REMARKS ABOUT EQUILIBRIUM CONFIGURATIONS OF CRYSTALS

BY

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Remarks about equilibrium configurations of crystals

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1. Introduction

The morphology of a crystal may show several phases and these may be altered with changes in its mechanical or thermal environment. For example, some crystals may be deformed to consist of several twin related phases. Indeed, our interest is to study defect structures in materials which have mobile phase boundaries whose existence, position, and orientation are sensitive to applied loads, temperature, and electromagnetic fields.

To set these phenomena into the context of thermoelectricity theory, Ericksen ([19],[20],[21],[22]) has derived a stored energy density which exhibits invariance with respect to change of the crystallographic lattice basis of the material. Such a density is invariant with respect to an infinite discrete group as well as frame indifferent. A body governed by it is rendered highly unstable with respect to certain motions. For example, at a smooth local minimum of energy in a constant temperature heat bath, the Cauchy stress reduces to a pressure, cf. Ericksen [18]. So it seems unlikely that even setting homogeneous boundary conditions leads to a homogeneous extremal.

In this note we take up a direct method for finding and analyzing equilibrium configurations under displacement loading conditions. We favor this approach as a means of surmounting the difficulties imposed by the defect structures on the stability of smooth solutions. We are able to illustrate how an important role in the thermodynamics of the crystal is played by its subenergy. This concept, related to the traditional free energy used by many workers, was introduced by Ericksen [23] and is based in part on a method of Flory [30]. Often the energy assumed by a configuration is its subenergy and its stress is a pressure determined by it. This may be reconciled with one common thermodynamic view where
phase diagrams are expressed in terms of pressure, or specific volume, and temperature.

The equilibrium configuration is characterized by a minimizing sequence, rather than just its limit. A convenient way of expressing this is through Young's idea of a parametrized measure. With this measure, energy and stress may be calculated. Morphology may be ascertained by inspection of the linearized equation that the parametrized measure provides. We may regard this measure as an accounting device to summarize the properties of a minimizing sequence.

What emerges of these considerations is a coarse theory which in some manner accommodates information from a finer structure to yield macroscopic properties. A limit configuration found in this way may be a macroscopically homogeneous but infinitely twinned array of states of minimum energy. It would appear that the material seeks to assume the lowest energy available to it by suffering small, kinematically admissible shears. Of course, a physical crystal cannot be infinitely twinned, but what we are able to construct may offer an approximation to the actual body.

This paper is primarily a report on [12]. Our remarks here will be a summary of

- a brief background of the theory
- the minimum energy calculation
- the existence of solutions and the notion of a parametrized measure solution
- the analysis of parametrized measure minima
- the analysis of the energy density at an equilibrium configuration
- brief examples related to phase transitions.

There are two facets to these questions as topics in the calculus of variations. One is to consider energy functions in general in order to seek those properties of material symmetry and continuity which permit is to determine minimum energy configurations. Fonseca [32],[33] has undertaken an analysis in this direction. Another is to restrict our attention to the elastic crystal to assess the behavior of minimizing sequences and their various state functions. This is our topic here. The two methods are complementary and they agree in their calculation of the
minimum energy available to a configuration.

It would be out of place for us to attempt to mention here the body of work devoted to the challenging questions which Ericksen’s ideas have stimulated. We might suggest to the interested reader consultation of some work of Ericksen [18–29], James [36–41], Parry [52], and Pitteri [56–60]. Ball and James study fine twinning in [7]. We show how our ideas are consistent with theirs in §6. Mathematical analysis of the dead loading problem and related issues is due to Fonseca [31]. Additional questions are considered by Fonseca and Tartar [34]. One interesting feature of the theory is that it may be used to derive the relations of Muller’s interaction theory for the ferroelectric transition in Rochelle salt, cf. [43]. An interesting earlier work about phase transitions is Tisza [64].

Given a bounded domain $\Omega \subset \mathbb{R}^n (n = 2 \text{ or } 3)$ with adequately smooth boundary $\partial \Omega$ and a stored energy density $W(F)$, we investigate deformations $y$ of $\Omega$ satisfying

$$\delta \int_\Omega W(\nabla y) \, dx = 0$$  \hspace{1cm} (1.1)

or

$$\int_\Omega W(\nabla y) \, dx = \inf \int_\Omega W(\nabla v) \, dx$$ \hspace{1cm} (1.2)

where the admissible variations belong to a class

$$\mathcal{A} = \{ v \in H^{1,\infty}(\Omega) : v = y_0 \text{ on } \partial \Omega \}$$

with $y_0$ prescribed (1).

