INTERFACIAL ENERGY AND THE MAXWELL RULE

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Research Report No. 88-18 2

May 1988

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1. INTRODUCTION.

A typical problem of phase transitions consists in minimizing an energy functional

$$J(u) := \int_{\Omega} W(u)\, dx,$$

where $\Omega \subset \mathbb{R}^n$ is an open bounded smooth domain, $u : \Omega \to \mathbb{R}^N$ and W supports more than one phase (i.e. $W \geq 0$ and there exist $a \neq b$ such that $W(a) = 0 = W(b)$).

When interfaces are allowed to form without an increase in energy there generally results a striking nonuniqueness of equilibria. Recently, several authors have studied this question from different points of view, the common feature being the search for a model which penalizes the formation of interfaces, hopefully to predict those solutions most likely to be observed.

There is an extensive bibliography concerning the Van der Waals-Cahn-Hilliard theory of phase transitions for fluids. Here N = 1, W has exactly two potential wells and the asymptotic behavior of minimizers of a perturbed problem is studied (see CARR, GURTIN & SLEMROD [8], GURTIN [20], KOHN & STERNBERG [26], MODICA [28], OWEN [29], [30], OWEN & STERNBERG [31], STERNBERG [35]). More recently, FONSECA & TARTAR [16] and STERNBERG [36] treated the case where N is arbitrary.

A different approach is undertaken by GURTIN [18], [19], where the interfaces are directly penalized.

Due to necessary compatibility conditions, none of these theories has been successfully applied to nonlinear elasticity, where u is a deformation gradient. In this paper we study the role played by a class of surface energies in the metastability of piecewise smooth configurations of a homogeneous elastic material. We adopt the point of view that, for dead loading, equilibria correspond to local minima of an energy functional

$$\int_{\Omega} W(\nabla u)\, dx + \sum_{I \in \mathcal{F}} \int_{I} \Gamma\, dS - \int_{\Omega} f.u\, dx - \int_{\partial\Omega_2} t.u\, dS,$$

where W is the strain energy density, Γ is a surface energy density accounting for jumps in deformation gradient, $\mathcal{F}$ is the family of phase boundaries, f represents the body forces and t is the surface traction on a portion $\partial\Omega_2$ of the boundary $\partial\Omega$ of Ω. Although most of our results are valid for non ordered materials, they may give some insight to questions of metastability of solids with crystalline structure. Problems related to equilibria, stability and metastability of elastic crystals have been addressed by BALL & JAMES [4], CHIPOT & KINDERLEHRER [9], ERICKSEN [12], [13], JAMES [24], KINDERLEHRER [25], PARRY [32] and PITTERI [33].

In order to describe phenonema like twinning and martensitic phase transitions, ERICKSEN [13] proposed a continuum theory based on nonlinear elasticity. This framework leads to variational problems that escape the classical hypotheses of the calculus of variations (see ERICKSEN [13], KINDERLEHRER [25]); such problems are highly unstable and previous results (see CHIPOT & KINDERLEHRER [9], FONSECA [14], [15]) suggest that the inclusion of interfacial energy might render them more stable.

In Section 2 we introduce the interfacial energy density Γ. The constitutive hypotheses for Γ are motivated by previous work of HERRING [23] and PARRY [32], who based their analysis on molecular considerations in which surface energies arise from interatomic interaction of finite range in solid crystals. Here it seems natural to attribute to Γ a lack of differentiability with respect to certain crystallographically simple directions (see CAHN & HOFFMAN [6], [7]).

In Proposition 3.2 we obtain new necessary conditions for metastability of piecewiese C^2 deformations that complement the ones previously deduced by ALEXANDER & JOHNSON [1], [2], GURTIN [21], GURTIN & MURDOCH [22], LEO [27], PARRY [32] and PITTERI [33] (see Proposition 3.1 and Proposition 3.2 (ii)). As a consequence, in Corollary 3.6 we conclude that the lack of differentiability of Γ permits the selection of a finite number of interfacial directions n for which the gradients F_+ and F_- of the deformations that form the adjoint phases of a piecewise homogeneous local minimizer do not satisfy the Maxwell rule (see CAHN & HOFFMAN [6], [7]). This confirms PARRY's [32] conjecture for the arrangement of thin shear bands in unloaded crystals, namely "...One is tempted, then, to suppose that stable shear bands çorrespond to 'inward pointing' cusps in the θ-plot ...". We note that configurations of that sort are likely to occur. As it was pointed out by PARRY [32], the strain energy densities of the deformation gradients F_+ and F_- in the photographs of RICHMAN [34] are generally unequal (they are not symmetry related). Hence, as it is reasonable to suppose that they are local minima of W, we deduce that F_+ and F_- cannot verify the Maxwell rule.

Moreover, using any reasonable notion of metastability wide enough to allow movement of the interfaces, we show (Proposition 3.7) that there is "neck forming" near the phase boundary of a two-phase deformation. Precisely, we have that either $\Gamma = 0$ or

$$\limsup_{\rho \to 0^-} \frac{A(\rho) - A(0)}{\rho} \leq 0 \leq \liminf_{\rho \to 0^+} \frac{A(\rho) - A(0)}{\rho}$$

where $A(t) := \text{area}\{x \in \Omega \mid x.n = k + t\}$ and $\{x \in \Omega \mid x.n = k\}$ is the interface with normal n.

In Remark 3.9 (ii) we examine the sufficient conditions for strong metastability proposed by PARRY [32]. Under his assumptions, we show that the lack of differentiability of Γ with respect to the interfacial normal is an essential requisite to prevent $W(F_+) = W(F_-)$.

In Section 4 we analyze the quasiconvexity condition in the presence of the interfacial energy. This property plays a crucial role in the calculus of variations, since it is a necessary condition for lower semicontinuity of multiple integrals (see BALL & MURAT [5], DACOROGNA [11]). Also, disregarding the interfacial energy contribution, if u is a relative minimizer with respect to the norm $\|\cdot\|_\infty + \|\cdot\|_{1,p}$ and if u is C^1 near x_0, then W is quasiconvex at $\nabla u(x_0)$ (see BALL [3]).

It turns out that a similar result holds for minimizers of $E(\cdot)$. In fact, in Proposition 4.3 we derive an analog of the quasiconvexity condition for Γ. This result, together with one of the hypotheses considered in Remark 3.9 (ii), implies that the Maxwell rule holds for piecewise C^2 relative minimizers (see Remark 4.4 (ii)).

Exploring frame indifference, we deduce (Proposition 5.1) that at metastable states the matrix

$$\frac{\partial \Gamma}{\partial F} F_-^T$$

is symmetric, i. e. we recover the analog to the symmetry of the Cauchy stress tensor (see GURTIN & MURDOCH [22] and LEO [27]). Further, for elastic crystals the quasiconvexity properties of Γ together with material symmetry imply that at metastable states

$$\frac{\partial \Gamma}{\partial F} F_-^T$$

reduces to a "pressure" up to a rank-one matrix (Proposition 5.3). Recall that, in the absence of interfacial energy, the Cauchy stress tensor is a hydrostatic pressure (see ERICKSEN [12]).

Finally, (Proposition 5.11) we prove that the Maxwell rule holds for a piecewise C^2 relative minimizer u whenever $\det \nabla u$ is continuous across the interface. It is worth noticing that for ordered materials the condition $\Gamma \geq 0$ at metastable states follows from material symmetry (Remark 5.13).

2. STATEMENT OF THE PROBLEM. INTERFACIAL ENERGY DENSITY.

In what follows, M^{3x3} denotes the set of all 3x3 real matrices, and $O^+(3)$ is the proper orthogonal group,

$M^{3x3}{}_+ := \{F \in M^{3x3} \mid \det F > 0\}$,

$G^+ := \{M \in M^{3x3} \mid M_{ij} \in \mathbb{Z},\ i, j = 1, 2, 3 \text{ and } \det F = 1\}$,

$X := \{(F; a, n) \in M^{3x3} x\, \mathbb{R}^3 x\, \mathbb{R}^3 \mid \det F > 0 \text{ and } \det(F + a\otimes n) > 0\}$.

We consider a hyperelastic solid which (in a fixed reference configuration) occupies an open bounded strongly Lipschitz domain $\Omega \subset \mathbb{R}^3$.

Throughout this paper, an *admissible deformation* is a mapping $u \in W^{1,\infty}(\Omega; \mathbb{R}^3)$ such that there exist a finite partition of Ω, $\{\Omega_i\}_{i=1,\dots,M}$ and a set $\mathcal{E} \subset \Omega$ such that:

Ω_i is a domain for all $i = 1,\dots, M$,

area $(\bar{\mathcal{E}}) = 0$,

$u \in C^2(\bar{\Omega}_i; \mathbb{R}^3)$ and $\det \nabla u > 0$ on $\bar{\Omega}_i$, $i = 1, \dots, M$,

$I_{i,j} := \partial\Omega_i \cap \partial\Omega_j \cap \Omega$, $1 \le i < j \le M$, is a C^2 surface at every $x \in I_{i,j} \setminus \mathcal{E}$ and

area $(I_{i,j} \cap I_{k,l}) = 0$ if $(i, j) \neq (k, l)$.

We call the surfaces $I_{i,j}$, $1 \le i < j \le M$, the *interfaces of u*. In most cases of interest, $\mathcal{E}$ reduces to a finite union of piecewise C^2 curves. The simplest example of admissible deformations are continuous piecewise affine deformations.

As a kinematical restriction, an admissible deformation must satisfy the well known compatibility condition

$$\nabla u_i = \nabla u_j + a_{i,j} \otimes n_{i,j} \quad \text{on } I_{i,j} \tag{2.1}$$

where $1 \le i < j \le M$, the amplitude vectors $a_{i,j} : I_{i,j} \to \mathbb{R}^3$ are continuous, u_i denotes the restriction of u to Ω_i, and $n_{i,j}$ is the normal to $I_{i,j}$ pointing into Ω_i. If u is piecewise affine then ∇u_i are constant, the interfaces are planar and $a_{i,j}$ are constant, $i,j = 1, \dots, M$.

When there is no possibility of confusion, drop the subscripts i and j and write

$I := I_{i,j}$,

$\Omega_+ := \Omega_i$,

$\Omega_- := \Omega_j$,

$F_+ := \nabla u_i$,

$F_- := \nabla u_j$,

so that (2.1) reduces to

$$F_+ = F_- + a \otimes n.$$

Accordingly, the *jump of a function h across I* is given by

$[h] := h_+ - h_-$.

We shall consider the mixed problem in which displacements are prescribed on a portion $\partial\Omega_1$ of of the boundary, and (dead load) tractions are assigned on the remainder $\partial\Omega_2$. Thus let $f \in L^q(\Omega; \mathbb{R}^3)$, $q > 3/2$, be the body force per unit volume in the reference configuration and let $t \in L^1(\partial\Omega_2; \mathbb{R}^3)$ be the surface traction per unit area of the undeformed configuration, where

$$\partial\Omega = \text{closure } (\partial\Omega_1 \cup \partial\Omega_2) \text{ and } \partial\Omega_1 \cap \partial\Omega_2 = \emptyset.$$

If $W : M^{3x3}{}_+ \to \mathbb{R}$ is the strain energy density per unit reference volume, then the *total energy of an admissible deformation u* is given by $\partial\Omega_2$

$$E(u) := \int_\Omega W(\nabla u)\, dx + \sum_{I \in \mathcal{F}} \int_I \Gamma\, dS - \int_\Omega f.u\, dx - \int_{\partial\Omega_2} t.u\, dS,$$

where $\mathcal{F}$ is the family of interfaces and $\Gamma: X \to \mathbb{R}$ is the surface energy density per unit area of the reference configuration.

