_1 + m_2 a_2 + m_3 a_3$$

with m_1, m_2, $m_3 \in \mathbb{Z}$. Clearly L is not unique and L' is another lattice matrix 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 [7], FONSECA [8], KINDERLEHRER [12]). A *defective crystal* is an array of atoms that cannot be mapped globally onto a space lattice, being such operation possible only locally and perhaps with the exclusion of some atoms. In this case the lattice vectors are actually averages over microscopic regions.

To connect the microscopic and macroscopic behaviors of the material, DAVINI [3] and in subsequent work DAVINI & PARRY [4], [5] introduced the kinematics of a model for defective crystals where the notion of defect relies on the assumption that deformations that leave a certain class of elastic invariants unchanged preserve the defectiveness. Within this theory, we take the viewpoint that equilibria correspond to minimizers of an energy functional

$$I(L) := \int_\Omega W(L(x)) \, dx$$

where L is a lattice matrix corresponding to a defect-preserving deformation of a perfect crystal with reference configuration Ω, and W represents the bulk energy density, which, due to (1.1) and to frame indifference, satisfies the invariance

$$W(RLH) = W(L) \quad \text{for all rotation } R \in O^+(3), L \in M_+^{3\times3}, H \in SL_3(\mathbb{Z}). \tag{1.2}$$

---

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

Irene Fonseca 1/3/91

1

Since W is not quasiconvex (see ERICKSEN [7], FONSECA [8], KINDERLEHRER [12]), the energy E(.,.) is not sequentially weakly lower semicontinuous and so, in general, we do not expect existence of minimizers. Following the work by CHIPOT & KINDERLEHRER [2] for elastic changes of state, we are interested in studying the behavior of minimizing sequences and their state functions rather than the macroscopic weak limit. Assuming that solutions may be measure-valued and using the parametrized probability measures of YOUNG [15] and the theory of compensated compactness of MURAT & TARTAR (see TARTAR [13]), we are able to calculate the energy and stresses of the deformed body when the class of variations includes non-elastic changes.

In Section 2 we give a brief description of the model for defective crystals proposed by DAVINI [3] and DAVINI & PARRY [4], [5]. Non-elastic defect-preserving deformations of a perfect crystal are called *neutral* and we show that, in the case of a perfect cubic crystal, the corresponding lattice matrix L can be written as

$$L(u(x)) = \nabla u(x) \{\nabla v(x)\}^{-1}, \qquad (1.3)$$

where $u : \Omega \to \mathbb{R}^3$ is the elastic deformation and v represents the slip or plastic deformation with det $\nabla v = 1$ a. e. in Ω (see FONSECA & PARRY [10]). Using the div-curl lemma (see TARTAR [13]) we prove that the class of neutral deformations is closed with respect to the weak * convergence in $W^{1,\infty}$ (see Proposition 2.7) and in Proposition 3.7 we show that the minors of L_n are weakly * continuous.

Due to (1.3) and assuming Dirichlet boundary conditions, we rewrite the energy I(.) as the functional

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

where (u, v) belong to the set of admissible pairs

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

which includes the elastic deformations in the case where v is the identity map.

In Section 3 we prove that the relaxation of the energy E(.,.) 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,

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

In Section 3 we show that the average weak limits of the Cauchy stress stress tensor corresponding to a minimizing sequence must be isotropic (see Theorem 3.1). ERICKSEN [6] had also remarked that perfect elastic crystals cannot support shear stresses (see FONSECA [8]) and later CHIPOT & KINDERLEHRER [2] showed that the average Cauchy stress for an elastic crystal is also a multiple of the identity. Moreover, DAVINI & PARRY [4] proved that, if we allow neutrally related states to compete, then some of the stress averages vanishe independently of the material symmetry hypotheses on W. In subsequent work (see FONSECA & PARRY [10], [11]) we study the effect caused by penalizing the energy using bulk energy or surface energy functionals.