The analytical difficulties encountered in the study of (1.1) or (1.2) are well publicized, by now, but may withstand a brief review. By an elastic crystal we understand a three dimensional lattice given by three independent lattice vectors $\{e_1, e_2, e_3\}$, written as a matrix $L = (e_1, e_2, e_3)$ with columns $e_i$. Owing to the frame indifference of the Helmholtz free energy $\Phi$, we may express

$$\Phi = \Phi(L^\top L).$$ \hspace{1cm} (1.3)

The lattice basis is not unique. Indeed, for any matrix $M$ having integer entries with $\det M = \pm 1$, the matrix
\( L^{-1} = LM \)

is another lattice basis, whence

\[ \Phi(L^T L) = \Phi(M^T L^T L M) \quad \text{for} \quad M \in \text{GL}(\mathbb{Z}^3) \]  \hspace{1cm} (1.4)

For a fixed \( L \) we define the elastic bulk energy of the crystal by

\[ W(F) = \Phi(L^T C L), \quad C = F^T F, \quad \det F > 0. \]  \hspace{1cm} (1.5)

Thus

\[ W(F) = W(QF\tilde{H}) \quad \text{for} \quad \det F > 0, \quad Q^T Q = I, \quad \det Q = 1, \quad H \in \mathbb{H}. \]  \hspace{1cm} (1.6)

where \( \mathbb{H} = L \text{GL}(\mathbb{Z}^3) L^{-1} \) is a conjugate group of \( \text{GL}(\mathbb{Z}^3) \). We impose on \( W \), or \( \Phi \), the conditions

\[ W(F) \geq 0, \quad W(I) = 0, \quad \text{and} \quad \lim_{\det F \to 0} W(F) = \infty. \]

More generally, \( \Phi \) may depend on temperature, polarization (when electromagnetic fields are active), or lattice shifts (for the case of complicated crystals.)

For any \( F, \det F > 0, \) and \( H = I + a \otimes n \in \mathbb{H} \), a direct calculation shows that

\[ W(F(1 + \lambda a \otimes n)), \quad -\infty < \lambda < \infty, \]  \hspace{1cm} (1.8)

is a periodic function of period 1. In particular this implies that there are points \( \lambda \) for which

\[ c_{ijk} a^i a^j n^k < 0, \]  \hspace{1cm} (1.9)

\[ c_{ijk} = \partial^2 W / \partial F_{ij} \partial F_{hk}(F(1 + \lambda a \otimes n)). \]

Thus \( W \) is not rank 1 convex, and in particular, neither quasiconvex nor lower semi-continuous. In fact the deformation satisfying (1.9) is infinitesimally unstable; whereas homogeneous deformations are minima of quasiconvex integrands by definition. A further contrast is afforded by the
The role of quasiconvexity, introduced by Morrey, cf. [50], in the investigation of isotropic elastic solids has been explored by Ball ([3],[4] for example.) We call the reader's attention to the work of Ball and Murat [8] and Dacorogna [14] as well. Although not pertinent to elasticity, the work of Meyers [48] sheds some light on these issues.

Moreover, the periodicity of \( W \) shows that the functional of (1.1) does not grow for all large values of \( |F| \). It is a dictum of the calculus of variations that rapid growth at infinity assists the finding of minima. Where growth is only linear, a minimizer need not be in an ordinary function space; its gradient may be a measure for example. This occurs in the classical theory of elastic-perfectly plastic deformation, cf. Temam [63] or [35]. When there is no growth at all, it may be even more difficult to characterize solutions. Our choice here is Young measures. We shall strive to convince the reader that the parametrized measure arises here in a very natural way which also is rather distinct from its use in the study of hyperbolic conservation laws. Its implementation there was suggested by Tartar [62] and it was further developed by DiPerna, for example [15]. Articles in the volume [61] are devoted to this subject; Slemrod [61] has written an expository one.

The notion of effective modulus, used in the theory of periodic structures, offers a point of comparison. The paper by Kohn and Milton [45] contains a very readable account of this. Given a tensor \( C(x) \), \( x \in Q \), a unit cube, its effective modulus tensor \( \overline{C} \) is

\[
\overline{C}A \cdot A = \inf_{H_{0}^{1}(Q)} \int_{Q} C(A + \nabla \zeta) : (A + \nabla \zeta) \, dx.
\]

If \( C(x) \) is constant, then \( \overline{C} = C \). In general \( \overline{C} \) is the tensor of coefficients of the homogenized operator associated to \( C \). Likewise, if \( W(A) \) is a variational integrand, we may call

\[
\overline{W}(A) = \inf_{H_{0}^{1}(Q)} \int_{Q} W(A + \nabla \zeta) \, dx
\]

its effective modulus in some sense. When \( W \) is quasiconvex, \( \overline{W} = W \). However, \( \overline{W}(A) \) is usually complicated and difficult to compute. One of the features of our \( W \), satisfying (1.5)-(1.7), is that \( \overline{W} \) is the subenergy
density which is a function of the determinant alone.

In the theory of effective moduli, one seeks to achieve the optimal coefficients of $\overline{C}$ in some sense by various constructions, cf. Milton [49] for example, or the papers in [45]. The question of whether or not there are optimal parametrized measure solutions for (1.1) or (1.2) has not yet been investigated. One connection between crystals and laminates has been explored in [13].