As it is common in nonlinear elasticity, we make the following hypotheses on W:

(H1) $W \geq 0$ and $W \in C^1(M^{3x3}{}_+; \mathbb{R})$;

(H2) (*frame indifference*) $W(RF) = W(F)$ for all $F \in M^{3x3}{}_+$, $R \in O^+(3)$.

Moreover, according to ERICKSEN [13], if the solid has a crystalline structure then W is invariant with respect to a conjugate group of G, precisely

(H3) (*invariance under the change of lattice basis*) $W(FM) = W(F)$ for all $F \in M^{3x3}{}_+$ and $M \in AG^+A^{-1}$, where the columns of the matrix A form a lattice basis for the crystal in the reference configuration.

For a detailed description of this model we refer the reader to ERICKSEN [13], FONSECA [14] and KINDERLEHRER [25]. For simplicity, we suppose that the reference configuration has cubic symmetry, so that A is the identity matrix.

Concerning the surface energy density Γ, our constitutive assumptions are based on molecular considerations for solid crystals outlined by HERRING [23] and PARRY [32]. Suppose that kinematically compatible lattices L_1 and L_2 coexist in equilibrium separated by a plane I' with normal n', and let the underlying pairwise homogeneous deformation have deformation gradients F and $F + a\otimes n$, where

$$n' = \frac{F^{-T}n}{\|F^{-T}n\|}.$$

HERRING [23] and PARRY [32] identify the surface energy with the energy of interaction of atoms in the lattice L_i, $i = 1,2$, with "virtual" atoms in a (non-existent) congruent lattice of identical atoms on the other side of the surface. Assuming that the atoms interact attractively in pairs by means of forces of finite range, and that the surface and interior lattice spacings are the same, they deduce that Γ is of the form

$$\Gamma(F;\, a,\, n) = \sum_{i=1}^{P} \gamma_i(F;\, a,\, n,\, r_i)\ |\cos(F^{-T}n,\, r_i)|$$

where $r_i = r_i\,(F;\, a,\, n)$ are smoothly varying vectors separating two atoms in the lattices L_j, $j=1,2$. The vectors r_i correspond to short bonds that cross I', while the functions γ_i are associated with the smooth potential energies of atomic interaction. Thus Γ is not differentiable with respect to n whenever $F^{-T}n$ is perpendicular to one of the vectors r_i, i.e.

$$\frac{\partial\Gamma}{\partial n}(F;\, a,\, n) \text{ does not exist if } n \in F^T\Pi_1 \cup F^T\Pi_2 \cup \ldots \cup F^T\Pi_P,$$

where Π_i is the plane through the origin with normal

$$\frac{r_i}{\|r_i\|},\ i = 1,\ldots,\, P.$$

We define the sets

$$X(F;\, a,\, n) := \{y \in \mathbb{R}^3 \mid y.\, F^{-1}r_i(F;\, a,\, n) = 0 \text{ for some } i \in \{1,\ldots,\, P\}\},$$

$$X^* := \{(F;\, a,\, n) \in X \mid n \in X(F;a,n)\}.$$

It is then natural to assume that:

(H'1) $\Gamma \geq 0$, $\Gamma \in W^{1,\infty}_{loc}(X;\, \mathbb{R}) \cap C^2(X \setminus X^*;\, \mathbb{R})$, $\Gamma(.;\, a,\, n) \in C^2$;

(H'2) $\Gamma(F;\, a,\, n) = \Gamma(F + a\otimes n;\, -a,\, n)$ for all $(F;\, a,\, n) \in X$;

(H'3) $\Gamma(F;\, \lambda a,\, n) = \Gamma(F;\, a,\, \lambda n)$ for all $F \in M^{3x3}{}_+$, $a \in \mathbb{R}^3$, $\lambda \in \mathbb{R}$ such that $(F;\, \lambda a,\, n) \in X$;

(H'4) $\Gamma(F;\, 0,\, n) = \Gamma(F;\, a,\, 0) = 0$ for all $(F;\, a,\, n) \in M^{3x3}{}_+ x\ \mathbb{R}^3 x\ \mathbb{R}^3$;

(H'5) (*frame indifference*) $\Gamma(RF;\, Ra,\, n) = \Gamma(F;\, a,\, n)$ for all $R \in O^+(3)$ and $(F;\, a,\, n) \in X$.

Further, for elastic crystals invariance with respect to changes in lattice basis imply (see PARRY [32])

(H'6) $\Gamma(FM;\, a,\, M^Tn) = \Gamma(F;\, a,\, n)$ for all $M \in G^+$ and $(F;\, a,\, n) \in X$.

As the matrices $\mathbb{1}$ and $\mathbb{1} + a \otimes b$, with $a, b \in \mathbb{Z}^3$ such that a.b=0, correspond to symmetry related variants, it would not be possible, at the molecular level, to distinguish the interface of a pairwise affine deformation with gradients F and $F(\mathbb{1} + a \otimes b)$. Thus, we assume

(H'7) $\Gamma(F; Fa, b) = 0$ for every $a, b \in \mathbb{Z}^3$ such that a.b=0.

We use the following notions of metastability for admissible deformations:

Definition 2.2.

(i) u is *weakly metastable* if there exists an $\varepsilon > 0$ such that $E(u) \leq E(u + \phi)$ for all $\phi \in C^\infty(\Omega; \mathbb{R}^3)$ such that $\phi = 0$ on $\partial\Omega_1$ and $||\phi||_{1,\infty} < \varepsilon$;

(ii) u is *metastable* if there exists an $\varepsilon > 0$ such that $E(u) \leq E(u + \phi)$ and $E(u) \leq E(u(. + \phi(.))$ for all $\phi \in C^\infty(\Omega; \mathbb{R}^3)$ such that $\phi = 0$ on $\partial\Omega_1$ and $||\phi||_{1,\infty} < \varepsilon$;

(iii) (PARRY [25]) u is *strongly metastable* if there exists an $\varepsilon > 0$ such that $E(u) \leq E(v)$ whenever $v(x + \varphi(x)) = u(x) + \phi(x)$ for all $x \in \Omega$, where $\varphi, \phi \in C^\infty(\Omega; \mathbb{R}^3)$ are such that $||\varphi||_{1,\infty} < \varepsilon$, $||\phi||_{1,\infty} < \varepsilon$ and $v(x) = u(x)$ on $\partial\Omega_1$;

(iv) If $1 \leq p < \infty$, u is said to be *p-weakly metastable* if there exists an $\varepsilon > 0$ such that $E(u) \leq E(u + \phi)$ for all $\phi \in C^\infty(\Omega; \mathbb{R}^3)$ such that $\phi = 0$ on $\partial\Omega_1$ and $||\phi||_{1,p} < \varepsilon$;

(v) If $1 \leq p < \infty$, u is *p -metastable* if there exists an $\varepsilon > 0$ such that $E(u) \leq E(u(. + \phi(.))$ for all $\phi \in C^\infty(\Omega; \mathbb{R}^3)$ such that $\phi = 0$ on $\partial\Omega_1$ and $||\phi||_{1,p} < \varepsilon$;

(v) u is *phase - metastable* if there exists an $\varepsilon > 0$ such that $E(u) \leq E(v)$ for all admissible deformation v with the same discontinuity surfaces of u and such that $||u - v||_{1,\infty} < \varepsilon$.

Remark 2.3.

Clearly, we have the following implications for a given admissible deformation:

strongly metastable $\Rightarrow$ metastable $\Rightarrow$ weakly metastable,

p-weakly-metastable $\Rightarrow$ weakly metastable, p-weakly-metastable and p-metastable $\Rightarrow$ metastable and

phase-metastable $\Rightarrow$ weakly metastable.

Next, we recall some results on surface integrals that we will use throughout this paper.

Let $I \subset \Omega$ be a C^2 surface with normal ν and mean curvature K. For $f : \Omega \to \mathbb{R}$ we define the *tangential derivatives*

$$\partial_i^t f := \frac{\partial f}{\partial x_i} - \frac{\partial f}{\partial \nu}\nu_i,$$

where the *normal derivative* is given by

$$\frac{\partial f}{\partial \nu} := \frac{\partial f}{\partial x_i}\nu_i.$$

Here we use the summation convention for repeated indices. Moreover, if f takes values in $\mathbb{R}^3$, we denote its *tangential divergence* by

$$\mathrm{Div}_t\, f := \mathrm{div}\, f - \frac{\partial f}{\partial \nu}.\nu.$$

If $f \in C^1$ and if ϕ is a diffeomorphism, then (see CIARLET [10])

$$\int_{\phi(I)} f(y)\, dS(y) = \int_I f(\phi(x))\, \|\mathrm{adj}(\nabla\phi(x))\, \nu(x)\|\, dS(x) \tag{2.4}$$

where adj(A) is the matrix of cofactors of A.

Also, if $f : \Omega \to \mathbb{R}^3$ is a C^1 function vanishing on ∂I, then

$$\int_I \mathrm{Div}_t\, f\, dS = -2\int_I f.\nu\, K\, dS, \tag{2.5}$$

from which follows immediatly that

$$\int_I g\mathrm{Div}_t\, f + \nabla^t g.f\, dS = -2\int_I gf.\nu\, K\, dS \tag{2.6}$$

whenever $gf = 0$ on ∂I.

Finally, it is easy to show that if $D \subset \mathbb{R}^3$ is an open bounded domain and if $f : D \to \mathbb{R}^3$ is a continuous function then

$$\lim_{\varepsilon \to 0} \int_{D \cap \frac{I - x_0}{\varepsilon}} f\, dS = \int_{D \cap \{x \mid x.\nu(x_0) = 0\}} f\, dS \tag{2.7}$$

for every $x_0 \in I$.

3. NECESSARY CONDITIONS FOR METASTABLE EQUILIBRIA.

In the sequel u is an admissible deformation, I is an interface of u and S is the *first Piola-Kirchhoff stress tensor*, i.e.

$$S_{kl} := \frac{\partial W}{\partial F_{kl}} \quad \text{for } k, l = 1, 2, 3.$$

The proof of the following proposition can be found in FONSECA [14] (parts (i), (ii)), PARRY [32] and PITTERI [33] (parts (iii) and (iv)). See also ALEXANDER & JOHNSON [1], [2], GURTIN [21], GURTIN & MURDOCH [22] and LEO [27].

Proposition 3.1.

Let u be weakly metastable. If (H1), (H'1) and (H'2) hold then

(i) $-\operatorname{div} S(\nabla u) = f$ in Ω_i, $i = 1,\dots,M$;

(ii) $S(\nabla u)\nu = t$ on $\partial\Omega_2$, where ν is the outward unit normal to $\partial\Omega$;

(iii) $\frac{\partial \Gamma}{\partial F}(F_-; a, n)\, n = 0$ a.e. on I;

(iv) $\mathrm{Div}_t \frac{\partial \Gamma}{\partial F}(F_-; a, n) + [S(\nabla u)]\, n = 0$ a.e. on I.