2. DEFECTIVE CRYSTALS AND NEUTRAL DEFORMATIONS.

We give a brief description of a mathematical model for defective crystals proposed by DAVINI [3] and DAVINI & PARRY [4], [5]. For more details see FONSECA & PARRY [10]. In the sequel, Ω is a bounded, open, strongly Lipschitz domain in $\mathbb{R}^3$, $M^{3\times3}$ denotes the space of real 3x3 matrices and $M_+^{3\times3} := \{ F \in M^{3\times3} \mid \det F > 0\}$.

Let Ω represent the macroscopic placement of a non-defective cubic crystal and consider a change of state from the reference state $\Sigma_0 := \{\Omega, \mathbb{1}\}$ to $\Sigma := \{u(\Omega), L\}$, where the macroscopic deformation $u : \Omega \to u(\Omega)$ is a Lipschitz function with $\det \nabla u > 0$ a. e. in Ω and $L(u(x))$ represents averages values over microscopic regions of the lattice vectors around $u(x)$ defining the lattice cell at the atomic scale. In this theory the evolution of defects is supposed to account for the discrepancy between the macroscopic deformation and the lattice vectors as they come from averaging at different scales. The main feature of the work of DAVINI [3] and DAVINI & PARRY

[4], [5] is the introduction of a class of changes of state which strictly includes the elastic ones and which, at least intuitively, leave the defectiveness unchanged as they correspond to elastic deformations followed by rearrangements at the microscopic level.

Definition 2.1.

We say that Σ_0 and Σ are *elastically related* if the Cauchy - Born hypothesis is satisfied, namely $L(u(x)) = \nabla u(x)$ a. e. $x \in \Omega$.

Since elastically related states preserve the defectiveness (see TAYLOR [14]), it is natural to search for those integrals of the type

$$\int_c f(\Delta).dx \ , \ \int_s f(\Delta).v(x) \, d\sigma(x), \ \int_V f(\Delta) \, dx$$

where $\Delta := \{L, \nabla L\}$ represents a *local state of the crystal*, which will remain invariant under elastic deformations. 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.

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

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

Also for $i, j \in \{1, 2, 3\}$ we define the following densities, where $y = u(x)$:

$b_i := \text{curl}_y \, d_i$	(*Burger's vectors*)
$\sigma_{ij} := b_i.d_j$	(components of *Bilby's dislocation tensor*)
$n := 1/\det L = \det D$	(the number of cells per unit volume)

$$m := \frac{1}{n \ \det \nabla u(x)} \qquad \text{(atomic mass of an average cell)}$$

$$g_i := \nabla_y m.l_i$$

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

Theorem 2.2. (DAVINI [3])

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

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

where H_2 is the 2-dimensional Hausdorff measure and $v(x)$ 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

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

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 2.5).

Definition 2.3.

The states Σ and Σ^* are said to be *neutrally related* if they are not elastically related although the integrals (2.2) remain invariant.

We obtain the following characterization for neutral states. For its proof we refer the reader to FONSECA & PARRY [10].

Proposition 2.4.

Σ_0 and $\Sigma = \{u(\Omega), L\}$ 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. $L(u(x)) = \nabla u(x) \{\nabla v(x)\}^{-1}$;

2. $\det \nabla v(x) = 1$.

We give some examples of neutrallly related states.

Example 2.5.

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

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

where $a, b \in \mathbb{R}^3$ are such that $a.b = 0$. By Proposition 2.4 it follows that Σ_0 and Σ are neutrally related.

(2) Let $\Sigma = \{u(\Omega), \mathbb{1}\}$, where $u(x) = x + x_3 e_2 = (\mathbb{1} + e_2 \otimes e_3)x$ and $v = u$. Σ is a special type of *rearrangement* of Σ_0, designated by *slip* in the classic phenomenological plasticity theories.

It turns out that if Σ_0 and Σ are neutrally related then they are locally elastically related, i. e. 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

$$L((u \circ g)(x)) = \nabla(u \circ g)(x) \text{ for almost all } x \in U_1.$$

Hence, it is natural to assume that neutrally related states preserve the defectiveness.

Next, we want 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

Irene Fonseca 1/3/91

6

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 [15] and TARTAR [13]) as it shows the work of CHIPOT & KINDERLEHRER [2] 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 [13]).