The illustration on p.151 of [49] shows a laminate construction which turns out to be similar to the construction used by us to find parametrized measure solutions. It is not dissimilar to what is seen under the microscope in the laboratory, say, of a specimen of shape memory material untreated to render it a single crystal, cf. eg., Barrett and Massalski [9], p. 527.

2. Minimum energy

The minimum energy available to a configuration turns out to be its subenergy, or related to it. For a given $W(F)$ this subenergy is defined to be

$$\phi(t) = \inf_{\det A = t} W(A)$$  \hspace{1cm} (2.1)

For the moment let us suppose fixed a bounded open set $\Omega$ with piecewise smooth boundary $\partial \Omega$ and $y_0$ a Lipschitz deformation of $\overline{\Omega}$ with $\det \nabla y_0 > 0$. Let us set

$$E_0(y_0) = \inf_{A(y_0)} \int_{\Omega} W(\nabla v) \, dx$$  \hspace{1cm} (2.2)

$$A(y_0) = \{ v \in H^{1,*}(\Omega) : \det \nabla v > 0 \text{ in } \Omega \text{ and } v = y_0 \text{ on } \partial \Omega \}$$  \hspace{1cm} (2.3)

We may state this result.

Assume that $\phi(t)$ is convex and $\Omega$ and $y_0$ are as above. Then

$$E_0(y_0) = \inf_{A(y_0)} \int_{\Omega} \phi(\nabla v) \, dx$$  \hspace{1cm} (2.4)
In the case where \( y_0(x) = Fx \) is a homogeneous deformation and \( \phi \) is convex, by Jensen’s inequality and (2.1),

\[
\int_{\Omega} W(\nabla v) \, dx \geq \int_{\Omega} \phi(\nabla v) \, dx
\]

\[
\geq \phi\left( |\Omega|^{-1} \int_{\Omega} \det \nabla v \, dx \right) |\Omega|
\]

\[
\geq \phi\left( |\Omega|^{-1} \int_{\Omega} \det F \, dx \right) |\Omega|
\]

\[
= \phi(\det F) |\Omega|.
\]

Thus from (2.4),

\[
E_\Omega(Fx) = \phi(\det F) |\Omega|.
\]  

(2.5)

The idea of the proof of (2.4) is to show (2.5) first and then to approximate. There are two ideas involved, both elementary, so we might mention them.

Let \( \Omega \subset \mathbb{R}^3 \) be a bounded open domain with piecewise smooth boundary as before. Let

\[
F_0, \det F_0 > 0,
\]

\[
B = I + a \otimes b, \det B = 1 + a \cdot b > 0, \text{ and}
\]

\[
\theta, 0 < \theta < 1,
\]

be given and consider

\[
F = F_0(1 + \theta a \otimes b) = (1 - \theta)F_0 + \theta F_0 B.
\]  

(2.6)

We assume that \( |b| = 1 \). Let \( x(t) \) be the characteristic function of the interval \( (0,\theta) \subset (0,1) \) and extend it to be a \( 1 \)-periodic function on \( \mathbb{R} \). It is easy to check that

\[
f^k(x) = x(kx \cdot b), \; k = 1,2,3, ...
\]

satisfy
Equilibrium configurations of crystals 8

November 25, 1986

\[ f^k \to \theta \text{ in } L^\infty(\mathbb{R}^3) \text{ weak }^* \text{ as } k \to \infty. \quad (2.7) \]

Let us recall that this means that for any ball \( B \),

\[ \int_B f^k \, dx \to \theta \text{ as } k \to \infty, \]

or equivalently, that

\[ \int_\Omega f^k \zeta \, dx \to \theta \int_\Omega \zeta \, dx \text{ as } k \to \infty \text{ for any } \zeta \in L^1(\Omega). \]

Setting

\[ u(y) = F_0(y + \int_0^r x(t) \, dt \cdot a), \quad r = y \cdot b, \]

and

\[ u^k(x) = k^{-1} u(kx), \quad (2.8) \]

it is clear that

\[ u^k \to Fx \text{ in } H^{1, \infty}(\Omega) \text{ weak }^* \quad (2.9) \]

This means that

\[ u^k \to Fx \text{ uniformly in } \overline{\Omega} \text{ and } \]

\[ F^k = \nabla u^k = F_0(1 + f^k a \otimes b) = (1 - f^k)F_0 + f^k F_0 B \to F \text{ in } L^\infty(\Omega) \text{ weak }^*. \]

Now

\[ W(F^k) = (1 - f^k)W(F_0) + f^k W(F_0 B), \]

whence

\[ W(F^k) \to (1 - \theta)W(F_0) + \theta W(F_0 B) \text{ in } L^\infty(\Omega) \text{ weak }^*. \]

A particular consequence of this is that whenever

\[ F = (1 - \theta)F_0 + \theta F_0 B, \quad B = 1 + a \otimes b, \]

then
\[ E_0(Fx) \leq (1 - \theta)W(F_0) + \theta W(F_0B). \]  

(2.10)

If \( W(F_0) = \phi(\det F_0) \) and \( B = H = 1 + a \otimes n \in H \), the symmetry group of \( W \), then

\[ W(F_0H) = W(F_0) = \phi(\det F_0) = \phi(\det F), \]

from which it follows that

\[ E_0(Fx) \leq |\Omega| \phi(\det F). \]

In the special case \( F_0 = 1 \) and \( W(F) \geq W(1) = 0 \) for all \( F \), then

\[ E_0((1 + \theta a \otimes n)x) = 0. \]

To attempt a first motivation of our idea, observe that this minimum has been calculated via a minimizing sequence without regard to the numerical value of \( W(1 + \theta a \otimes n) \).

This computation, although illustrative, is not sufficient to establish (2.5). There must be some iterative argument; care must be exercised with boundary conditions, and so forth. We found useful this fact about matrices: For any matrix \( A, \det A > 0 \), there are vectors \( a_i, n_i, i = 1,2 \), and a rotation \( Q \) such that

\[ A = (\det A)^{1/4} Q(1 + a_2 \otimes n_2)(1 + a_1 \otimes n_1). \]

(2.11)

\[ a_i \cdot n_i = 0, \quad i = 1,2. \]

In general there need only be one iteration. A similar fact is proved in Fonseca [33].

Returning to the idea behind (2.10), let \( \psi(A) \) be any continuous function on \( M \), the set of matrices with positive determinant. Then the sequence \( (\psi(F^k)) \) is bounded in \( L^\infty(\Omega) \) and indeed

\[ \psi(F^k) = (1 - f^k) \psi(F_0) + f^k \psi(F_0B) \rightarrow (1 - \theta) \psi(F_0) + \theta \psi(F_0B) \quad \text{in} \quad L^\infty(\Omega) \text{ weak*}. \]
Now we may by leap of imagination write

\[(1 - \theta) \psi(F_0) + \theta \psi(F_0B) = \int_M \psi(A) \, d\nu \tag{2.12}\]

for

\[\nu = (1 - \theta)\delta_{F_0} + \theta \delta_{F_0B},\]

where \(\delta_A\) denotes the Dirac delta measure at the matrix \(A\). The measure \(\nu\) is called a parametrized measure or Young measure [65] for the sequence \((u^k)\).

Reconsidering the case where \(B = H = I + a \otimes \epsilon H\) and \(W(F_0) = \phi(\det F_0)\) realizes the value of the subenergy, we find that \((u^k)\) is a minimizing sequence and we may refer to \(\nu\) as a parametrized measure minimum.

The formula (2.12) may be used to evaluate various state functions. For example, the Piola-Kirchhoff stress \(S(F) = \partial W/\partial F(F)\) and the linear elasticity tensor \(S'(F) = \partial S(F)/\partial F = \partial^2 W(F)/\partial F^2\) are given by

\[
\tilde{S} = \int_M S(A) \, d\nu
\]

and

\[
\tilde{S}' = \int_M S'(A) \, d\nu \tag{2.13}
\]

Observe that \(F\) itself is given by

\[
F = \int_M A \, d\nu .
\]

It is not clear which matrices \(F\) give rise to minimizing Young measures. In view of (2.11), a dense set in \(M\) is given by those of the form

\[
F = QF_0(I + \theta_2 a_2 \otimes n_2)(I + \theta_1 a_1 \otimes n_1) \tag{2.14}
\]

where \(W(F_0) = \phi(\det F_0), \ \theta_1 \in \Re, \ Q^T Q = I, \) and

\[
H_i = I + a_i \otimes n_i \in H .
\]
The proof of this is analogous to the proof of (2.5) and the measure \( \nu \) associated to \( F \) is

\[
\nu = (1 - \theta_1)(1 - \theta_2)\delta_{QF_0} + \theta_1(1 - \theta_2)\delta_{QF_0H_1} + \theta_2(1 - \theta_1)\delta_{QF_0H_2} + \theta_1\theta_2\delta_{QF_0H_2H_1}
\]

(2.15)

More generally if

\[
H_i = 1 + a_i \otimes n_i \in H \text{ and } \theta_i \in \mathbb{R}, \ i = 1, \ldots, N,
\]

then

\[
F = QF_0 \prod_i (1 + \theta_i a_i \otimes n_i)
\]

determines a Young measure minimum given by a formula analogous to (3.15).

We might say a few words about the case when the subenergy \( \phi \) is not assumed convex. In this situation (2.4) must be modified to

\[
E_\Omega(y_0) = \inf_{\mathcal{A}(y_0)} \int_\Omega \phi^{**}(\nabla v) \, dx
\]

(2.16)

where \( \phi^{**} \) is the convex minorant of \( \phi \). There are several ways to show this. The easiest relies on the formula (2.10) in the case where \( a, b \) are not necessarily orthogonal and a result of Ball and Murat, [8] p. 240. Another proof may be given using Mascolo and Schianchi [47] and Moser [51].

3. Properties of minimum energy configurations

Ericksen's deduction [18] that the Cauchy stress of a minimizing configuration is a constant pressure turns out to be valid under arbitrary deformation, at least in some sense. To discuss this, we might first agree on what we mean by a parametrized measure minimum and subsequently on what we mean by a stable minimum.
Let us say that a sequence \((u^k)\) in \(H^1(\Omega)\) determines the parametrized measure \((\nu_x)_{x \in \Omega}\) provided that there is a \(y \in H^1(\Omega)\) such that

\[
u_x \to y \quad \text{in } H^1(\Omega) \text{ weak*}
\]

\[
\phi^k = \nabla u^k \quad \text{satisfy } \det \phi^k > 0 ,
\]

\[
\mathcal{E}_\Omega(y) = \lim_{k \to \infty} \int_\Omega W(\phi^k) \, dx ,
\]

and for any continuous function \(\psi(A)\),

\[
\psi(\phi^k) \to \psi \quad \text{in } L^\infty(\Omega) \text{ weak* where}
\]

\[
\psi(x) = \int_\Omega \psi(A) \, d\nu_x .
\]

Since the \(\|\phi^k\|_{L^\infty(\Omega)}\) are bounded, the support of any parametrized measure is compact.

Note that if \(y(x), x \in \Omega\), is a Lipschitz minimum, it is also a parametrized measure minimum with

\[
\mu_x = \delta_{F(x)} .
\]

However there may be sequences \((u^k)\) convergent to \(y\) which determine measures \((\nu_x)\) different from \((\mu_x)\) above. This is an essential feature of the parametrized measure as a macroscopic device for recording properties of the smaller scale structure.

When \(\phi\) is convex it is possible to check that \(W(A)\) is \(d\nu_x\) integrable and

\[
\mathcal{E}_\Omega(y) = \lim_{k \to \infty} \int_{\Omega} \phi(\phi^k) \, dx .
\]

Moreover,

\[
W(F(x)) = \phi(\det F(x))
\]

\[
(3.4)
\]

\[
(3.5)
\]
\[ \text{supp } \nu_x \subset \{ A : \det A = \det F(x) \} \text{ a.e. in } \Omega. \]

From (3.5), it follows easily that for a subsequence of \( k \),

\[ \det F^k \to \det F \text{ a.e. in } \Omega \text{ and in } L^p(\Omega), \ 1 \leq p < \infty. \]

Since \( \text{adj} \nabla \nu \) is a weak* continuous function, the above implies that

\[ (F^k)^{-1} \to F^{-1} \text{ in } L^\infty(\Omega) \text{ weak*}. \quad (3.6) \]

Most desirably, an equilibrium solution renders stationary the energy functional within a suitable class of disturbances. This is an attribute of stability which is not necessarily conferred on a state which realizes minimum energy. Much has been written about this, especially by Ball [4],[5], and it is fair to report that our difficulties here are connected to the growth of \( W \) as \( \det F \to 0 \). For example, that \( (\nu_x)_x \in \Omega \) is a parametrized measure minimum ought to mean that

\[ \int_{\Omega} \overline{W} \, dx \leq \int_{\Omega} \int_{\partial \Omega} W(A + \nabla \zeta) \, d\nu_x \, dx, \quad \zeta \in H^{1,\infty}(\Omega), \]

at least for \( \| \zeta \|_{H^{1,\infty}(\Omega)} \) sufficiently small. Unfortunately, since nothing has been established about \( \det F \), it is not evident that there are any \( \zeta \) for which the right hand side is finite.

Conditions for variation of domain are the easiest to control, so our criteria will be expressed in these terms. We say that a parametrized measure minimum is stable provided that for each \( \zeta \in H^{1,\infty}(\Omega) \), there is an \( \epsilon_0 > 0 \) such that

\[ \int_{\Omega} \overline{W} \, dx \leq \int_{\Omega} \int_{\partial \Omega} W(A(1 + \epsilon \nabla \zeta)) \det(1 + \epsilon \nabla \zeta)^{-1} \, d\nu_x \, dx < \infty \]

for \( \epsilon < \epsilon_0 \). \quad (3.7)

From this we may infer a familiar form of the equilibrium equation:

\[ \int_{\Omega} \int_{\partial \Omega} \left\{ A^T S(A) : \nabla \zeta - W(A) \text{div } \zeta \right\} \, d\nu_x \, dx = 0 \text{ for } \zeta \in H^{1,\infty}(\Omega) \quad (3.8) \]

There are several conditions which guarantee that a minimum is stable. About the solution \( y(x) \), with \( F = \nabla y \), if
\[ \det F \geq c > 0 \quad \text{in } \Omega, \quad (3.9) \]

then the measure \((\nu_x)_x \epsilon \Omega\) is stable. This is true for any parametrized measure minimum whose underlying deformation gradient is \(F\).

Also note that if

\[ m \det(A)^{-\alpha} \leq W(A) \leq M \det(A)^{-\alpha} + C \quad (3.10) \]

holds for some \(0 < m \leq M\), \(\alpha > 0\), and \(C \geq 0\), then any parametrized measure minimum is stable. In fact, (3.10) need only hold on the support of \(\nu\).

The energy density derived in Eftis, McDonald, and Arkipic [16],[17] may be written in the form

\[ W(A) - g(\det A) \quad (3.11) \]

where \(W(A)\) satisfies (3.10) but \(g\) is a convex function of \(\det A\) which has the property

\[ \lim_{t \to 0} g(t) = +\infty. \]

The minima of interest to them are usually homogeneous, so (3.9) applies. More generally, as our result below makes clear, a parametrized measure minimum for \(W\) determines a stationary point of (3.11).

Stable minima have the property which Ericksen observed. We state this result.

Assume that \((\nu_x)_x \epsilon \Omega\) is a parametrized measure minimum in the sense of (3.1), (3.2), (3.3) which is stable in the sense of (3.7). Let the subenergy \(\phi\) be strictly convex. Then \(\det F\) and \(\phi(\det F)\) are constant in \(\Omega\) and the Cauchy stress

\[ T = \phi'(\det F)I \quad (3.12) \]

is a constant pressure.
There are some interpretations of this as well. Suppose our situation involves minimum energy configurations associated to $W(F, \theta)$, where $\theta$ is temperature. Then the entropy density at a minimum

$$\eta = -\partial W / \partial \theta (F, \theta) = -\partial \phi / \partial \theta (\det F, \theta)$$

(3.13)

and the specific heat, at constant volume say,

$$C_v = \partial^{-1} \partial \eta / \partial \theta$$

(3.14)

depend only on specific volume, that is $\det F$, not on the details of the boundary conditions.

For example, a Curie point associated to a singularity of the specific heat depends only on the specific volume, even though it may indicate a change of shape of the crystal. This is consistent with the traditional view of thermodynamicists who frequently write phase diagrams in terms of specific volume, pressure, and temperature, cf. Pippard [55], p.136 et. seq. for instance.

Many analytical questions now arise, for example regarding the form of a parametrized measure minimum. This is currently under investigation. For example, suppose that the measure $\nu$ corresponds to a homogeneous deformation $\nu = F x$ and

$$\nu = \mu \delta_{F_0 H},$$

that is

$$\int_M \psi(A) d\nu = \int_{SO(3)} \psi(QF_0 H) d\mu.$$

Then

$$F = \left( \int_{SO(3)} Q d\mu \right) F_0 H = PF_0 H,$$

and by weak continuity,

$$\det F = \int_{SO(3)} \det(QF_0 H) d\mu = \det F_0$$

and
\[ F^{-1} = \int_{\mathcal{M}} (QF_0H^{-1}) \, d\nu = H^{-1}F_0^{-1}P^T. \]

From this,
\[ 1 = \text{det} FF^{-1} = \text{det} P \text{det} P^T = (\text{det} P)^2, \]
so
\[ \text{det} P = 1. \]

Also,
\[ 1 = FF^{-1} = PP^T, \]

hence \( P \) is a rotation. Now \( \mu \) is a probability measure on the sphere of radius \( \sqrt{3} \) in \( \mathbb{R}^3 \), which is the convex hull of its extreme points. It follows that \( \mu \) is a delta measure at \( P \), so
\[ \nu = \delta_P \otimes \delta_{F_0H}. \]

Other characterizations in this spirit are also possible.

4. **Parametrized measure equilibria**

Some of the preceding conclusions remain valid when the measure does not provide an absolute minimum, but this depends on what is granted about equilibrium configurations. Surely they ought to be local minima in some sense, and the extent to which they are will determine their properties. While dynamical considerations may offer the most satisfactory notions of metastability, as developed in Ball and Andrews [2] and Pego [53],[54] for example, these are not yet available for our three dimensional problem.

Maintaining our static viewpoint, an alternative approach to the analysis of the measure is to investigate the behavior of the energy density at an equilibrium configuration. The essential features of the argument are illustrated by considering measures which minimize with respect to small compactly supported perturbations. Under these circumstances a form of quasiconvexity may be established. Similar considerations in a different context were initiated independently by Ball [6]. When the admissible perturbations are sufficiently large, conclusions
like (3.11)-(3.13) follow. Such may be seen as either a defect or an advantage of the theory.

We found this point of view to be a useful complement to the study of absolute minima, but in order to keep this presentation short, we shall omit the details.

5. Some example related to phase transitions

The phase transformations we have in mind involve the onset of a change of shape or other properties with little hysterisis as the crystal, or more general periodic structure, is slowly cycled through the transformation temperature. Let $\theta_0$ denote the critical temperature and suppose that $\Phi(L^T(\epsilon)L(\epsilon),\theta)$ is arranged so that the reference configuration is the stable homogeneous parent phase for $\theta \geq \theta_0$; i.e.,

$$F = 1 \quad \text{for} \quad \theta \geq \theta_0$$ (5.1)

is a minimum of $W(F,\theta)$.