In the next result, we need to ensure the existence of $\partial\Gamma/\partial n$ and $\partial\Gamma/\partial a$ and so, according to (H'1),we define the set

$$\Omega_0 := \{x \in \Omega \setminus \mathcal{E} \mid x \in I_{i,j} \text{ and } (\nabla u_j(x); a_{i,j}(x), n_{i,j}(x)) \in X \setminus X^* \text{ for some } 1 \le i < j \le M\}.$$

Conditions analogous to Proposition 3.2 (ii) were derived in ALEXANDER & JOHNSON [1],[2], GURTIN [21] and LEO [27].

Proposition 3.2.

Let (H1), (H'1) and (H'2) be satisfied and let u be metastable.Then

(i) $\frac{\partial \Gamma}{\partial n}.n = 0$ on $I \cap \Omega_0$,

and, granted (H'3),

$\frac{\partial \Gamma}{\partial a}.a = 0$ on $I \cap \Omega_0$;

(ii) $$W(F_+) - W(F_-) - S(F_+).(F_+ - F_-) + 2K\,\Gamma(F_-; a, n) - \mathrm{Div}_t\left(\frac{\partial \Gamma}{\partial n}\right) = 0 \tag{3.2}$$

on $I \cap \Omega_0$, where K is the mean curvature of I.

Proof. Let $x_0 \in I \cap \Omega_0$; since $X \setminus X^*$ is open and F_- is continuous, let $\varepsilon_0, \varepsilon_1 > 0$ be such that

$$\| (F; b, m) - (F_-(x_0); a(x_0), n(x_0)) \| < \varepsilon_0 \Rightarrow (F; b, m) \in X \setminus X^*$$

and

$$\| x - x_0 \| < \varepsilon_1 \Rightarrow \| (F_-(x); a(x), n(x)) - (F_-(x_0); a(x_0), n(x_0)) \| < \varepsilon_0/2$$

if $x \in I \cap \Omega_0$. Let $\phi \in C^\infty(\Omega; \mathbb{R}^3)$ with supp $\phi \subset B(x_0; \varepsilon_1/2)$ and choose ε small enough so that

$$w_\varepsilon : \Omega \to \Omega \text{ is a diffeomorphism,}$$

$$w_\varepsilon(B(x_0; \varepsilon_1/2)) \subset B(x_0; \varepsilon_1),$$

$$\varepsilon \|\nabla\phi\|_\infty (\|F_-\|_\infty + 1) < \varepsilon_0/2$$

and

$$E(u) \leq E(u_\varepsilon),$$

where $w_\varepsilon(x) := x + \varepsilon\phi(x)$ and $u_\varepsilon(x) := u(w_\varepsilon(x))$. As u is a metastable deformation, using (2.4) we obtain

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0}(J_1 + J_2 + J_3) = 0 \tag{3.3}$$

where

$$J_1 := \int_{\Omega_+ \cup \Omega_-} W(F(x)\,\nabla w_\varepsilon(w_\varepsilon^{-1}(x))\, \det \nabla w_\varepsilon^{-1}(x)\, dx,$$

$$J_2 := \int_I \Gamma(F_-(x)\,\nabla w_\varepsilon(w_\varepsilon^{-1}(x)); a(x), \nabla w_\varepsilon^T(w_\varepsilon^{-1}(x))\, n(x))\ \|(\mathrm{adj}\nabla w_\varepsilon^{-1}(x))\, n(x)\|\, dS$$

and

$$J_3 := -\int_\Omega f(x)\, .u(w_\varepsilon(x))\, dx.$$

On the other hand, from the identity

$$\mathrm{adj}\,(A^{-1}) = \frac{A^T}{\det A},$$

it follows that

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \det\,(\mathbb{1} + \varepsilon\nabla\phi(w_\varepsilon^{-1}(x)) = \mathrm{div}\,\phi(x),$$

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \mathrm{adj}\,(\nabla w_\varepsilon^{-1}(x)) = \nabla\phi^T(x) - \mathrm{div}\,\phi(x)\mathbb{1}$$

and

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \|\mathrm{adj}\,(\nabla w_\varepsilon^{-1}(x))\, n(x)\| = n(x)\,.\,[\nabla\phi^T(x)n(x) - \mathrm{div}\,\phi(x)n(x)]$$

$$= -\operatorname{Div}_t \phi(x).$$

Hence, we conclude that

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} J_1 = \int_\Omega S(F).\, F(\nabla\phi)\, dx - \int_\Omega W(F) \operatorname{div} \phi \, dx$$

and, by (2.6) and Proposition 3.1 (iii), we obtain

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} J_2 = \int_I \frac{\partial\Gamma}{\partial F} . F_-(\nabla\phi)\, dS + \int_I \left(n\otimes\frac{\partial\Gamma}{\partial n}\right). \nabla\phi \, dS - \int_I \Gamma \operatorname{Div}_t\phi \, dS$$

$$= \int_I -\operatorname{Div}_t\left(F_-^T \frac{\partial\Gamma}{\partial F}\right). \phi\, dS + \int_I \left(n\otimes\frac{\partial\Gamma}{\partial n}\right). \nabla\phi\, dS + \int_I \nabla^t\Gamma.\phi\, dS + 2\int_I K\,\Gamma\, \phi.n\, dS.$$

Finally, as

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} J_3 = -\int_\Omega f.\nabla\phi\, dx,$$

(3.3) and Proposition 3.1 (i), (iii) yield

$$0 = \int_I \{W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) + 2K\,\Gamma(F_-; a, n)\}\, \phi\, .\, n\, dx - \int_I [S(F)]\, n\, .\, F_+\phi\, dS$$
$$- \int_I \operatorname{Div}_t\left(F_-^T \frac{\partial\Gamma}{\partial F}\right). \phi\, dS + \int_I \left(n\otimes\frac{\partial\Gamma}{\partial n}\right). \nabla\phi\, dS + \int_I \nabla^t\Gamma.\phi\, dS. \tag{3.4}$$

Clearly, from (3.4) we deduce that

$$\frac{\partial\Gamma}{\partial n}.n = 0$$

which, together with (H'3), implies that

$$\frac{\partial\Gamma}{\partial a}.a = 0.$$

Therefore,

$$\int_I \left(n\otimes\frac{\partial\Gamma}{\partial n}\right). \nabla\phi\, dS = -\int_I \operatorname{Div}_t\left(n\otimes\frac{\partial\Gamma}{\partial n}\right). \phi\, dS$$

and (3.4) reduces to

$$0 = \{W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) + 2K\,\Gamma(F_-; a, n)\}\, n - F_+^T\, [S(F)]\, n$$
$$-\operatorname{Div}_t\left(F_-^T \frac{\partial\Gamma}{\partial F}\right) - \operatorname{Div}_t\left(n\otimes\frac{\partial\Gamma}{\partial n}\right) + \nabla^t\Gamma. \tag{3.5}$$

As $\|n\| = 1$, we obtain

$$\operatorname{Div}_t\left(n\otimes\frac{\partial\Gamma}{\partial n}\right).n = \operatorname{Div}_t\left(\frac{\partial\Gamma}{\partial n}\right)$$

and the inner-product of (3.5) by n yields

$$0 = W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) + 2K\,\Gamma(F_-; a, n) - [S(F)]\, n.\, F_+n$$
$$- \operatorname{Div}_t\left(F_-^T\frac{\partial\Gamma}{\partial F}\right).n - \operatorname{Div}_t\left(\frac{\partial\Gamma}{\partial n}\right).$$

Finally, by Proposition 3.1 (iii, iv) we have

$$- \operatorname{Div}_t\left(F_-^T\frac{\partial\Gamma}{\partial F}\right).n = [S(F)]\, n\, .\, F_-n$$

which, together with the previous formula, implies (3.2).

It follows immediatly from Propositions 3.1 and 3.2 that for piecewise-affine, metastable deformations the traction is continuous across the interface and the Maxwell rule holds.

Corollary 3.6.

Let u be a piecewise affine metastable deformation. If (H1), (H'1) and (H'2) hold, then

(i) $[S(F)]\, n = 0$ on I;

(ii) $W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) = 0$ if $(F_-; a, n) \in X \setminus X^*$.

Next, we show that the boundary of Ω near the interface of a two-phase, affine, strongly metastable deformation is qualitatively predictable. Precisely, we prove that there is "neck formation" at the phase boundary.

Proposition 3.7.

Let u be a two-phase, affine, strongly metastable deformation and let $I = \{x \in \Omega \mid x.n + k\}$be the interface of u. Assume that (H1), (H'1) and (H'2) are verified and that $(F_-; a, n) \in X \setminus X^*$.

If $\bar{I} \cap \partial\bar{\Omega}_1 = \varnothing$, then either $\Gamma(F_-; a, n) = 0$ or

$$\limsup_{\rho \to 0^-} \frac{A(\rho) - A(0)}{\rho} \le 0 \le \liminf_{\rho \to 0^+} \frac{A(\rho) - A(0)}{\rho},$$

where $A(t) := \text{area}\, \{x \in \Omega \mid x.n = k + t\}$.

Proof. Assume that $\partial\Omega_1 \subset\subset$ closure (Ω_+), where $\Omega_+ := \{x \in \Omega \mid x.n > k\}$, $\Omega_- := \{x \in \Omega \mid x.n < k\}$, $F_+ = F_- + a \otimes n$ and

$$u(x) = \begin{cases} F_+ x & \text{if } x.n > k \\ \\ F_- x + ka & \text{if } x.n \le k. \end{cases}$$

We define

$$w_\rho^+(x) := \begin{cases} 0 & \text{if } x.n > k + \rho \\ (k + \rho)a - (x.n)a & \text{if } k < x.n < k + \rho \\ \rho a & \text{if } x.n < k \end{cases}$$

and

$$u_\rho^+ := u + w_\rho^+(x).$$

As u is strongly metastable and since

$$u_\rho^+(x + \rho n) = u(x) + \rho(F_- n + a),$$

for ρ sufficiently small, we have

$$E(u) \le E(u_\rho^+);$$

i. e.,

$$\int_{\Omega_{+\rho}} W(F_+)\, dx + \int_I \Gamma(F_-; a, n)\, dS - \int_{\partial\Omega_2 \cap \Omega_{+\rho}} t.u\, dS - \int_{\partial\Omega_2 \cap \Omega_-} t.u\, dS \le$$

$$\int_{\Omega_{+\rho}} W(F_-)\, dx + \int_{I_\rho} \Gamma(F_-; a, n)\, dS - \int_{\partial\Omega_2 \cap \Omega_{+\rho}} t.[u + (k + \rho - x.n)a]\, dS - \int_{\partial\Omega_2 \cap \Omega_-} t.(u + \rho a)\, dS,$$

where

$$\Omega_{+\rho} := \{x \in \bar{\Omega} \mid k < x.n < k + \rho\} \text{ and } I_\rho := \{x \in \Omega \mid x.n = k + \rho\}.$$

Hence

$$\text{meas }(\Omega_{+\rho})\, (W(F_+) - W(F_-)) \le \Gamma(F_-; a, n)\, (A(\rho) - A(0)) + \int_{\partial\Omega_2 \cap \Omega_{+\rho}} t.(x.n - k)a\, dS$$

$$- \rho \int_{\partial\Omega_2 \cap \Omega_{+\rho}} t.a\, dS - \rho \int_{\partial\Omega_2 \cap \Omega_-} t.a\, dS,$$

which, dividing by ρ and letting $\rho \to 0^+$, yields

$$A(0)\, (W(F_+) - W(F_-)) \le \Gamma(F_-; a, n) \liminf_{\rho \to 0^+} \frac{A(\rho) - A(0)}{\rho} - \int_{\partial\Omega_2 \cap \Omega_-} t.a\, dS. \tag{3.8}$$

By Proposition 3.1 (i), (ii) and Corollary 3.6 (i), we have

$$\int_{\partial\Omega_2 \cap \Omega_-} t.a\, dS = -A(0)\, S(F_-).(F_+ - F_-)$$

and so, since the Maxwell rule is satisfied (see Corollary 3.6 (ii)),we conclude from (3.8) that either

$$\Gamma(F_-; a, n) = 0$$

or

$$\liminf_{\rho \to 0^+} \frac{A(\rho) - A(0)}{\rho} \ge 0.$$

In a similar way, if we consider variations

$$u_\rho^- := u + w_\rho^-(x)$$

with ρ > 0 and

$$w_\rho^-(x) := \begin{cases} 0 & \text{if } x.n > k \\ (x.n - k)a & \text{if } k - \rho < x.n < k \\ -\rho a & \text{if } x.n < k - \rho, \end{cases}$$

we conclude that

$$\Gamma(F_-; a, n) \limsup_{\rho \to 0^-} \frac{A(\rho) - A(0)}{\rho} \leq 0.$$

Remarks 3.9.

(i) It is natural to suppose that the homogeneous deformations forming the different phases of a metastable, piecewise affine, deformation u correspond to local minima of the energy density W (see PARRY [32]). If F_- and $F_+ = F_- + a \otimes n$ are the gradients of adjoint variants of u and if $(F_-; a, n) \in X \setminus X^*$, then, by Corollary 3.6 (ii), we would obtain

$$W(F_+) = W(F_-). \tag{3.10}$$

However, the photographs of RICHMAN [34] of twinned cubic crystals seem to suggest that F^+ and F^- are not symmetry related, and so (3.10) is, in general, violated.

We therefore obtain a confirmation of PARRY's conjecture: namely, the gradients of a metastable, piecewise affine, deformation correspond to points where the interfacial energy Γ is not differentiable. This fact could explain the preferred directions of the phase boundaries (see CAHN & HOFFMAN [6], [7]).

(ii) In [32] PARRY derives sufficient conditions for strong metastability of an undeformed shear band under null loading; among those we have

(1) F_- and $F_- + a \otimes n$ provide local minima of W;

(2) $\Gamma(F_-; a, n') \leq \Gamma(F; \lambda a, n')$ for all (F, n', λ) close enough to $(F_-, n, 1)$;

(3) $(F_-; a, n) \in X^*$;

(4) (*local Wulff's condition*) If $\|v\| = 1 = \|w\|$, $\|v - n\|$ and $\|w - n\|$ are sufficiently small, and if $\lambda, \mu \geq 0$ and $\lambda v + \mu w = n$, then

$$\Gamma(F_-; a, n) < \lambda\, \Gamma(F; a, v) + \mu\, \Gamma(F_-; a, w).$$

In (i) we remarked that (1) would imply (3.10) if (3) was violated. We now examine conditions (2) and (4) in the inhomogeneous case in which (3) fails.

Let u be a metastable deformation and let $x_0 \in I$ be such that:

(2') $\Gamma(F_-(x); a(x), n(x) + \varepsilon n') \leq \Gamma(F_-(x) + \varepsilon c \otimes d; a(x), n(x) + \varepsilon n')$ for all $\varepsilon \in [-\varepsilon_0, \varepsilon_0]$, c, d, $n' \in \partial B(0, 1)$ and $x \in B(x_0, \varepsilon_0) \cap I$, (3') $(F_-(x_0); a(x_0), n(x_0)) \in X \setminus X^*$,

(4') For every $x \in B(x_0, \varepsilon_0) \cap I$ there exists $\varepsilon > 0$ such that if $\|v\| = 1 = \|w\|$, $\|v - n(x)\| < \varepsilon$, $\|w - n(x)\| < \varepsilon$, $\lambda, \mu \geq 0$ and $\lambda v + \mu w = n(x)$ then

$$\Gamma(F_-(x); a(x), n(x)) \leq \lambda\, \Gamma(F_-(x); a(x), v) + \mu\, \Gamma(F_-(x); a(x), w).$$

By (2') we have

$$\frac{\partial \Gamma}{\partial F}(F_-(x); a(x), n(x)) \,.\, c \otimes d = 0$$

for all $c, d \in \partial B(0, 1)$ and $x \in B(x_0, \varepsilon_0) \cap I$. Therefore,

$$\frac{\partial \Gamma}{\partial F}(F_-(x); a(x), n(x)) = 0$$

and from Proposition 3.1 (iv) and Proposition 3.2 (ii) we deduce that

$$[S(\nabla u)]\, n = 0$$

on $B(x_0, \varepsilon_0) \cap I$. Hence, since $X \setminus X^*$ is an open set,

$$W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) + 2K\, \Gamma(F_-; a, n) - \mathrm{Div}_t\left(\frac{\partial \Gamma}{\partial n}\right) = 0. \tag{3.11}$$

It turns out if that I is a surface of minimal area (see FONSECA & TARTAR [16], GURTIN [17], [18], [19], [20], KOHN & STERNBERG [26], MODICA [28], OWEN [29], [30], OWEN & STENBERG [31] and STERNBERG [35], [36]), then (3.11) reduces to

$$W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) - \mathrm{Div}_t\left(\frac{\partial \Gamma}{\partial n}\right) = 0.$$

Finally, we show that (4') implies that

$$\Gamma(F_-(x); a(x), n(x)) + \frac{\partial^2 \Gamma}{\partial n^2}(F_-(x); a(x), n(x))\, \xi.\xi \geq 0 \tag{3.12}$$

for all ξ such that $\|\xi\| = 1$, $\xi.n(x) = 0$. Fix $x \in B(x_0, \varepsilon_0) \cap I$, $k \in \mathbb{N}$ and let

$$w(t) := \frac{n + tk\xi}{1 + t^2k^2}.$$

Let μ be a smooth function such that

$$0 < \mu(0) < 1$$

and define

$$\lambda(t) := \|\mu(t)w(t) - n\|$$

and

$$v(t) := \frac{n - \mu(t)w(t)}{\lambda(t)}.$$

By (4') and Proposition 3.2 (i),

$$0 \le \frac{d^2}{dt^2}\Big|_{t=0}\{\lambda(t)\,\Gamma(F_-;\, a, v(t)) + \mu(t)\,\Gamma(F_-;\, a, w(t))\}$$

$$=(\lambda''(0) + \mu''(0))\left(\Gamma(F_-;\, a, n) - \frac{\partial\Gamma}{\partial n}(F_-;\, a, n).n\right) + k^2\frac{\mu(0)}{1-\mu(0)}\,\frac{\partial^2\Gamma}{\partial n^2}(F_-;\, a, n)\,\xi.\,\xi$$

$$= \frac{\mu(0)}{1-\mu(0)}\left\{(\mu'(0)^2 + k^2)\,\Gamma(F_-;\, a, n) + k^2\,\frac{\partial^2\Gamma}{\partial n^2}(F_-;\, a, n)\,\xi.\,\xi\right\}.$$

Dividing the previous inequality by k^2 and letting $k \to \infty$, we obtain (3.12).

4. QUASICONVEXITY OF THE SURFACE ENERGY DENSITY Γ.

It is well known that if u is p-weakly-metastable and if $x_0 \in \Omega_i$ for some $i = 1, \ldots, M$, then W is *quasiconvex at F*, where $F = \nabla u(x_0)$, i. e.

$$\int_D W(F + \nabla\varphi(x))\,dx \ge W(F)\,\mathrm{meas}D \tag{4.1}$$

for every bounded open set $D \subset \mathbb{R}^3$ and for every $\varphi \in \mathcal{D}(D;\, \mathbb{R}^3)$ satisfying $\det(F + \nabla\varphi(x)) > 0$ for all $x \in D$ (see BALL [3]). Also, if (4.1) holds, then W is *rank one convex at F*; i. e.,

$$W(F) \le \theta\, W(F + c\otimes d) + (1-\theta)\, W\!\left(F - \frac{\theta}{1-\theta}c\otimes d\right) \tag{4.2}$$

for all $\theta \in [0, 1)$ and for all $c, d \in \mathbb{R}^3$ such that $\det(F + \alpha\, c \otimes d) > 0$ with $\alpha \in \{1, \theta(\theta - 1)^{-1}\}$. In this section we obtain conditions analogous to (4.1) and (4.2) for the interfacial energy density Γ.

Let I be an interface of u and let $x_0 \in I$. In the sequel we will use the notation

$(F_-;\, a, n) := (F_-(x_0);\, a(x_0), n(x_0))$

and, for D a subset of $\mathbb{R}^3$, we define

$D^* := \{x \in D \mid x.n(x_0) = 0\}$.

Proposition 4.3.

Let u be p-weakly-metastable and assume that (H1), (H'1) and (H'2) hold. If $x_0 \in I$ then

(i) (*Quasi convexity*)

$$\int_{D^*} \Gamma(F_- + \nabla\varphi(y); a, n)\, dS \geq \text{area } (D^*)\, \Gamma(F_-; a, n)$$

for every bounded open set $D \subset \mathbb{R}^3$ and for every $\varphi \in \mathcal{D}(D; \mathbb{R}^3)$ satisfying $\det (F_+ + \nabla\varphi(x)) > 0$ and $\det (F_- + \nabla\varphi(x)) > 0$ for all $x \in D$;

(ii) (*Rank one convexity*)

$$\Gamma(F_-; a, n) \leq \theta\, \Gamma(F_- + c\otimes d; a, n) + (1-\theta)\, \Gamma\left(F_- - \frac{\theta}{1-\theta} c\otimes d; a, n\right)$$

for all $\theta \in [0, 1)$ and for all $c, d \in \mathbb{R}^3$ such that $\det (F_+ + \alpha\, c \otimes d) > 0$ and $\det (F_- + \alpha\, c \otimes d) > 0$ with $\alpha \in \{1, \theta(\theta - 1)^{-1}\}$.

Proof. (i) Let $D \subset \mathbb{R}^3$ be a bounded open set and let $\varphi \in \mathcal{D}(D; \mathbb{R}^3)$ be such that $\det (F_+ + \nabla\varphi(x)) > 0$ and $\det (F_- + \nabla\varphi(x)) > 0$ for all $x \in D$. Consider the variations

$$u_\varepsilon(x) := u(x) + \varepsilon\varphi\left(\frac{x - x_0}{\varepsilon}\right).$$

For $|\varepsilon|$ sufficiently small we have $E(u) \leq E(u_\varepsilon)$; i.e.,

$$\int_{x_0+\varepsilon D} W(\nabla u(x))\, dx + \int_{I\cap(x_0+\varepsilon D)} \Gamma(F_-(x); a(x), n(x))\, dS \leq$$

$$\int_{x_0+\varepsilon D} W\left(\nabla u(x) + \nabla\varphi\left(\frac{x - x_0}{\varepsilon}\right)\right) dx + \int_{I\cap(x_0+\varepsilon D)} \Gamma\left(F_-(x) + \nabla\varphi\left(\frac{x - x_0}{\varepsilon}\right); a(x), n(x)\right) dS$$

$$- \varepsilon\int_{x_0+\varepsilon D} f(x).\varphi\left(\frac{x - x_0}{\varepsilon}\right) dx.$$

Using the change of variable $x = x_0 + \varepsilon y$, we obtain, using (2.4),

$$\varepsilon^3\int_D W(\nabla u(x_0 + \varepsilon y))\, dy + \varepsilon^2\int_{D\cap\frac{I-x_0}{\varepsilon}} \Gamma(F_-(x_0 + \varepsilon y); a(x_0 + \varepsilon y), n(x_0 + \varepsilon y))\, dS \leq$$

$$\varepsilon^3 \int_D W(\nabla u(x_0 + \varepsilon y) + \nabla\varphi(y))\, dy + \varepsilon^2\int_{D\cap\frac{I-x_0}{\varepsilon}} \Gamma(F_-(x_0 + \varepsilon y) + \nabla\varphi(y); a(x_0 + \varepsilon y), n(x_0 + \varepsilon y))\, dS$$

$$- \varepsilon^4\int_D f(x_0 + \varepsilon y).\varphi(y)\, dy.$$

Dividing the previous inequality by ε^2 and letting $\varepsilon \to 0$, by (2.7) we conclude that

$$\int_{D^*} \Gamma(F_- + \nabla\varphi(y); a, n)\, dS \geq \text{area } (D^*)\, \Gamma(F_-; a, n).$$

(ii) Let $c, d \in \mathbb{R}^3$ and $\theta \in [0, 1)$ be such that $\|d\| = 1$, $\det(F_+ + \alpha c \otimes d) > 0$ and $\det(F_- + \alpha c \otimes d) > 0$ with $\alpha \in \{1, \theta(\theta - 1)^{-1}\}$. Due to the continuity of Γ, with no loss of generality we can assume that d is not parallel to n. We consider the construction made in FONSECA [15], Theorem 2.4; precisely, let $\{v, w, d\}$ be an orthonormal basis of $\mathbb{R}^3$ and let $k_0 \in \mathbb{N}$ be such that

$$\det\left(F_+ + \frac{2\theta}{k} c\otimes v\right) > 0 \text{ and } \det\left(F_- + \frac{2\theta}{k} c\otimes v\right) > 0$$

for all $k \in \mathbb{N}$, $k \geq k_0$, and for every $v \in \mathbb{R}^3$ with $\|v\| = 1$. For $k \geq k_0$ let Q_k be the parallelepiped

$$Q_k := \left\{ x \in \mathbb{R}^3 \mid |x.v| \leq \frac{k}{2},\ |x.w| \leq \frac{k}{2} \text{ and } \theta - 1 \leq x.d \leq \theta \right\}$$

with vertices

$$A_1^k = \left(\frac{k}{2}, \frac{k}{2}, \theta\right), A_2^k = \left(-\frac{k}{2}, \frac{k}{2}, \theta\right), A_3^k = \left(-\frac{k}{2}, -\frac{k}{2}, \theta\right), A_4^k = \left(\frac{k}{2}, -\frac{k}{2}, \theta\right)$$

and

$$A_5^k = \left(\frac{k}{2}, \frac{k}{2}, \theta-1\right), A_6^k = \left(-\frac{k}{2}, \frac{k}{2}, \theta-1\right), A_7^k = \left(-\frac{k}{2}, -\frac{k}{2}, \theta-1\right), A_8^k = \left(\frac{k}{2}, -\frac{k}{2}, \theta-1\right).$$

In addition, we consider the following points in Q_k:

$$B_1^k = \left(\frac{k-k_0}{2}, \frac{k-k_0}{2}, 0\right), B_2^k = \left(-\frac{k-k_0}{2}, \frac{k-k_0}{2}, 0\right), B_3^k = \left(-\frac{k-k_0}{2}, -\frac{k-k_0}{2}, 0\right)$$

and

$$B_4^k = \left(\frac{k-k_0}{2}, -\frac{k-k_0}{2}, 0\right).$$

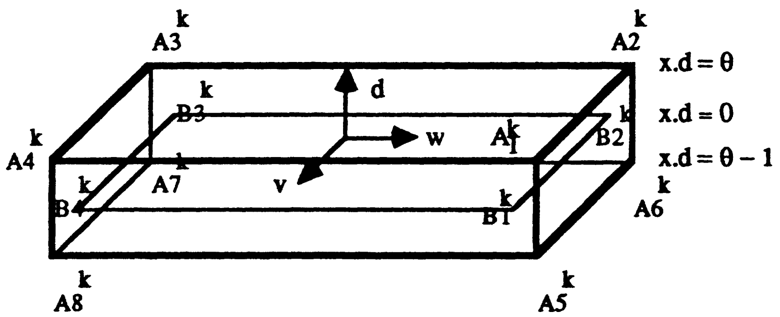

Fig. 1

We decompose Q_k as

$$Q_k = Q_k^+ \cup Q_k^- \bigcup_{i=1}^{4} T_i^k,$$

where

$$Q_k^+ := \text{convex hull } \{A_1^k, A_2^k, A_3^k, A_4^k, B_1^k, B_2^k, B_3^k, B_4^k\},$$

$Q_k^- :=$ convex hull $\{A_5^k, A_6^k, A_7^k, A_8^k, B_1^k, B_2^k, B_3^k, B_4^k\}$,
$T_1^k :=$ convex hull $\{A_1^k, A_4^k, A_5^k, A_8^k, B_1^k, B_4^k\}$,
$T_2^k :=$ convex hull $\{A_1^k, A_2^k, A_5^k, A_6^k, B_1^k, B_2^k\}$,
$T_3^k :=$ convex hull $\{A_2^k, A_3^k, A_6^k, A_7^k, B_2^k, B_3^k\}$,
$T_4^k :=$ convex hull $\{A_3^k, A_4^k, A_7^k, A_8^k, B_3^k, B_4^k\}$.

Next, we define the functions

$$w_k(x) := \begin{cases} c\otimes d\, x - \theta c & \text{if } x \in Q_k^+ \\ \dfrac{\theta}{\theta-1} c\otimes d\, x - \theta c & \text{if } x \in Q_k^- \\ \dfrac{2\theta}{k_0} c\otimes v\, x - \dfrac{\theta k}{k_0} c & \text{if } x \in T_1^k \\ \dfrac{2\theta}{k_0} c\otimes w\, x - \dfrac{\theta k}{k_0} c & \text{if } x \in T_2^k \\ -\dfrac{2\theta}{k_0} c\otimes v\, x - \dfrac{\theta k}{k_0} c & \text{if } x \in T_3^k \\ -\dfrac{2\theta}{k_0} c\otimes w\, x - \dfrac{\theta k}{k_0} c & \text{if } x \in T_4^k \\ 0 & \text{otherwise.} \end{cases}$$

If $\mathcal{S}_k$ denotes the set of interfaces of w_k, then there exists a sequence $\varphi_{m,k} \in C^1(\mathbb{R}^3; \mathbb{R}^3)$ such that

$$\operatorname{supp} \varphi_{m,k} \subset Q_{2k},$$

$$\varphi_{m,k} \to w_k \text{ in } L^\infty,$$

$$\nabla\varphi_{m,k} \to \nabla w_k \text{ for all } x \notin \mathcal{S}_k,$$
$$\sup_{m,k} \|\nabla\varphi_{m,k}\|_\infty < \infty$$

and

$$\inf_{m,k,x} \{\det (F_+ + \nabla\varphi_{m,k}(x)), \det (F_+ + \nabla\varphi_{m,k}(x))\} > 0.$$

Moreover, since d is not parallel to $n(x_0)$, for k large enough we have

$$\text{area}\, (Q_{2k}^* \cap \mathcal{S}_k) = 0.$$

Therefore, by (i),

$$\Gamma(F_-; a, n)\, \text{area}\, (Q_{2k}^*) \le \int_{Q_{2k}^*} \Gamma(F_- + \nabla\varphi_{m,k}(x); a, n)\, dS$$

and so, passing to the limit in m, we deduce that

$$\Gamma(F_-; a, n) \le \frac{1}{\text{area}\, (Q_k^*)} \int_{Q_k^*} \Gamma(F_- + \nabla w_k(x); a, n)\, dS.$$

Hence, by the definition of w_k,

$$\Gamma(F_-; a, n) \leq \frac{\text{area }(Q_k^+)^*}{\text{area }(Q_k^*)}\,\Gamma(F_- + c\otimes d; a, n) + \frac{\text{area }(Q_k^-)^*}{\text{area }(Q_k^*)}\,\Gamma\left(F_- - \frac{\theta}{1-\theta}\,c\otimes d; a, n\right)$$
$$+ \sum_{i=1}^{4} \frac{\text{area }(T_i^k)^*}{\text{area }(Q_k^*)} \max\left\{\Gamma\left(F_- \pm \frac{2\theta}{k_0}\,c\otimes v; a, n\right), \Gamma\left(F_- \pm \frac{2\theta}{k_0}\,c\otimes w; a, n\right)\right\}.$$

Finally, letting $k \to \infty$,

$$\Gamma(F_-; a, n) \leq \theta\,\Gamma(F_- + c\otimes d; a, n) + (1-\theta)\,\Gamma\left(F_- - \frac{\theta}{1-\theta}\,c\otimes d; a, n\right).$$

Remark 4.4.

(i) Suppose that u is p-weakly-metastable. If $u \in C^1$ near x_0, then (4.2) yields

$$W(\nabla u(x_0) + c\otimes d) - W(\nabla u(x_0)) - S(\nabla u(x_0))\,.\,c\otimes d \geq 0 \tag{4.5}$$

for all $c, d \in \mathbb{R}^3$ such that $\det(\nabla u(x_0) + c\otimes d) > 0$. Hence, if we disregard the contribution of the surface energy, the traction is continuous across the interface (see Proposition 3.1 (iv)) and from (4.5) it follows that the Maxwell rule holds (see JAMES [24]); namely, if $x_0 \in I$, then

$$[S(\nabla u(x_0))]\,n(x_0) = 0$$

and

$$W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) = 0. \tag{4.6}$$

Consider sequences $x_m \in \Omega_i$ and $y_m \in \Omega_j$ converging to x_0. By (4.5)

$$W(\nabla u(x_m) - a(x_0)\otimes n(x_0)) - W(\nabla u(x_m)) + S(\nabla u(x_m))\,.\,a(x_0)\otimes n(x_0) \geq 0$$

and

$$W(\nabla u(y_m) + a(x_0)\otimes n(x_0)) - W(\nabla u(y_m)) - S(\nabla u(y_m))\,.\,a(x_0)\otimes n(x_0) \geq 0.$$

Letting $m \to +\infty$, we conclude that

$$W(F_-) - W(F_+) - S(F_+).(F_- - F_+) \geq 0$$

and (4.7)

$$W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) \geq 0.$$

It is clear that $(4.7)_{1,2}$ are still valid when we include the interfacial energy term in the total energy functional.

(ii) Let u be p-weakly-metastable and assume that (H1), (H'1) and (H'2) are satisfied. Let $x_0 \in I$ and, as in Remark 3.9 (ii), consider the following hypothesis:

(2") $\Gamma(F_-(x); a(x), n(x)) \le \Gamma(F_-(x) + \varepsilon c \otimes d; a(x), n(x))$

for all $\varepsilon \in [-\varepsilon_0, \varepsilon_0]$, $c, d \in \partial B(0, 1)$ and $x \in B(x_0, \varepsilon_0) \cap I$. Then (2") holds if and only if

$$\frac{\partial \Gamma}{\partial F}(F_-; a, n) = 0 \tag{4.8}$$

on $B(x_0, \varepsilon_0) \cap I$. It is clear that (2") implies (4.8). Conversely, by Proposition 4.3 (ii),

$$\frac{d}{d\theta}\Big|_{\theta=0}\left\{ \theta\, \Gamma(F_- + \varepsilon c \otimes d; a, n) + (1-\theta)\, \Gamma\left(F_- - \frac{\theta}{1-\theta}\, \varepsilon c \otimes d; a, n\right)\right\} \ge 0,$$

which, together with (4.8), yields (2"). Therefore, if (2") holds then by Proposition 3.1 (iv), (4.7) and (4.8) we conclude that the traction is continuous across the interface, i.e.

$$[S(\nabla u(x_0))]\, n(x_0) = 0$$

and the Maxwell rule (4.6) is satisfied.

Next, we deduce corresponding quasiconvexity and rank one convexity conditions for a p-metastable deformation.

Proposition 4.9.

Let u be p-metastable and assume that (H1), (H'1) and (H'2) hold. If $x_0 \in I$, then

(i) (*Quasi-convexity*)

$$\int_{D^{**}} \Gamma(F_-(\mathbb{1} + \nabla\varphi(y));\; a, (\mathbb{1} + \nabla\varphi^T(y))n)\, dS \ge \text{area}(D^*)\, \Gamma(F_-; a, n)$$

for every bounded open set $D \subset \mathbb{R}^3$ and for every $\varphi \in \mathcal{D}(D; \mathbb{R}^3)$ satisfying $\det(\mathbb{1} + \nabla\varphi(y)) > 0$ for all $y \in D$, with $D^{**} := \{y \in D \mid (y + \varphi(y)).n = 0\}$;

(ii) (*Rank one convexity*)

$$\Gamma(F_-; a, n) \le \theta\, \|n + (c.n)d\|\, \Gamma(F_-(\mathbb{1} + c \otimes d); a, (\mathbb{1} + d \otimes c)n)$$
$$+ \|n - \theta(n + (c.n)d)\|\, \Gamma\left(F_-\left(\mathbb{1} - \frac{\theta}{1-\theta} c \otimes d\right); a, \left(\mathbb{1} - \frac{\theta}{1-\theta} d \otimes c\right) n\right)$$

for all $\theta \in [0, 1)$ and for all $c, d \in \mathbb{R}^3$ such that $\det(\mathbb{1} + \alpha\, c \otimes d) > 0$ with $\alpha \in \{1, \theta(\theta - 1)^{-1}\}$.

Proof. (i) For $|\varepsilon|$ sufficiently small, consider the deformations

$$u_\varepsilon(x) := u\left(x + \varepsilon\varphi\left(\frac{x - x_0}{\varepsilon}\right)\right).$$

Then $E(u) \le E(u_\varepsilon)$; i. e.,

$$\int_{x_0+\varepsilon D} W(\nabla u(x))\,dx + \int_{I\cap(x_0+\varepsilon D)} \Gamma(F\_(x); a(x), n(x))\,dS - \int_{x_0+\varepsilon D} f(x).u(x)\,dx$$

$$\le \int_{x_0+\varepsilon D} W\left(\nabla u\left(x+\varepsilon\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right)\left(\mathbb{1}+\nabla\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right)\right) dx$$

$$+\int_{I_\varepsilon}\Gamma\left(F\_\left(x+\varepsilon\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right)\left(\mathbb{1}+\nabla\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right);\ a\left(x+\varepsilon\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right),\left(\mathbb{1}+\nabla\varphi^T\left(\frac{x-x_0}{\varepsilon}\right)\right)n\left(x+\varepsilon\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right)\right)dS$$

$$-\int_{x_0+\varepsilon D} f(x).u\left(x+\varepsilon\varphi\left(\frac{x-x_0}{\varepsilon}\right)\right) dx,$$

where

$$I_\varepsilon := \left\{x \in x_0+\varepsilon D \mid x+\varepsilon\varphi\left(\frac{x-x_0}{\varepsilon}\right) \in I\right\}.$$

Making the change of variables

$$y = \frac{x-x_0}{\varepsilon}$$

and setting

$$w(y) := y + \varphi(y)$$

we obtain

$$\varepsilon^3\int_D W(\nabla u(x_0+\varepsilon y))\,dy + \varepsilon^2\int_{D\cap\frac{I-x_0}{\varepsilon}} \Gamma(F\_(x_0+\varepsilon y); a(x_0+\varepsilon y), n(x_0+\varepsilon y))\,dS$$

$$-\varepsilon^3\int_D f(x_0+\varepsilon y)\,.u(x_0+\varepsilon y)\,dy$$

$$\le \varepsilon^3\int_D W(\nabla u(x_0+\varepsilon w(y))\nabla w(y))\,dy$$

$$+\varepsilon^2\int_{D\cap w^{-1}\left(\frac{I-x_0}{\varepsilon}\right)} \Gamma(F\_(x_0+\varepsilon w(y))\nabla w(y); a(x_0+\varepsilon w(y)), \nabla w^T(y)\, n(x_0+\varepsilon w(y)))\,dS$$

$$+\varepsilon^3\int_D f(x_0+\varepsilon y).u(x_0+\varepsilon w(y))\,dy.$$

Dividing the previous inequality by ε^2 and letting $\varepsilon \to 0$, by (2.7), we deduce that

$$\text{area}(D^*)\,\Gamma(F\_; a, n) \le \lim_{\varepsilon\to 0}\int_{D\cap w^{-1}\left(\frac{I-x_0}{\varepsilon}\right)} \Gamma(F\_\nabla w(y); a, \nabla w^T(y)\, n)\,dS$$

$$= \lim_{\varepsilon\to 0}\int_{w(D)\cap\frac{I-x_0}{\varepsilon}} \Gamma(F\_\nabla w(w^{-1}(x)); a, \nabla w^T(w^{-1}(x))\, n)\,\|\text{adj}\nabla w^{-1}(x)\nu(x)\|\,dS$$

$$= \int_{w(D)\cap\{x \mid x.n=0\}} \Gamma(F\_\nabla w(w^{-1}(x)); a, \nabla w^T(w^{-1}(x))\, n)\,\|\text{adj}\nabla w^{-1}(x)n\|\,dS$$

$$= \int_{D^{**}} \Gamma(F\_\nabla w(y); a, \nabla w^T(y)\, n)\, dS.$$

(ii) Here we use the same construction of the proof of Proposition 4.3 (ii) and, in a similar way, we assume (without loss of generality) that $||d|| = 1$ and that d is not parallel to n. Also, we can suppose that $(n.v)v + (n.w)w$ is not parallel either to $v + w$ or to $v - w$. By part (i),

$$\begin{aligned} \text{area}(Q_k^*)\, \Gamma(F\_; a, n) &\le \int_{Q_k^{**}} \Gamma(F\_(\mathbb{1} + \nabla w_k(y)); a, (\mathbb{1} + \nabla w_k^T(y))n)\, dS \\ &\le \text{area}\, (Q_k^+)^{**}\, \Gamma(F\_(\mathbb{1} + c\otimes d); a, (\mathbb{1} + d\otimes c)n) \\ &+ \text{area}\, (Q_k^-)^{**}\, \Gamma\left(F\_\left(\mathbb{1} - \frac{\theta}{1-\theta}\, c\otimes d\right); a, \left(\mathbb{1} - \frac{\theta}{1-\theta}\, d\otimes c\right)n\right) \\ &+ \text{Const.} \sum_{i=1}^{4} \text{area}\, (T_i^k)^{**}. \end{aligned} \tag{4.10}$$

Clearly,

$$\begin{aligned} \limsup_{k\to+\infty} \frac{\text{area}\, (Q_k^+)^{**}}{\text{area}(Q_k^*)} &\le \lim_{k\to+\infty} \frac{\text{area}\, \{y \in Q_k \mid 0 \le y \le \theta \text{ and } y.(n + (c.n)d) = \theta\, c.n\}}{\text{area}\, \{y \in Q_k \mid y.n = 0\}} \\ &= \lim_{k\to+\infty} \frac{\text{area}\, \{y \in Q_k \mid 0 \le y \le \theta \text{ and } y.(n + (c.n)d) = 0\}}{\text{area}\, \{y \in Q_k \mid y.n = 0\}}. \end{aligned} \tag{4.11}$$

We claim that

$$\lim_{k\to+\infty} \frac{\text{area}\, \{y \in Q_k \mid 0 \le y \le \theta \text{ and } y.(n + \alpha d) = 0\}}{\text{area}\, \{y \in Q_k \mid y.n = 0\}} = \theta\, ||n + \alpha d|| \tag{4.12}$$

for all $\alpha \in \mathbb{R}$. In fact, by the assumptions made on n, d, v and w, for k large enough

$$\text{area}\, \{y \in Q_k \mid 0 \le y.d \le \theta \text{ and } y.(n + \alpha d) = 0\} = ||C - O||\, ||A_k - B_k||$$

and

$$\text{area}\, \{y \in Q_k \mid y.n = 0\} = ||A - B||\, ||A_k - B_k||,$$

where we have used the notation of Figures 2 and 3. Since

$$||A - B|| = \frac{1}{|\sin \beta|} = \frac{1}{\sqrt{1 - (d.n)^2}}$$

and

$$\begin{aligned} ||C - O|| &= \frac{\theta}{|\sin \gamma|} \\ &= \frac{\theta}{\sqrt{1 - \dfrac{((n + \alpha d).d)^2}{||n + \alpha d||^2}}} \\ &= \frac{\theta\, ||n + \alpha d||}{\sqrt{1 - (d.n)^2}} \end{aligned}$$

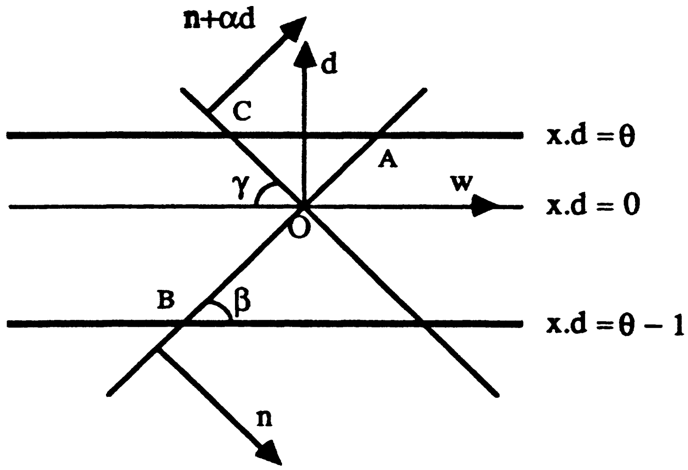

Fig. 2. Intersection of the planes $\{y.(n + \alpha d) = 0\}$ and $\{y.n = 0\}$ with $Q_k \cap \text{Span}\,\{d, n\}$.

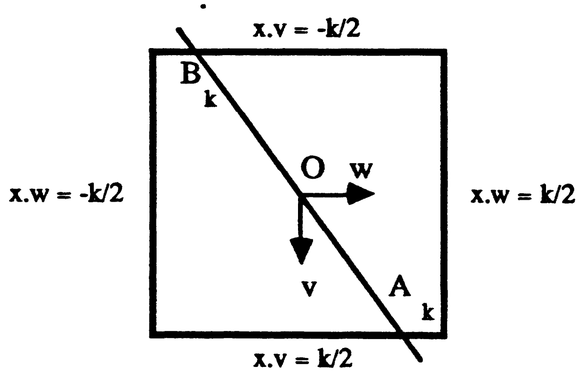

Fig.3. Intersection of the planes $\{y.(n + \alpha d) = 0\}$ and $\{y.n = 0\}$ with $\{y \in Q_k \mid y.d = 0\}$.

we obtain (4.12). Hence, by (4.11) and (4.12),

$$\limsup_{k \to +\infty} \frac{\text{area}\,(Q_k^+)^{**}}{\text{area}(Q_k^*)} \leq \theta \,\|\, n + (c.n)d\| \tag{4.13}$$

and, in a similar way, we have

$$\begin{aligned}\limsup_{k \to +\infty} \frac{\text{area}\,(Q_k^-)^{**}}{\text{area}(Q_k^*)} &\leq (1 - \theta)\, \|n - \frac{\theta}{1-\theta}(c.n)d\| \\ &= \|n - \theta(n + (c.n)d)\|. \end{aligned} \tag{4.14}$$

Finally, as

$$\limsup_{k \to +\infty} \frac{\sum_{i=1}^{4} \text{area}(T_i^k)^{**}}{\text{area}(Q_k^*)} = 0$$

by (4.10), (4.13) and (4.14) we conclude that

$$\Gamma(F_-; a, n) \leq \theta \, \|n + (c.n)d\| \, \Gamma(F_-(\mathbb{1} + c\otimes d); a, (\mathbb{1} + d\otimes c)n)$$
$$+ \|n - \theta(n + (c.n)d)\| \, \Gamma\Big(F_-\Big(\mathbb{1} - \frac{\theta}{1-\theta} c\otimes d\Big); a, \Big(\mathbb{1} - \frac{\theta}{1-\theta} d\otimes c\Big)n\Big).$$

5. CONSEQUENCES OF THE RANK ONE CONVEXITY OF Γ.

It is well known that, due to frame indifference, the Cauchy stress tensor

$$\frac{1}{\det F} \frac{\partial W}{\partial F} F^T$$

is symmetric. We now show that frame indifference effects in a similar way, the tensor

$$\frac{\partial \Gamma}{\partial F} F^T.$$

Proposition 5.1.

Let (H1), (H2), (H'1), (H'2), (H'3) and (H'5) hold. Then

(i) $\frac{\partial \Gamma}{\partial F}(F; a,n)\, F^T + \frac{\partial \Gamma}{\partial a}(F; a, n)\otimes a$ is a symmetric matrix for all $(F; a, n) \in X \setminus X^*$;

(ii) if u is phase-metastable, then

$$\frac{\partial \Gamma}{\partial F}(F_-; a, n)\, F_-^T \text{ is a symmetric matrix}$$

and

$$\text{either } \Gamma(F_-; a, n) = 0 \quad \text{or} \quad \frac{\partial \Gamma}{\partial a}(F_-; a, n) = 0$$

for all $x \in I \cap \Omega_0$.

Proof. (i) Let Λ be a skew-symmetric matrix. By (H'5),

$$\Gamma(e^{\varepsilon\Lambda}F; e^{\varepsilon\Lambda}a, n) = \Gamma(F; a, n);$$

thus, differentiating with respect to ε at $\varepsilon = 0$,

$$\Big(\frac{\partial \Gamma}{\partial F} F^T + \frac{\partial \Gamma}{\partial a} \otimes a\Big).\Lambda = \frac{\partial \Gamma}{\partial F} .\Lambda F + \frac{\partial \Gamma}{\partial a} .\Lambda a = 0,$$

which proves part (i).

(ii) Let $g : \mathbb{R} \to \mathbb{R}$ be a smooth function such that

$$g(s) = 0 \text{ if } s > 1 \text{ and } \int_0^1 s^2 g'(s)\, ds \neq 0$$

and define

$$g_r(s) := r\, g\left(\frac{s}{r}\right) \text{ for } r > 0.$$

Let Λ be a skew-symmetric matrix and let $x_0 \in I$. Consider the variations

$$u_{\varepsilon,r}(x) := \begin{cases} u(x_0) + e^{\varepsilon \Lambda g_r(|x - x_0|)}(u(x) - u(x_0)) & \text{if } |x - x_0| < r \\ \\ u(x) & \text{otherwise.} \end{cases}$$

As

$$\|u_{\varepsilon,r} - u\|_{1,\infty} \text{ converges to } 0 \text{ as } \varepsilon \to 0^+,$$

we obtain

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} E(u_{\varepsilon,r}) \geq 0.$$

Since

$$\nabla u_{\varepsilon,r}(x) := \begin{cases} e^{\varepsilon \Lambda g_r(|x - x_0|)}\left(\nabla u(x) + \varepsilon\Lambda(u(x) - u(x_0)) \otimes g'\left(\frac{|x - x_0|}{r}\right)\frac{x - x_0}{|x - x_0|}\right) & \text{if } |x - x_0| < r \\ \\ \nabla u(x) & \text{otherwise} \end{cases}$$

and as $-\Lambda$ is also skew-symmetric, by (H2) and (H'5),

$$0 = \int_{B(x_0,r)} \frac{\partial W}{\partial F}(F(x)).\left[\Lambda(u(x) - u(x_0)) \otimes g'\left(\frac{|x - x_0|}{r}\right)\frac{x - x_0}{|x - x_0|}\right] dx$$
$$+ \int_{I \cap B(x_0,r)} \frac{\partial \Gamma}{\partial F}(F_-(x); a(x), n(x)).\left[\Lambda(u(x) - u(x_0)) \otimes g'\left(\frac{|x - x_0|}{r}\right)\frac{x - x_0}{|x - x_0|}\right] dx$$
$$- \int_{B(x_0,r)} f(x).\left(r\, \Lambda\, g\left(\frac{|x - x_0|}{r}\right)(u(x) - u(x_0))\right).$$

Making the change of variables

$$x - x_0 = ry,$$

dividing through the previous equation by r^3, and letting $r \to +\infty$, we obtain

$$\frac{\partial \Gamma}{\partial F} \cdot \left(\Lambda F_- \int_{\{y \mid |y|<1,\ y.n=0\}} y \otimes g'(|y|)\, \frac{y}{|y|}\, dS(y)\right) = 0. \tag{5.2}$$

Finally, as

$$\int_{\{y \mid |y|<1,\ y.n=0\}} y \otimes g'(|y|)\, \frac{y}{|y|}\, dS(y) = \pi \int_0^1 s^2 g'(s)\, ds\, (\mathbb{1} - n\otimes n),$$

Proposition 3.1 (iii) and (5.2) yield

$$0 = \frac{\partial \Gamma}{\partial F} \cdot \Lambda F_-\, (\mathbb{1} - n\otimes n) = \frac{\partial \Gamma}{\partial F} F_-^T \cdot \Lambda.$$

Hence $(\partial\Gamma/\partial F)\, F_-^T$ is a symmetric matrix which, together with part (i), implies that $\partial\Gamma/\partial a$ is parallel to a.

From Proposition 3.2 (i) we conclude that either $a = 0$ or $\partial\Gamma/\partial a = 0$.

ERICKSEN [12] proved that, when there is no interfacial energy contribution, if u is metastable relative to large disturbances, then the Cauchy stress tensor reduces to a hydrostatic pressure:

$$\nabla u^T S(\nabla u) = \alpha \mathbb{1} \text{ a.e. in } \Omega, \text{ for some } \alpha \in \mathbb{R}.$$

This remains valid when the surface term Γ is present. We now show that an analog of this condition is satisfied on the phase boundaries, where

$$\frac{\partial\Gamma}{\partial F}$$

plays the role of S(F).

Let

$$I^* := I \cap \text{closure}\left\{ x \in I \cap \Omega_0 \mid \text{there exists } b \in \mathbb{Z}^3 \setminus\{0\} \text{ such that } n(x) = \frac{b}{\|b\|} \right\},$$

and note that if the surface is not degenerate near $x \in I$, then $x \in I^*$.

Proposition 5.3.

Let u be p-weakly-metastable and assume that (H1), (H'1), (H'2) and (H'6) hold. There exists $\mu : I^* \to \mathbb{R}^3$ continuous such that

$$F_-^T \frac{\partial\Gamma}{\partial F}(F_-; a, n) = -\, n.\mu \mathbb{1} + n \otimes \mu \quad \text{on } I^*. \tag{5.3}$$

Proof. The estimate

$$\|-\, n.\mu \mathbb{1} + n \otimes \mu\| \geq \|\mu\|^2$$

and a continuity argument allow us to restrict attention to the case where

$$n(x) = \frac{b}{\|b\|} \quad \text{for some } b \in \mathbb{Z}^3\setminus\{0\}.$$

Let $c, d \in \mathbb{Z}^3$ be such that $c.d = c.b = 0$. By Proposition 4.3 (ii),

$$\Gamma(F_-; a, n) \leq \theta\, \Gamma(F_- + F_- c \otimes d; a, n) + (1-\theta)\, \Gamma\left(F_- - \frac{\theta}{1-\theta} F_- c \otimes d; a, n\right)$$

which, together with (H'6), yields

$$\Gamma(F_-; a, n) \leq \Gamma\left(F_- - \frac{\theta}{1-\theta} F_- c \otimes d; a, n\right)$$

for all $\theta \in [0, 1)$. Hence,

$$F_-^T \frac{\partial\Gamma}{\partial F}(F_-; a, n) \,.\, c \otimes d = 0$$

for all c, d $\in \mathbb{R}^3$ such that c.d = c.b = 0. Therefore, there are functions μ and ν satisfying

$$F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) = -\nu \, \mathbb{1} + n \otimes \mu.$$

Finally, since by Proposition 3.1 (iii)

$$\frac{\partial \Gamma}{\partial F}(F_-; a, n)\, n = 0,$$

we conclude that

$$\nu = n . \mu.$$

In what follows we will use the notation of Proposition 5.3.

Corollary 5.4.

Let u be phase metastable and p-weakly-metastable and assume that (H1), (H2), (H'1), (H'2), (H'3), (H'4), (H'6) and (H'7) are verified. If $x \in I^*$ then

(i) $0 \le \Gamma(F_-; a, n) \le -n.\mu$;

(ii) there exists $\lambda \in \mathbb{R}$ such that $\mu = \lambda\, (F_-^T F_-)^{-1} n$.

Proof. (i) As in the proof of Proposition 5.3, we assume that

$$n(x) = \frac{b}{\|b\|} \quad \text{for some } b \in \mathbb{Z}^3\backslash\{0\}.$$

Suppose in addition that $\Gamma(F_-; a, n) > 0$ and fix $v \in \mathbb{Z}^3$ with v.n = 0. By (H'4) we have $a \neq 0$ and so there exist $v' \in \{v, -v\}$ and $w \in \mathbb{R}^3$ such that

$$\frac{F_-^{-1} a . w}{v' . w} > 0.$$

On the other hand, since

$$\frac{F_+^{-1} a . w}{v' . w} = \frac{F_-^{-1} a . w}{v' . w} \cdot \frac{\det F_-}{\det F_+}$$

we deduce that

$$\frac{F_+^{-1} a . w}{v' . w} > 0.$$

Defining the sequence of vectors

$$c_k := \frac{a}{k\|b\|(v'.w)} - \frac{F_- v'}{v'.w} \quad \text{for } k \in \mathbb{N},$$

by Proposition 4.3 we have that

$$\Gamma(F_-; a, n) \le \theta \Gamma(F_- + c_k \otimes w; a, n) + (1-\theta)\, \Gamma\left(F_- - \frac{\theta}{1-\theta} c_k \otimes w; a, n\right)$$

for $\theta \in [0, 1)$ small enough. By (H'3) and (H'7),

$$\Gamma(F_- + c_k \otimes w; a, n) = \Gamma(F_- + c_k \otimes w; (F_- + c_k \otimes w)v', kb) = 0$$

and so,

$$0 \leq \frac{d}{d\theta}|_{\theta=0}\left\{ (1-\theta)\, \Gamma\left(F_- - \frac{\theta}{1-\theta} c_k \otimes w; a, n\right)\right\} = -\Gamma - \frac{\partial \Gamma}{\partial F}(F_- ; a, n).\, (c_k \otimes w).$$

Letting $k \to +\infty$, by Proposition 5.3 we obtain

$$\Gamma \leq F_-^T \frac{\partial \Gamma}{\partial F}(F_- ; a, n).\, \frac{v' \otimes w}{v'.w} = -\, n.\mu.$$

(ii) By Proposition 5.1 (ii) and Proposition 5.3,

$$\frac{\partial \Gamma}{\partial F} F_-^T = -(n.\mu)\mathbb{1} + F_-^{-T} n \otimes F_- \mu$$

is a symmetric matrix; hence there is a $\lambda \in \mathbb{R}$ such that $F_- \mu = \lambda F_-^{-T} n$.

Proposition 5.5.

Let u be phase-metastable and p-metastable. If (H1), (H2), (H'1), (H'2), (H'3) and (H'6) hold and if $x \in I \cap \Omega_0$, then

(i) $\Gamma(F_-; a, n)\, [\, \|n + (c.n)d\| - 1 - (c.n)(d.n)] - \left(F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n)\right).\, (c \otimes d) \geq 0$

for all $c, d \in \mathbb{Z}^3$ such that $c.d = 0$;

(ii) $\Gamma(F_-; a, n)\, [\, |c.n|\, \|d\| - (c.n)(d.n)] - \left(F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n)\right).\, (c \otimes d) \geq 0$

for all $c, d \in \mathbb{R}^3$ such that $c.d = 0$;

(iii) $F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n) = -(n.\xi)\mathbb{1} + n \otimes \xi$

for some $\xi \in \mathbb{R}^3$, with $\|\, \Gamma(F_-; a, n)n + \xi\, \| \leq \Gamma(F_-; a, n)$. If in addition (H2) and (H'5) are satisfied and if $\Gamma(F_-; a, n) = 0$ then

$$\frac{\partial \Gamma}{\partial F}(F_-; a, n) = 0 \text{ and } \frac{\partial \Gamma}{\partial n}(F_-; a, n) = 0.$$

Proof. (i) If $c, d \in \mathbb{Z}^3$ are such that $c.d = 0$ then, by Proposition 4.9 (ii),

$$\Gamma(F_-; a, n) \leq \theta\, \|n + (c.n)d\|\, \Gamma(F_- (\mathbb{1} + c \otimes d); a, (\mathbb{1} + d \otimes c)n) + \\ + \|n - \theta\,(n + (c.n)d)\|\, \Gamma\left(F_-\left(\mathbb{1} - \frac{\theta}{1-\theta}\, c \otimes d\right); a, \left(\mathbb{1} - \frac{\theta}{1-\theta}\, d \otimes c\right) n\right)$$

for all $\theta \in [0, 1)$. Differentiating the right hand side of this inequality with respect to θ at $\theta = 0$, and using (H'6), we deduce that

$$\Gamma(F_-; a, n)\,[\,\|n + (c.n)d\| - 1 - (c.n)(d.n)] - \left(F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n)\right) . (c \otimes d) \geq 0.$$

(ii) Take c, d $\in \mathbb{Z}^3$ such that c.d = 0 and apply the formula in part (i) to kc and d, with k $\in \mathbb{N}$.

Dividing through by k and letting $k \to \infty$,

$$\Gamma(F_-; a, n)\,[\,|c.n|\,\|d\| - (c.n)(d.n)] - \left(F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n)\right) . (c \otimes d) \geq 0,$$

which, by a density argument, is still valid for c, d $\in \mathbb{R}^3$ with c.d = 0.

(iii) If in (ii) we choose $\pm$c, d $\in \mathbb{R}^3$ such that c.d = 0 and c.n = 0, then

$$\left(F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n)\right) . (c \otimes d) = 0$$

and so there are $\alpha, \xi \in \mathbb{R}^3$ such that

$$F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n) = \alpha \mathbb{1} + n \otimes \xi. \tag{5.6}$$

Therefore, by Proposition 3.1 (iii) and Proposition 3.2 (i), we deduce that

$$\alpha n + (\xi.n)n = 0$$

and (5.6) reduces to

$$F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) + n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n) = -(n.\xi)\mathbb{1} + n \otimes \xi.$$

This result, together with (ii), yields

$$\Gamma(F_-; a, n)\,[\,|c.n|\,\|d\| - (c.n)(d.n)] - (c.n)(d.\xi) \geq 0$$

for all c, d $\in \mathbb{R}^3$ such that c.d = 0. Hence, either

$$\Gamma(F_-; a, n) = 0 \text{ and } \xi = 0 \tag{5.7}$$

or

$$\Gamma(F_-; a, n) > 0 \text{ and } \left\| n + \frac{\xi}{\Gamma(F_-; a, n)} \right\| \leq 1. \tag{5.8}$$

Clearly, (5.7) and (5.8) imply that

$$\| \Gamma n + \xi \| \leq \Gamma(F_-; a, n).$$

If $\Gamma(F_-; a, n) = 0$ then (5.7) yields

$$F_-^T \frac{\partial \Gamma}{\partial F}(F_-; a, n) = -\, n \otimes \frac{\partial \Gamma}{\partial n}(F_-; a, n). \tag{5.9}$$

Therefore, if, in addition, (H2) and (H'5) hold, then, by Proposition 5.1 (ii), there is a $\lambda \in \mathbb{R}^3$ such that

$$F_- \frac{\partial \Gamma}{\partial n}(F_-; a, n) = \lambda F_-^{-T} n. \tag{5.10}$$

Taking the inner product by $F_-^{-T} n$ on (5.10), by Proposition 3.2 (i), we have that $\lambda = 0$ and so, (5.9) and

(5.10) imply that

$$\frac{\partial\Gamma}{\partial F}(F_-; a, n) = 0 \text{ and } \frac{\partial\Gamma}{\partial n}(F_-; a, n) = 0.$$

Proposition 5.11.

Let u be phase-metastable and p-metastable. Assume that (H1), (H2), (H'1), (H'2), (H'3), (H'4), (H'5) and (H'6) are satisfied and let $x \in I \cap \Omega_0$.

(i) If $\det F_- = \det F_+$ then

$$\Gamma(F_-; a, n) = 0, \frac{\partial\Gamma}{\partial F}(F_-; a, n) = 0 \text{ and } \frac{\partial\Gamma}{\partial n}(F_-; a, n) = 0.$$

(ii) If $\det \nabla u_- = \det \nabla u_+$ in a neighborhood of x in I then

$$[S(F)]n = 0$$

and the Maxwell rule holds:

$$W(F_+) - W(F_-) - S(F_-).(F_+ - F_-) = 0.$$

Proof. (i) By Proposition 5.5 (iii) it suffices to show that $\Gamma(F_-; a, n) = 0$. If $a = 0$ then (H'4) yields the desired result. Assume that $a \neq 0$ and choose $\omega, \tau \in \mathbb{Z}^3$ such that

$$\omega.\tau = 0, \tau.n \neq 0 \text{ and } \frac{\omega \,.\, F_-^{-1}a}{\tau.n} < 0. \tag{5.12}$$

Fix $t \in \mathbb{R}$ and define

$$c := \frac{\tau - t F_-^{-1}a}{\tau.n}, \quad d := t\omega - n.$$

Then, since $\det F_- = \det F_+$,

$$F_-^{-1}a \,.\, n = 0$$

and

$$\det(\mathbb{1} + c\otimes d) > 0 \text{ and } \det\left(\mathbb{1} - \frac{\theta}{1-\theta}\, c\otimes d\right) > 0$$

for $\theta \geq 0$ sufficiently small. Moreover, (H'7) implies that

$$\Gamma(F_-(\mathbb{1} + c\otimes d); a, (\mathbb{1} + c\otimes d)n) = \Gamma(F_-(\mathbb{1} + c\otimes d); (\mathbb{1} + c\otimes d)\tau, \omega) = 0.$$

Hence, by Proposition 4.9 (ii) we obtain

$$\Gamma(F_-; a, n) \leq \|n - \theta\,(n + (c.n)d)\|\, \Gamma\left(F_-\left(\mathbb{1} - \frac{\theta}{1-\theta}\, c\otimes d\right); a, \left(\mathbb{1} - \frac{\theta}{1-\theta}\, d\otimes c\right) n\right).$$

Differentiating the right hand side of the previous inequality with respect to θ at $\theta = 0$, by Proposition 5.5 (iii) we conclude that

$$t\,\{\Gamma(F_-;\, a,\, n)n + \xi\}.\omega + t^2\,(n.\xi)\,\frac{\omega\,.\,F_-^{-1}a}{\omega.\tau} \le 0$$

for all $t \in \mathbb{R}$. Therefore (5.12) implies that

$$\Gamma(F_-;\, a,\, n)n + \xi = 0 \;\text{ and }\; n.\xi \ge 0.$$

On the other hand, since by Proposition 5.5 (iii)

$$\|\,\Gamma(F_-;\, a,n)n + \xi\,\| \le \Gamma(F_-;\, a,n),$$

it follows that $n.\xi \le 0$; thus

$$n.\xi = 0 \text{ and } \Gamma(F_-;\, a,\, n) = 0.$$

(ii) By (i),

$$\mathrm{Div}_t \frac{\partial\Gamma}{\partial F} = 0 \text{ near } x$$

and so, by Proposition 3.1 (iv),

$$[S(F)]n = 0.$$

The Maxwell rule follows from (i) and Proposition 3.2 (ii).

Remark 5.13.

We used only the hypothesis

$$\Gamma \ge 0 \tag{5.14}$$

on part (iii) of Proposition 5.5 (see (5.7) and (5.8)). Moreover, (5.14) can be obtained directly from Proposition 5.5 (ii). Indeed, if we add the inequalities corresponding to (c, d) and (-c, d) we deduce (5.14).

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