2.6 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 $u_n \to u_\infty$ and $v_n \to v_\infty$ in L^∞ weak $*$. If, in addition, $\{\text{div } u_n\}$ and $\{\text{curl } v_n\}$ are bounded sequences in $H^{-1}_{loc}(\Omega)$ then $u_n \cdot v_n \to u_\infty \cdot v_\infty$ weakly $*$.

Proposition 2.7

Let $\Sigma_n = \{u_n(\Omega), L_n\}$ be a sequence of states neutrally related to Σ_0 and let $v_n : \Omega \to \mathbb{R}^3$ be such that $L_n(u(x)) = \nabla u_n(x) \{\nabla v_n(x)\}^{-1}$, $\det \nabla v_n(x) = 1$ for almost all $x \in \Omega$. If $u_n \to u_\infty$ and $v_n \to v_\infty$ in $W^{1,\infty}$ weak $*$ then

1. $\det \nabla v_\infty(x) = 1$ a. e. in Ω ;

2. $L_n(x) \to L_\infty(x) := \nabla u_\infty(x)\{\nabla v_\infty(x)\}^{-1}$ in L^∞ weak $*$.

Proof. (1) follows immediatly from the fact that $F \to \det F$ is a null lagrangian. Also, as

$$\{\nabla v_n(x)\}^{-1} = \{\text{adj } \nabla v_n(x)\}^T$$

Irene Fonseca 1/3/91

7

with the rows of $\nabla u_n(x)$ curl free and the rows of adj $\nabla v_n(x)$ divergence free[2], we obtain (2) from the div-curl lemma.

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 2.8.

If $\{u_\eta\}$ is a bounded sequence in $L^\infty(\Omega, \mathbb{R}^p)$ then there exists a subsequence $\{u_\epsilon\}$ and a family of probability measures $\{\mu_x\}_{x \in \Omega}$ (*Young measure*) such that if $f \in C(\mathbb{R}^p)$ then $\{f(u_\epsilon)\}$ 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 Proposition 2.7, consider a sequence of states $\Sigma_n = \{u_n(\Omega), L_n\}$ neutrally related to $\Sigma = \{u(\Omega), L\}$ and let $v_n : \Omega \to \mathbb{R}^3$ be such that $L_n(u(x)) = \nabla u_n(x) \{\nabla v_n(x)\}^{-1}$, det $\nabla v_n(x) = 1$ for almost all $x \in \Omega$. Let $u_n \to u_\infty$, $v_n \to v_\infty$ in L^∞ weak *, $L_n(x) \to L_\infty(x) := \nabla u_\infty(x) \{\nabla v_\infty(x)\}^{-1}$ in L^∞ weak * and let $\{\mu_x\}_{x \in \Omega}$ be the Young's measure corresponding to $\{L_n\}$. If the change is elastic then $L_n = \nabla u_n$, $L_\infty = \nabla u_\infty$, and as $M \to \det(M)$ and $M \to \text{adj} M$ are null lagragians it follows that

$$\det \left(\int_{M^{3x3}} M \, d\mu_x(M) \right) = \int_{M^{3x3}} \det M \, d\mu_x(M) \qquad (2.1)$$

and

$$\text{adj} \left(\int_{M^{3x3}} M \, d\mu_x(M) \right) = \int_{M^{3x3}} \text{adj} M \, d\mu_x(M). \qquad (2.2)$$

---

[2]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 $A.B := \text{tr}(A^T B)$.

The analysis of CHIPOT & KINDERLEHRER [2] relies heavily on (3.3) and (3.4). Next we show that (3.3) and (3.4) still hold for neutrally related states.

Proposition 2.9.