The symmetry group of a homogeneous configuration with deformation gradient $F$ is

$$\mathcal{L} = \{ H \in \mathbb{H}: H^TCH = C, \ C = F^TF \}.$$ (5.2)

We assume that the symmetry group of (5.1) is constant for $\theta \geq \theta_0$,

$$\mathcal{L}_1 = \{ H \in \mathbb{H}: H^TH = I \}.$$ (5.2)

Below $\theta_0$, there is a stable homogeneous daughter phase

$$F = F_0(\theta), \ C_0(\theta) = F_0(\theta)^TF_0(\theta)$$ (5.3)

whose symmetry group is properly contained in $\mathcal{L}_1$. Other daughter phases with Cauchy-Green tensors $C$ are related to $F_0(\theta)$ by symmetry, namely, in such a way that

$$C = H^TC_0H \quad \text{for some} \quad H \in \mathcal{L}_1.$$ (5.4)
The phases may coexist at critical temperature. These concepts are explained by Ericksen [21]. To simplify matters let us think that

\[ W(1, \theta) = 0 \quad \text{for} \quad \theta \geq \theta_0 \]
\[ W(F_0(\theta), \theta) = 0 \quad \text{for} \quad \theta \leq \theta_0 . \]

(5.5)

Our sketch of the profile of \( W \) as a function of \( \theta \) is the standard austenite/martensite one.

We may discuss the transition in terms of the extent of kinematic compatibility between parent and daughter phases.

Case 1. Second order transition

\[ F_0(\theta_0) = 1 \quad \text{although} \quad F_0(\theta) \neq 1 \quad \text{for} \quad \theta < \theta_0 . \]

Examples of this are rare. For practical purposes, the ferroelectric transition in Rochelle salt is one. Here the linearized equation exists at the critical temperatures, however it necessarily exhibits certain degeneracies which are generalized Clausius-Clapeyron relations or Ehrenfest relations. These are the Muller relations, cf. Lines and Glass [46] or Tisza [64]. In [43], the ferroelectric transition is discussed in particular and it is shown that Agmon-Douglas-Nirenberg conditions [1] must fail for certain boundary value problems at critical temperature.

Case 2. Kinematically compatible first order transition

\[ F_0(\theta_0) - 1 \quad \text{is rank 1} \]

Although the starting point of James' discussion in [40], this analysis does not abide by the parent/daughter symmetry breakdown described above. The daughter phases are actually certain types of aggregate phases, perhaps the sort which we shall encounter in Case 3. One possible configuration is given in Figure 7, [40]. There is a possibility of piecewise affine, hence Lipschitz, solutions. At the critical temperature, the domain \( \Omega \) may be decomposed into disjoint subdomains \( \Omega_i, \ i = 1, ..., n \), with

\[ F = x_{o_1} 1 + \sum_{2 \leq i \leq n} x_{o_i} F_i , \]

(5.6)

where, say, \( F_2 = F_0(\theta_0) \) and the \( F_i, i > 2 \), are variants of \( F_2 \) with respect
to some group action. State functions may be determined by evaluation
directly on $F$. In other words, the parametrized measure is merely

$$
\nu = x_{\omega_i} \delta_i + \sum_{2 \leq i < n} x_{\omega_i} \delta_{F_i}.
$$

We are not presently aware of any examples where this behavior
takes place in crystals. When $F_0 = 1 + a \otimes b$, then

$$
C_0 = (1 + a \otimes b)(1 + b \otimes a)
$$

has an eigenvector $p = a \wedge b$ of eigenvalue 1. It is not difficult to check
that if the parent phase is a primitive cubic lattice, then the daughter
phase is not likely to be a primitive tetragonal lattice. In this case, 1
would be an eigenvalue of $C_0$ with multiplicity two.

Case 3. Kinematically incompatible parent and daughter phases
fine phase twinning

This is the subject addressed by Ball and James [7]. Here we wish
to point out that our ideas are consistent with theirs. In fine twinning, a
homogeneous laminate constructed of daughter phases is compatible with
the parent phase across the parent/daughter interface. We refer to the
parent phase as austenite and the daughter phase as martensite. The
phenomena is rather widespread, indeed, typical of many
austenite/martensite transitions. Indium-thallium [10],[11] is an example
and the ferroelectric transition in Barium titanate is another [42]. The
martensite, to render itself kinematically compatible with the austenite,
appears to average itself among twin related phases.
fine twinning with martensite/austenite interface

Suppose we are given a plane $x \cdot m = 0$ in $\Omega$ to serve as the austenite/martensite interface and require that

$$x \cdot m > 0 \quad \text{in the austenite and} \quad x \cdot m < 0 \quad \text{in the martensite.}$$

In experience, the possibilities for this plane will be limited by the symmetry considerations mentioned at the beginning of this section. We suppose that $F_0$ and $F_{00} = F_0(1 + a \otimes n)$, $1 + a \otimes n \in H$, are daughter phases and that for some $\theta$, $0 < \theta < 1$, the sequence $(u^k)$ of (2.8) satisfies

$$u^k \rightharpoonup y \quad \text{in } H^{1,\infty}(\Omega) \text{ weak*} \quad (5.7)$$

where

$$y(x) \text{ and } x \text{ are kinematically compatible across } x \cdot m = 0.$$

Thus

$$y(x) = (1 + a \otimes b)x = Fx \quad (5.8)$$

for some $b \in \mathbb{R}^3$. We may take $|m| = 1$.

Our first observation is that the sequence $(u^k)$ may be slightly altered to form a minimizing sequence. Let

$$0 \quad t < -1$$
\[ \eta(t) = \begin{cases} t + 1 & -1 \leq t \leq 0 \\ 1 & t > 0 \end{cases} \quad (5.9) \]

Set \( \eta^k(x) = \eta(kx \cdot m), k = 1, 2, 3, \ldots, \) and

\[ v^k(x) = (1 - \eta^k(x))u^l(x) + \eta^k(x)x \quad (5.10) \]

for a \( j = j(k) \) which we shall specify now. Indeed, since \( u^k \to y \) uniformly as \( k \to \infty \), it is easy to check that we may choose a subsequence \( (u^l) \) of \( (u^k) \) such that

\[ v^k \to x \quad x \cdot m \geq 0 \quad \text{in } H^1(\Omega) \text{ weak*}. \quad (5.11) \]

This implies, cf. § 3,

\[ \det \nabla v^k \to \det F \quad \text{a.e. in } \{x \cdot m < 0\} \cap \Omega, \]

so that owing to the form of \( \nabla v^k \), \( \det \nabla v^k \geq \frac{1}{2} \det F > 0 \) for \( k \) sufficiently large. It follows that

\[ \int_{\Omega} W(\nabla v^k) \, dx = \int_{\Omega \cap \{x \cdot m < -1/k\}} W(F^k) \, dx \]

\[ + \int_{\Omega \cap \{-1/k < x \cdot m < 0\}} W(\nabla v^k \cdot x) \, dx + \int_{\Omega \cap \{x \cdot m > 0\}} W(1) \, dx \]

\[ \to 0 \]

as \( k \to \infty \) since the first and last integrals vanish and the middle one may be estimated by

\[ \left| \int_{\Omega \cap \{-1/k < x \cdot m < 0\}} W(\nabla v^k) \, dx \right| \leq \text{const.}/k . \]

Now the limit of the \( (u^k) \) is given by (2.6), so

\[ F_0(1 + \theta a \cdot n) = 1 + b \cdot m . \quad (5.12) \]

Let \( p = m \cdot n \). The equation (5.12) implies that
Equilibrium configurations of crystals

\[ F_0 \mathbf{p} = \mathbf{p} \]

so \( F_0 - 1 \) is of rank 2 and its range is in the plane spanned by \( \mathbf{m} \) and \( \mathbf{n} \). We write

\[ F_0 = 1 + c_0 \mathbf{n} + b_0 \mathbf{m} \]

The same holds for \( F_{00} \) since

\[ F_{00}(1 + (\theta - 1)\mathbf{a} \cdot \mathbf{n}) = 1 + b \mathbf{m}, \]

so

\[ F_{00} = 1 + c_{00} \mathbf{n} + b_{00} \mathbf{m}. \]

Substituting in here the equation defining \( F_{00}, F_{00} = F_0(1 + \mathbf{a} \cdot \mathbf{n}), \) we see immediately that \( b_0 = b_{00} = b \).

Expressing \( u^k \) by

\[ u^k(x) = F_0(x + k^{-1}w(kx)a), \]

where

\[ k^{-1}w(kx) \rightarrow \theta x \cdot \mathbf{n} \quad \text{uniformly,} \]

one checks that

\[ u^k(x) - y(x) = c_0 x \cdot \mathbf{n} + k^{-1}w(kx)F_0 a, \]

so that

\[ 0 = \lim (u^k(x) - y(x)) = c_0 x \cdot \mathbf{n} + \theta x \cdot \mathbf{n}F_0 a. \]

Consequently, \( c_0 = -\theta F_0 a \). Also, \( c_{00} = (1 - \theta)F_0 a \). Setting \( c = F_0 a \), we obtain the representation [7]

\[ F_0 = 1 - \theta c \mathbf{n} + b \mathbf{m}, \]

\[ F_{00} = 1 + (1 - \theta)c \mathbf{n} + b \mathbf{m}. \quad (5.13) \]

With the representation (5.13) in hand, one may begin to consider
the issues posed by the symmetries of the austenite and the martensite to determine, for example, the relationships among the vectors \( m \) and \( n \) and the proportion \( \theta \). This has been done in [7] to excellent agreement with experiment. A parametrized measure minimum is given by the measure

\[
v = (1 - \chi_n)((1 - \theta)\delta_{F0} + \theta\delta_{F00}) + \chi_n\delta_1,
\]

(5.14)

where \( \chi_n \) is the characteristic function of \{\( x \cdot m > 0 \) \} \( \cap \Omega \).

\(^{(1)}\) The space \( H^{1,p}(\Omega) \) is the Sobolev space of functions in \( L^p(\Omega) \) whose derivatives are in \( L^p(\Omega) \), \( 1 < p < \infty \).

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