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

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

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

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

Proof. By Propositions 2.7 and 2.8 we have

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

and

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

and in a similar way

$$
\begin{aligned}
\operatorname{adj} \left(\int_{M^{3x3}} M \, d\mu_x(M) \right) &= \operatorname{adj} L_\infty(x) \\
&= \operatorname{adj} \nabla u_\infty(x) \{ \nabla v_\infty(x) \}^T
\end{aligned}
$$

with the rows of $\operatorname{adj} \nabla u_\infty$ divergence free and the rows of $\nabla \varphi_\infty(x)$ curl free. By the div-curl lemma we conclude that

$$\operatorname{adj} \left(\int_{M^{3x3}} M \, d\mu_x(M) \right) = w.^* \text{limit} \operatorname{adj} \nabla u_n(x) \{ \nabla v_n(x) \}^T$$

$$= w.*\text{limit adj } L_n(x)$$

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

3. RELAXATION OF THE BULK ENERGY.

Here we take the viewpoint that crystal equilibria correspond to extremals of some energy functional. Taking into account Proposition 2.4, we assume that the bulk energy associated to a neutral state $\Sigma = \{u(\Omega), L\}$ is given by

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

where $L(u(x)) = \nabla u(x)\{\nabla v(x)\}^{-1}$, $\det \nabla v(x) = 1$ a. e. in Ω, and W is the stored energy density satisfying (1.2). Also, as it is usual, in order to make it energetically impossible to compress part of the body to zero volume or to change its orientation we suppose that

$$W(L) \to 0^+ \text{ as } \det L \to 0^+. \tag{3.1}$$

We consider Dirichlet boundary conditions, where Σ is an admissible change if $(u, v) \in \mathscr{A}(u_0)$ and

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

This class includes the elastic deformations in the case where v is the identity map. Here $u_0 \in C^1(\overline{\Omega}, \mathbb{R}^3)$ is one-to-one in Ω, $\det \nabla u_0 > 0$ in Ω and

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

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

In particular, these conditions imply that if $(u, v) \in \mathscr{A}(u_0)$ then u is invertible a. e. (see BALL [1]). Using Lagrange multipliers, DAVINI & PARRY [4] showed that, independently of the boundary conditions and of the symmetry invariance, at a smooth local minimizer we must have

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

---

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

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

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

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 (1.2), ERICKSEN [6] proved that for elastic crystals at equilibrium the Cauchy stress reduces to a pressure,

$$T = -p\mathbb{1} \tag{3.2}$$

and later CHIPOT & KINDERLEHRER [2] recovered (3.2) 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,

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

$$= (g^{**})'(\det \nabla u_\infty(x)) \, \mathbb{1} \text{ a. e. in } \Omega \tag{3.3}$$

where g is the *subenergy function* introduced by ERICKSEN and FLORY,

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

Here we will show that (3.3) still holds even when neutrall changes of state are allowed to compete. Let $\Sigma_n = \{u_n(\Omega), L_n\}$ be a minimizing sequence for $I(.)$. with $(u_n, v_n) \in \mathscr{A}(u_0)$ 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 Proposition 2.7 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 3.1

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

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

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

We start by obtaining the relaxation of the bulk energy functional.

Theorem 3.2.

Let $A \in M_+^{3\times 3}$ and let $\mathscr{A}(A) := \{(\xi, v) \in W^{1,\infty}(\Omega, \mathbb{R}^3) \times W^{1,\infty}(\Omega, \mathbb{R}^3) | \, \xi(x) = Ax \text{ on } \partial\Omega,$

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

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

This result was proven by CHIPOT & KINDERLEHRER [2] and FONSECA [9] in the case where only elastic changes are admissible :

$$\inf \left\{ \int_\Omega W(\nabla\xi(x)) \, dx \mid \xi \in Ax + W_0^{1,\infty}(\Omega, \mathbb{R}^3) \right\} = \text{meas } (\Omega) \, g^{**}(\det A). \qquad (3.4)$$

Proof of Theorem 3.2. Clearly, by (3.4)

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

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

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

$$\int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1}) \, dx \geq \int_\Omega g^{**}(\det \nabla\xi(x) \det \nabla v(x)^{-1}) \, dx$$

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

$$\geq \text{meas } (\Omega) \, g^{**}\left(\frac{1}{\text{meas}(\Omega)} \int_\Omega \det \nabla\xi(x) \, dx \right)$$

$$= \text{meas}(\Omega) \, g^{**}(\det A).$$

12

From Theorem 3.2 and using the same argument as in CHIPOT & KINDERLEHRER [2] we obtain the following generalization to the case of inhomogeneous boundary conditions.

Proposition 3.3.

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

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

Proposition 3.4

1. $$\int_\Omega \overline{W}(x)\ dx = \int_\Omega \left(\ \int_{M^{3\times3}} W(M)\ d\mu_x(M)\ \right)\ dx$$

$$\leq \inf\left\{\ \int_\Omega W(\nabla\xi(x)\{\nabla v(x)\}^{-1})\ dx\ |\ (\xi, v) \in \mathcal{A}(u_0)\right\}\ ;$$

2. $\text{supp}\ \mu_x \subset M_+^{3\times3}$ and $\det\nabla u_\infty > 0$ a. e. in Ω.

Proof. Part (1) is proven exactly as in CHIPOT & KINDERLEHRER [2] and (3.1) and (1) imply that $\text{supp}\ \mu_x \subset M_+^{3\times3}$. Finally, by Theorem 3.2

$$\nabla u_\infty(x)\ \{\nabla v_\infty(x)\}^{-1} = L_\infty(x)$$

$$= \int_{M^{3\times3}} M\ d\mu_x$$

which, together with Proposition 2.9 (1), yields

$$\det\nabla u_\infty(x) = \int_{M^{3\times3}} \det M\ d\mu_x > 0\quad \text{a. e. in}\ \Omega.$$

Corollary 3.5

Under the hypotheses of Proposition 3.3

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

Proof. Using the same argument as in CHIPOT & KINDERLEHRER [2], by Proposition 3.4 we have det $\nabla u_\infty > 0$ a. e. in Ω and so, since g is convex and det $\nabla u_n \to$ det ∇u_∞ weakly *, by Proposition 3.3 we conclude that

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

$$\leq \lim \inf \int_\Omega g^{**}(\det \nabla u_n(x)) \, dx$$

$$\leq \lim \inf \int_\Omega W(L_n(x)) \, dx$$

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

Proposition 3.6

1. $\overline{W}(x) = \overline{g}(x) = \overline{g^{**}}(x) = g^{**}(\det \nabla u_\infty(x))$ a. e. in Ω ;

2. supp $\mu_x \subset \{M \in M_+^{3\times3} \mid \alpha(x) \leq \det M \leq \beta(x)\}$ 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 supp μ_x.

Proof. The argument is essentially the same as in CHIPOT & KINDERLEHRER [2], where we must use Proposition 2.9 (1).

Finally, we give the proof of Theorem 3.1.

Proof of Theorem 3.1. By Proposition 3.6 (3), if $M \in$ supp μ_x then

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

and so

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

Also, by Proposition 3.6 (2)

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

Irene Fonseca 1/3/91

14

and we deduce that

$$S(M) = (g^{**})'(\det \nabla u_\infty(x)) \text{ adj } M, \tag{3.5}$$

hence, by Proposition 2.9 (2),

$$\overline{S}(x) = \int_{M^{3x3}} (g^{**})'(\det \nabla u_\infty(x)) \text{ adj } M \, d\mu_x(L)$$

$$= (g^{**})'(\det \nabla u_\infty(x)) \text{ adj } L_\infty(x). \tag{3.6}$$

Finally, by (3.5) and for almost all $x \in \Omega$

$$\overline{T}(x) = \int_{M^{3x3}} T(M) \, d\mu_x(L) = \int_{M^{3x3}} \frac{1}{\det M} S(M) \, M^T \, d\mu_x(M)$$

$$= (g^{**})'(\det \nabla u_\infty(x)) \int_{M^{3x3}} \frac{1}{\det M} \text{ adj} M \, M^T \, d\mu_x(M)$$

$$= (g^{**})'(\det \nabla u_\infty(x)) \, \mathbb{1}$$

and by (3.6)

$$\frac{1}{\det L_\infty(x)} \overline{S}(x) \, L_\infty^T = \frac{1}{\det L_\infty(x)} (g^{**})'(\det \nabla u_\infty(x)) \text{ adj } L_\infty(x) \, L_\infty^T$$

$$= (g^{**})'(\det \nabla u_\infty(x)) \, \mathbb{1}.$$

REFERENCES.

[1]   BALL, J. M. "Global invertibility of Sobolev functions and the interpenetration of matter", Proc. Roy. Soc. Edinburgh **88A** (1981), 315-328.

Irene Fonseca 1/3/91

[2]   CHIPOT, M. and D. KINDERLEHRER "Equilibrium configurations of crystals", Arch. Rat. Mech. Anal. **103** (1988), 237-277.

[3]   DAVINI, C. "A proposal for a continuum theory of defective crystals", Arch. Rat. Mech. Anal. **96** (1986), 295-317.

[4]   DAVINI, C. & G. PARRY "On defect-preserving deformations in crystals", Int. J. of Plasticity **5** (1989), 337-369.

[5]   DAVINI, C. & G. PARRY "A complete list of invariants for defective crystals", to appear.

[6]   ERICKSEN, J. L. "Loading devices and stability of equilibrium", in *Nonlinear Elasticity,* Academic Press, N. Y. (1973), 161-173.

[7]   ERICKSEN, J. L. "Twinning of crystals I", in *Metastability and Incompletely Posed Problems, IMA Vol. in Appl. Math* **3** (1987), 77-96.

[8]   FONSECA, I. "Variational methods for elastic crystals", Arch. Rat. Mech. Anal. **97** (1987), 189-220.

[9]   FONSECA, I. "The lower quasiconvex envelope of the stored energy function for an elastic crystal", J. Math. Pures et Appl. **67** (1988), 175-195.

[10]   FONSECA, I. & G. PARRY "Equilibrium configurations of defective crystals", to appear.

[11]   FONSECA, I. & PARRY, G. "On a class of invariant integrals", to appear.

[12]   KINDERLEHRER, D. "Twinning of crystals II", in *Metastability and Incompletely Posed Problems, IMA Vol. in Appl. Math* **3** (1987), 185-211.

[13]   TARTAR, L. "Compensated compactness and applications to partial differential equations," Nonlinear analysis and mechanics : Heriot-Watt Symposium, vol. IV, Res. Notes in Math. **39**, Pitman, 1979, 136-212.

[14]   TAYLOR, G. I. "The mechanism of plastic deformation of crystals", I, II, Proc. Roy. Soc. A **145** (1934), 362-387, 388-404.

[15]   YOUNG, L. C., "Generalized surfaces in the calculus of variations I, II", Ann. of Math. **43** (1942), 84-103, 530-544.

REPORT DOCUMENTATION PAGE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302 and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE March 1991	3. REPORT TYPE AND DATES COVERED

4. TITLE AND SUBTITLE Remarks on variational problems for defective crystals	5. FUNDING NUMBERS
6. AUTHOR(S) Irene Fonseca and Gareth Parry	

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Carnegie Mellon University Department of Mathematics Pittsburgh, PA 15213	8. PERFORMING ORGANIZATION REPORT NUMBER NAMS-21

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U. S. Army Research Office P. O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.	12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

In the context of a continuum theory of crystals with defects, one can define a particular list of tensors which remain unchnaged when the crystal is deformed elastically. In our model, the defect notion relies on the assumption that deformations that leave these elements invariant do not change the defects. This class of deformations strictly includes the elastic deformations; nonelastic defect-preserving deformations are called neutral and generally involve some kind of rearrangement, or slip, of the crystal lattice. Here we deal with slightly defective crystals, i.e. where defects are so few that a lattice is distinguishable at the microscopic scale. We factor neutral deformations into components which are exclusively elastic at the macroscopic level or exclusively slip at the microscopic level. Using direct methods of the calculus of variations we determine equalibrium configurations for defective crystals. As in Chipot & Kinderlehrer, we study the behavior of minimizing sequences and their state functions, and in order to take into account possible oscillations of the minimizing sequences we assume that solutions may be measure-valued.

14. SUBJECT TERMS defective crystals, neutral states, div-curl lemma			15. NUMBER OF PAGES 16
			16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL