Some Methods of Analysis in the Study of Microstructure

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1. Introduction

Fine scale morphology or microstructure is implicated in the macroscopic behavior of many materials, but the manifestations of this are often unclear. We are in need of improved methods for studying this frequently encountered situation. In this report we describe in an expository fashion the initial developments of one such technique which has been applied in several instances especially related to certain alloys or other crystalline materials. Good examples where defect structures consisting of fine scale morphology are relatively simple are certain phase transformations of displacive or structural type and the mechanical behavior of shape memory alloys. Martensitic materials, in particular, exhibit fine twinned microstructures, often appearing as layers or layers within layers. Although we often refer to microstructure, we are confronted with a primarily continuum phenomenon for which some authors use the term mesoscale. In these considerations, one issue is paramount: the presence of spatially oscillatory behavior and the means of understanding it constitutes the bridge from the fine scale to the large scale.

Crystals are idealized as materials with a high degree of configurational order. As a consequence, the continuum energy densities ascribed to them are invariant under discrete groups and have multiple potential wells. Such densities are not lower semicontinuous. The infimum of energy may be obtained only in some generalized sense, while a minimizing sequence may develop successively finer oscillations. Said in another fashion, when the material deforms owing to change in its environment, the configurational order acts as a constraint resulting in the creation of a defect structure, which in this case is a complicated spatially oscillatory fine structure. The limit

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1 Supported in part by the Army Research Office.
2 To appear in the proceedings of the Tenth Army Conference on Applied Mathematics and Computing.
3 For illustrations of oscillatory behavior in alloys and other materials see [1,23,4,5,27,53].
Some methods of analysis in the study of microstructure

2 11/2/92

Some methods of analysis in the study of microstructure

A feature of the constitutive theory under discussion is that surface energies, magnetic domain wall energies, and similar effects are neglected, although the highly nonlinear potential well structure for the material has a prominent role. Thus fine phase laminar twin systems and fine phase magnetic domain structures may tend to limits of infinite fineness. The theory in this formulation delivers useful information about variant arrangement and location as well as macroscopic state functions like energy and stress. It is particularly useful in deciding where in the body fine structure will arise.

At the analytical level, we apply a recently developed averaging method, briefly explained in §2 below, which accounts for rapidly spatially varying systems and accommodates the fine scale microstructure. A configuration which minimizes a given variational principle is described in terms of generalized moments of the minimizing sequence, or equivalently, oscillatory statistics. The most important property of the method is to unify energetic and kinematic considerations by compelling the statistics to be consistent with the variational principle.

Examples of this sort of analysis served to generalize the crystallographic theory of martensite, Ball and James [1], and to compute the relaxation of energy densities in the presence of symmetry, Chipot and Kinderlehrer [9] and Fonseca [26]. It has subsequently played a role in many discussions related to microstructure, eg, [2,4,5,10,12,13,14,15,25,27,28,30,31,32,33,35,39,40,41,45,47]. A treatment of the variational foundations of this method is given in [29,36,37,38]. Kohn [42,43] has shown how these ideas and those of relaxation in, general are consistent with the treatment of Khachaturyan and Roitburd, eg. [34,49]. Here we shall briefly explore two examples: a theory for highly magnetostrictive iron/rare earth alloys and a mathematical example of evolution of fine structure. A major impetus for these investigations is to provide a basis for the numerical computation of configurations with complicated microstructure. A few selected results of these efforts will be reported.

2. Local spatial averages Young measures. We describe the portrayal of microstructure or fine structure by local spatial averages or Young measures. We also explain the mechanism by which these averages serve to unify energetic and kinematic considerations. Since this may not be familiar to most readers, we give some examples as well. A bounded sequence of functions or more general fields, scalar, vector, or matrix valued,

\[ f_k: \Omega \rightarrow \mathbb{R}^N, \quad k = 1,2,\ldots, \]  

may describe a spatially oscillatory structure or system in the region \( \Omega \). For example, if \( \Omega \) is a cube, \( f_0 \) a fixed periodic function, and
Some methods of analysis in the study of microstructure

\[ f^k(x) = f_0(kx), \]

the system represents spatial oscillations modulated in some fashion by \( f_0 \). A specific one-dimensional example is

\[ f^k(x) = \sin \pi kx, \quad 0 \leq x \leq 1, \quad k = 1, 2, 3, \ldots \quad (2.2) \]

Another one is

\[
 f^k(x) = \begin{cases} 
 -1 & \frac{i-1}{k} < x < \frac{j-1}{k} \\
 1 & \frac{j-1}{k} < x \leq \frac{i}{k} 
\end{cases} \quad \frac{1}{k} \leq j, \quad 0 \leq x \leq 1. \quad (2.3)
\]

The general sequence \( \{f^k\} \) may fail to converge pointwise or even in the mean, as the examples (2.2) and (2.4) above illustrate. This, it turns out, is characteristic of the minimizing sequences for functionals which lack lower semicontinuity and in particular of variational problems associated to crystalline solids in the context of finite elasticity.

The behavior of the sequence may be grasped by computing limits of averages

\[
 \bar{f}(a) = \lim_{\rho \to 0} \int_{B_\rho(a)} x. \quad (2.4)
\]

where \( |B_\rho| \) stands for the volume of the ball of radius \( \rho \). This tells us only the average limit of the sequence, however, and does not inform us of its particular oscillatory behavior. The technical name for this convergence is weak* convergence. To overcome this, we calculate generalized moments. Let \( \psi \) be any continuous function and consider the sequence \( \psi(f^k) \). Although this sequence need not converge, we may ascertain, as above, a weak limit function

\[
 \bar{\psi}(a) = \lim_{\rho \to 0} \int_{B_\rho(a)} \psi(f^k) dx. \quad (2.5)
\]

The association

\[ \psi \to \bar{\psi}(a) \]

gives rise to an integral representation (a probability measure) on \( \psi \),

\[
 \bar{\psi}(a) = \int_{\mathbb{R}^N} \psi(\lambda) d\nu_a(\lambda) \quad (2.6)
\]

which has the property

\[
 \int_E \psi(f^k) dx \to \int_E \bar{\psi} dx \quad \text{for any subset} \quad E \subset \Omega. \quad (2.7)
\]
This collection of measures \( \nu = (\nu_x)_{x \in \Omega} \) summarizes the statistics of the spatial oscillations of the sequence. It was introduced by Young [54] to study control problems. Its first use in differential equations is due to Tartar [50,51] who studied hyperbolic conservation laws. They are measures defined on the range of the sequence \((f^k)\) which depend on the point \(x \in \Omega\).

In particular, it is generally incorrect to suppose that the limit of a minimizing sequence realizes the infimum of energy in a variational principle whose minimizing sequences are highly oscillatory. The minimum energy must be evaluated using (2.6).

Examples

For example, both the sequences of (2.2) and (2.3) have \( \bar{f}(x) = 0 \). On the other hand, for (2.2),

\[
\bar{\psi}(a) = \frac{1}{\pi} \int_{-1}^{1} \psi(\lambda) \frac{d\lambda}{\sqrt{1 - \lambda^2}}, \quad 0 < a < 1. \tag{2.8}
\]

while for (2.3),

\[
\bar{\psi}(a) = \frac{1}{2} (\psi(-1) + \psi(1)), \quad 0 < a < 1. \tag{2.9}
\]

The oscillatory statistics of the two sequences are thus quite different.

Let us now give a simple well known example of how oscillations may arise in the mathematical context. The first of these is the familiar Young-Zermelo tacking problem, [54]. Let \( \varphi(\lambda) \) be a double well potential with equal wells at \(-1\) and \(1\) as depicted in Figure 1 and, with \(\Omega = (0,1)\) an interval, set

\[
I(v) = \int_{\Omega} (\varphi(v') + v^2) \, dx. \tag{2.10}
\]

A minimizing sequence \((u^k)\) for this functional wishes to enjoy both \(\frac{du^k}{dx} = \pm 1\) for all \(k\) and \(u^k \to 0\) in \(\Omega\). The result is the generation of oscillations, with a typical minimizing sequence given by \(u^k\) with

\[
\frac{du^k}{dx} = f^k \text{ in } \Omega, \tag{2.11}
\]
with the $f^o$ defined in (2.3). The Young measure solution of the minimization problem is given by, cf. (2.9),

$$v = \frac{1}{2}(8.i + 5.i). \quad (2.12)$$

In this example, oscillations are created by competition between the two terms of the functional. In multivariable problems, side conditions, like boundary conditions, are sufficient to give rise to an oscillatory structure.

Interestingly, it is difficult to decide this from a computational standpoint because the additional competition between the grid orientation and the particular kinematics organization of the configuration requires a sufficiently large computational domain as well as certain other features. We are examining these issues with Nicolaides.

The propagation of oscillations, and even the convection of oscillations is an important issue. Tartar has investigated this in some detail [52], recently introducing the H measure to account for aspects of the frequency distribution of a sequence as well.

3. Magnetostriction A remarkable feature of ferromagnetic materials is that the single domain state is generally unstable. This constrasts with martensite, where the single variant configuration is stable for arbitrarily large samples. In the blue phase of cholesteric liquid crystals, the failure of stability of the uniform state relative to an array of defects is a frustration. Our theory here could be interpreted as one possible interpretation of this phenomenon at a macroscopic scale. The frustration in our system arises from the competition of an anisotropy energy which demands constant magnetization strength and direction with an induced field energy which prefers to tend to zero. A consequence of this is to promote development of a fine scale structure which seeks to compromise the constraint of constant magnetization strength.

Certain iron/rare earth alloys display both frustration and a huge magnetostriction. There are cubic Laves phase RFe2 (R = rare earth) compounds, for example, where magnetically induced strains "overwhelm the conventional thermal expansion of the material*, Clark [11]. TbDyFe2 (terfenol) solidifies from the melt with a complex highly mobile domains consisting of structural domains and magnetic domains. Typical growth habits result in configurations with parallel twinned layers, cf. Figure 2, that persist in the magnetostrictive process. We have been
Some methods of analysis in the study of microstructure

studying this with a theory of magnetoelastic interactions based on the micromagnetics of W. F. Brown, Jr. [6,7,8] and the symmetry considerations introduced by Ericksen [16-24]. For a complete discussion, we refer to James and Kinderlehrer [32]. It has some similarities with Toupin's theory of the elastic dielectric [54]. We then apply it to the equilibrium microstructure of TbDyFe$_2$. The primary mechanism of magnetostriction appears to be an exchange of stability of mechanical variants under the influence of a change in the magnetic field, but we do not discuss this in detail here.

For relatively rigid materials one may assume the free energy to depend on magnetization alone, [30,31]. The theory in this case gives good qualitative agreement with experiment, explaining why cubic magnets have a few large domains and why uniaxial ones have a fine structure. Domain refinement at the boundary is also predicted when the normal to the boundary has a suitable orientation with relative to the crystal axes, in agreement with observations.

The variational principle is formulated in terms of a stored energy density which depends on the deformation gradient $F \in \mathbb{M}$, 3 x 3 matrices, magnetization (per unit mass) $m \in \mathbb{R}^3$, and temperature $\theta \in \mathbb{R}$. We suppose it given by a nonnegative function

$$W(F, m, \theta) \quad F \in \mathbb{M}, \quad m \in \mathbb{R}^3, \quad \theta \in \mathbb{R},$$

subject to the condition of frame indifference

$$W(QF, mQ^T, \theta) = W(F, m, \theta), \quad Q \in \text{SO}(3),$$

and material symmetry

$$W(FP, m, \theta) = W(F, m, \theta), \quad P \in \mathbb{P},$$

where $\mathbb{P}$ is a crystallographic point group.

Requiring $W$ to depend on the deformation gradient $F = \nabla y$ and magnetization $m$ but not on $\nabla^2 y$ and $\nabla m$ indicates that any energy associated with mechanical twin walls and Bloch walls is neglected. In this formulation, there may be infinitely fine twins or infinitely fine magnetic
domains, as we have suggested earlier. Since on a macroscopic level, the materials of interest display highly mobile domain configurations, any wall energies need be very small. The analytical benefit is that in the limit of infinite fineness we are able to determine rather accurately the arrangement and location of variants within the material, although not their dimensions.

Let \( y \) denote the spatial variable and \( H \) and \( M \) denote the magnetic field and the magnetization (dipole moment per unit volume), respectively. In the spatial configuration, Maxwell's equations hold. In addition, material is magnetically saturated. For an appropriate choice of units, and introducing \( U(y) \) as a potential for \( H \),

\[
\text{div}_y (-\nabla_y U + M) = 0 \quad \text{in} \ R^3, \tag{3.4}
\]

and the field energy density is given by

\[
\frac{1}{2} |H|^2 = \frac{1}{2} |\nabla_y U|^2.
\]

The saturation constraint leads to

\[
\frac{|M|}{\rho} = f(\theta) \quad \text{in the body}, \tag{3.5}
\]

where \( \rho \) is the density.

The domain \( \Omega \) is interpreted as an undistorted single crystal above the Curie temperature. By an abuse of notation, let \( y(x) \) denote the deformation of \( \Omega \) to \( y(\Omega) \), assumed for the purposes of discussion to be 1:1. Since \( \rho(x) = 1/\det \nabla y(x) \), the magnetization per unit mass previously introduced, \( m = \det \nabla y M \), so the constraint (3.5) assumes the form

\[
|m| = f(\theta).
\]

We assume \( f(\theta) = 1 \), without loss in generality.

In this fashion we may write the virtual energy of the configuration \( y = y(x), \ m = m(x) \) in the mixed reference/spatial form

\[
E(y, m) = \int_\Omega W(\nabla y, m, \theta) \, dx + \frac{1}{2} \int_{R^3} |\nabla_y U|^2 \, dy \tag{3.6}
\]

subject to the constraints,

\[
\text{div}_y (-\nabla_y U + \frac{1}{\det \nabla y} m) = 0 \quad \text{in} \ R^3. \tag{3.7}
\]

\[
|m| = 1 \quad \text{in} \ y(\Omega).
\]

From (3.7), we may also write the energy in the form
E(y,m) = \int f w(\nabla y, m, e) \, dx + \int_\Omega f \frac{1}{2} m \cdot \nabla y U \, dy. \quad (3.8)

Both for computational and analytical reasons, it is useful to express this in terms of reference variables alone. For this, introduce \( u(x) = U(y(x)) \), so \( \nabla u(x) = \nabla y U(y(x)) F(x) \). With \( C \ll F \), the constraint equation (2.9) becomes

\[
\text{div}(-\nabla u C^{-1} \det F + m F^{-1}) = 0 \quad \text{in} \quad \mathbb{R}^3, \quad (3.9)
\]

and the saturation condition is simply

\[
I_{ml} = 1 \quad \text{in} \quad Q. \quad (3.10)
\]

The virtual energy of \( y = y(x), \quad m = m(x) \) in reference form is

\[
E(y, m) = \int f w(\nabla y, m, 9) \, dx + \int_\mathbb{R}^3 f \nabla u C^{-1} \nabla u \det F \, dx, \quad (3.11)
\]

subject to (3.9) and (3.10). Analogous to (3.8), we may also write (3.11) as

\[
E(y, m) = \int f w(\nabla y, m, 9) \, dx + \int_\mathbb{R}^3 f \nabla u m F^{-1} \, dx. \quad (3.12)
\]

The symmetry condition (3.3) induces a potential well structure on \( W \). The arrangement of these potential wells determines the possible fine structure. Our schema for understanding this well structure begins by choosing for \( P \) the symmetry group of a putative high temperature non-magnetic parent phase of the material. For example, in the case we shall consider here, \( P \) is the cubic group of order 24: relative to a cubic basis, these are the proper orthogonal matrices of the form \( P = (p_{ij}), \quad p_{ij} \in \{ \pm 1, 0 \} \). This is the appropriate assumption for TbDyFe2. For \( 9 < 6_0 \), we assume there exists a pair \( (U_i, m_i) \) with \( I_{mI} = 1 \) and \( U_i = U_i^T \) positive definite satisfying

\[
W(U_i, m_i, 9) \leq W(F, m, e) \quad \text{for} \quad F, D, \quad I_{mI} = 1. \quad (3.13)
\]

Generally, \( U_i \) and \( m_i \) depend on temperature. The conditions (3.2) and (3.3) imply the existence of other minima by (2.9). Assume that the full set of minima is determined by the orbits of \( (U_i, m_i) \) under these actions. Thus

\[
\inf W = W(RU_i H, m_i R T, e) < W(F, m, 9) \quad \text{for} \quad R \in \text{SO}(3), \quad H \in P
\]

and Fe M, \( I_{mI} = 1 \), with \( (F, m) \neq (R U_i H, m_i R T) \). \quad (3.14)

The potential wells are described as

\[
(RU_i, m_I R T), \quad R \in \text{SO}(3),
\]
Some methods of analysis in the study of microstructure

\( (RU_2m_2R^T), \ R \in SO(3), \)

\( (RU_nmnR^T), \ R \in SO(3), \)

where\( \{ (U_1,m_1), (U_2,m_2), \ldots (U_n,m_n) \} = \{ (QU_1Q^T,m_1Q^T): Q \in P \}. \)

An orbit of the form \( (RU_i,miR^T), R \in SO(3), \) will be called a variant by analogy to martensitic transformations.

Our idea of a variational principle is to find a pair \( \text{yon} \) such that

\[ E(\text{yon}) = \inf_{EOM} (TUO \text{ subject to } (3.9)) \]

However, in our situation, with the material, in essence, uniaxial, this will not be possible. Instead we must content ourselves with this result, whose verification relies on an explicit construction:

\[ \inf E = \min W \text{fftl}. \quad (3.15) \]

4. The variational context

4.1 The variational context: energetics

Consider the minimization question associated to \( (3.8) \) subject to \( (3.9) \). By choosing a special sequence of magnetizations, one may show that

\[ \inf E(y,m) \sim \min W \text{LIQI}, \quad (4.1) \]

as discussed at the end of \$3. However, because of the competition between the field energy and the stored energy, there cannot be any pair \( (y^*,m^*) \) with \( y^* \) affine and

\[ E(y^*,m^*) = \min W \text{LIQI}. \quad (4.2) \]

We are led in this manner to consider a sequence of deformation fields and magnetization fields \( (y^k,m^k) \) subject to \( (3.9) \) for which (dependence on \( \psi \) suppressed)

\[ E(y^kn^k) \to \min W \text{LIQI}. \quad (4.3) \]

and

\[ \forall y^k \to \bar{y} \quad \text{and} \quad m^k \to \bar{m}, \]
Some methods of analysis in the study of microstructure

where the convergence is in the sense of (2.4), or equivalently, (2.7).

The only way for (4.3) to occur is if

\[ W(y^k, m^k) \to \min W \quad \text{and} \quad \frac{1}{2} \int_{\mathbb{R}^3} |\nabla y^k|^2 \, dy \to 0. \quad (4.4) \]

Since

\[ W(y^k, m^k) \to \bar{W}(x), \quad \text{for } x \in \Omega, \]

\[ \bar{W}(x) = \int_{M \times S^2} W(A, \mu) \, dv(A, \mu), \]

we must have that the set of \((A, \mu)\) charged by \(v\), that is the support of the measure \(v\), is contained in the minimum energy wells described by (3.17). In analytical terms we write

\[ \text{supp } v \subset \{(A, \mu) : W(A, \mu) = \min W \} = \Sigma. \quad (4.5) \]

In addition, (4.4) provides via the constraint equation in (3.9) that

\[ \text{div}_y \frac{1}{\det \nabla y^k} m^k \to 0 \quad \text{in } H^{-1}(\mathbb{R}^3). \quad (4.6) \]

(4.5) and (4.6) place severe constraints on the possible forms of \(\nabla y\) and \(\bar{m}\).

4.2 The variational context: kinematics

An easy integration by parts shows that if \((y^k)\) is a sequence of deformation fields with bounded derivatives, then for any minors \(M(\nabla y^k)\) of the matrices \(\nabla y^k\),

\[ M(\nabla y^k) \to M(\bar{\nabla y}) \]

in the sense of (3.4), that is, in the weak* sense. Thus minors are special functions \(\psi(A)\) which are continuous with respect to this convergence. They are, of course, the null-Lagrangians. The Young measure relation also holds. So, in the present situation, combining (4.5) with the Young measure representation gives

\[ \nabla \bar{y}(x) = \int_{\Sigma} A \, dv_x(A, \mu) , \quad (4.7) \]

\[ \text{adj } \nabla \bar{y}(x) = \int_{\Sigma} \text{adj } A \, dv_x(A, \mu) , \quad \text{and} \]

\[ \det \nabla \bar{y}(x) = \int_{\Sigma} \det A \, dv_x(A, \mu) . \quad (4.9) \]
Some methods of analysis in the study of microstructure

where adj A stands for the classical adjoint of A and det A stands for the determinant of A. Formula (4.7) is simply a restatement of (3.4) in this case and is included to provide a complete list of null-lagrangians. We refer to (4.7) - (4.9) as the minors relations.

These relations place extremely strong restrictions on the nature of possible equilibrium configurations because they assert that the limit statistics of equilibrium configurations must be compatible with the potential well structure of the macroscopic bulk energy.

It is worthwhile pointing out that for the special case of an infinitely fine laminate supported on two deformation gradients $M_1$ and $M_2$, that is,

$$f_v(A) dv_A(A,n) = (1-G)v(M_1) + 6y(M_2), \quad (4.10)$$

for some $0, 0 < \gamma < 1$, the minors relations imply that

$$M_2 - M_1 = a \otimes n = \text{rank one}, \quad (4.11)$$

and the $\{ M_j \}$ may represent the deformation gradients of twin related variants with normal $n$. A sequence of deformations which determines (4.10) with $\gamma = 1$ is given by

$$V_y(x) = M_i + \frac{\gamma}{2}(1 + f^\gamma(x-n))a \otimes n, \quad x \in \Omega, \quad (4.12)$$

where $f^\gamma$ is defined in (2.3).
The Phase Transition in TbDyFe$_2$

Figure 3 The phase transition in terfenol.

Analogous formulas hold for any problem in thermoelasticity, but in magnetostriction we also have a relation about magnetization owing to (3.12). This relation is most useful in reference coordinates. Recall that

$$\overline{m}(x) = \sum \mu \, dV_x(A, \mu) .$$

(4.13)

The new relation is that
\[ \bar{m}(x)V\bar{y}(x)-T = \sum_{i} UA \cdot T d v_{x}(A^{\circ}), \quad (4.14) \]

with
\[ \text{div}(\epsilon(V\bar{y}-T)) = 0 \quad \text{in} \ R^{3}. \quad (4.15) \]

4.3 Application

In Terfenol-D, onset of ferromagnetism is associated with a stretch of the unit cell along a main diagonal parallel to the magnetization. In simplified kinematics, we find a pair \((Uij,mi)\) satisfying (2.15) provided by

\[ U_{i} = 1 + \epsilon m_{i} \otimes m_{i} \quad \text{and} \quad m_{i} = -^{\wedge}(1,1,1), \; \epsilon \; \text{small}, \quad (4.1) \]

for a suitable choice of coordinates. The other potential wells are determined by

\[ U_{i} = 1 + \epsilon m_{i} \otimes m_{i}, \; i = 2,3,4, \; \text{with} \]
\[ m_{2} = \gamma = (-1,1,D, \; m_{3} = \frac{1}{3} U, \; m_{4} = \frac{1}{3} 1 - U), \; \nu = \frac{1}{3} (U - 1). \quad (4.2) \]

Since \(-m_{j}\) is also an admissible magnetization, there are a total of eight potential wells. We regard the coordinates chosen so that this represents the lower laminate in Figure 1. The upper laminate is obtained from it by a rotation about the \(m_{i}\) axis. Note that this is not a symmetry operation of the original energy and, although holding invariant the well of \((Uij,mi)\), gives a different set of wells. To save space, here we discuss only the lower laminate. To properly treat the entire system, we must introduce an inhomogeneous energy \(W(Fan,8,x), \; x \in \mathbb{R}^{2}\), cf. [32].

To establish our result we wish to check that we may produce a minimizing sequence \((y^{k}j_{n}^{k})\) for the energy \(E(yon)\) with the potential well structure determined by (4.1) and (4.2) whose statistics, as determined by the "minors relations" and their generalizations, \((3.13) - (3.15), (3.20), \) and \((3.21), \) deliver the observed crystallographic data, for example, of the lower laminate of Figure 1. We are able to do this using the wells determined by \((Ui,mi)\) and \((U_{2},m_{2})\).

Given any pair of transformation strains
\[ U_{i} \approx 1 + \epsilon \xi \otimes \xi \; \text{and} \; U_{2} = 1 + \epsilon \xi \otimes \xi \]
\[ I \; \xi I = 1, \; \xi \; \text{and} \; \xi \; \text{independent}, \]
then the type I and type II twins (or twins and reciprocal twins) have normals
\[ n^{+} = \xi + \%2 \; \text{and} \; n^{-} = \xi - \%2. \]
There are rotations $R^*e$ and vectors $tf^e$ with

$$ U_i = R \pm U_2 (1 + \mathbf{a} \otimes \mathbf{n}) $$

(4.3)

In this case with $x_i = m_i$, $n^+ = (100)$ and $n^- = <011>$, in agreement with the observations of D. Lord [44,53].

A coherent laminate may be constructed from the deformation gradients $U_1$ and $R+U_2$ or from the deformation gradients $U_1$ and $R-U_2$, cf. also (3.16) - (3.19). We may construct a compatible sequence of magnetizations $m^k$ with $m^k = \pm m_i$ in the $U_1$ regions and $m^k = \pm m_2(R^+)T$ in the $R^+U_2$ regions with the property that the limit average $\bar{m} = 0$ so that

$$ \lim E(yKm^k) = \min WI CI I, $$

cf. Figure 2 below.

![Figure 4](image-url)

Figure 4. The equilibrium microstructure of a laminate with parameters predicted by the theory. The gray arrows represent directions of the magnetization within the mechanical layers. In the $U_1$ layers they are $\pm m_i$ where $m_i$ is a $<111>$ direction and in the shaded layers they are $\pm m_2(R^+T)$ where $012$ is a $<-111>$ direction.

It is possible to deduce, moreover, that the only magnetization distributions consistent with the mechanical laminate have $\bar{m} = 0$. One may explicitly write a Young measure solution

$$ \nu_x = \frac{1}{2}(1 - \lambda)(\delta(U_1,m_i) + \delta(U_1,-m_i)) + \frac{1}{2}\lambda(\delta(R^+U_2,m_2(R^+T)) + \delta(R^+U_2,-m_2(R^+T)), x \in \Omega^*, $$

where $0 \leq X \leq 1$.

Our analysis suggests however that Figure 2 above is not the only solution and need not be the only one the laboratory photographs show either. A laminate may also be realized with
Some methods of analysis in the study of microstructure 15 11/2/92

decomposition gradients $U_3$ and $RU_4$ which has the same appearance on an $\langle 01-1 \rangle$ plane. Note that $m_3 + m_4 \parallel (100)$. This configuration has the property that it is exactly compatible across the $\langle 111 \rangle$ plane whereas compatibility of the $U_1$ and $RU_2$ laminate is only in the fine structure limit and requires $\lambda$ constant. Interestingly, the fine structure laminate might display greater magnetostriction.

The computation of configurations is underway by Ma, who has successfully reproduced hysteretic behavior in linearly magnetostrictive models. Previously, Luskin and Ma, [45], studied the rigid ferromagnet.

5. Evolution Evolution problems for potentials which are not convex may be considered within this framework. The basics of an existence theory were given in [40] and has been significantly advanced by Demoulini and Walkington, in work which has not been published. Walkington, in particular, has adapted method for computing solutions of the Young-Zermelo problem to evolution, for reasons which will become clear momentarily.

Consider $\varphi$ as in Figure 1, a scalar valued potential for example, and ask for a solution of the problem, $q(\lambda) = \varphi(\lambda)$,

$$-\text{div} \, q(\nabla u) + \frac{\partial u}{\partial t} = 0 \quad \text{in} \quad \Omega \times (0, \infty)$$

$$u \mid_{\Omega \times (0)} = u_0$$

$$u \mid_{\partial \Omega \times (0, \infty)} = 0$$

A classical solution need not exist because the equation may be backward parabolic in some regions, but we may seek a Young measure solutions along the lines we have been discussing. We find this solution by adapting an implicit scheme.

The functional

$$I(v) = \int_{\Omega} (\varphi(\nabla v) + \frac{1}{2h}(v - w)^2) \, dx, \quad h > 0,$$

is only slightly different from (2.10). Given $h > 0$, set $t_k = kh$ and $u^{h,0} = u_0$. Solve iteratively for Young measures $v^{h,k}$ and underlying deformations $u^{h,k}$ by the minimization procedure

$$\int_{\Omega} (\varphi(\nabla v) + \frac{1}{2h}(v - u^{h,k-1})^2) \, dx \rightarrow \min$$

where the competing $v \in H^1_0(\Omega)$, for example. The $v^{h,k}$ and $u^{h,k}$ satisfy
Some methods of analysis in the study of microstructure

\[ \int \left( \phi + i (v - i M^{-1})^2 \right) \, dx = \min, \]  
\( (5.4) \)

\[ \overline{q}(x) = \sum_{k} U(X) \mathbf{v}^k(X) , \]  
with
\[ \text{supp} v^h \subset \{ \lambda : \phi(\lambda) = \langle f^*(k) \rangle \}. \]  
\( (5.5) \)

where \( \phi^{**} \) denotes the convexified \( \phi \), which is its relaxation in this situation. Moreover, it is possible to show that
\[ -\text{div} \overline{q} + J(\mathbf{u}^h, k - \mathbf{u}^h, k - 1) = 0, \]  
where
\[ \overline{q}^h(x) \]  
\[ = \int q^h(X) \mathbf{v}^h(X) \, \mathbf{a} \]  
\( (5.6) \)

We next assemble the \( v^{*\lambda} \) and \( u^{h, k} \), defining \( u^n \) to be the linear interpolant of the \( (u^{h, k}) \) and \( v^h \) the piecewise constant in time measure equal to \( v^\lambda \) in \( (k - 1)h < t < kh \). We obtain in this fashion a family of approximants which are "maximally dissipative" because of (5.5) and converge to a Young measure solution of (5.1).

It turns out that the solution \( u^{*\lambda} \) of the basic variational principle is the unique solution of the relaxed problem for this principle which is strictly convex in \( v \), but not in \( Vv \). Some convex analysis that tells us that \( u^h \) is unique and so is its limit \( u \) as \( h \to 0 \). The Young measure need not be unique.

This is an opportunity to study the pure generation of oscillations in a new context. The underlying solution is known. What statistics are possible for the sequences which generate this solution and can we compute them? How do they evolve in time? Using an algorithm specifically designed to compute Young measures by Nicolaides and Walkington, Walkington has computed several examples of this behavior, shown in Figure 6. Although in these pictures, the solution decreases monotonically to its limit
\[ u(x, 0) = \begin{cases} 0^+ & 0 < x \leq 0.5 \\ 0^- & 0.5 < x < 1 \end{cases}. \]
$u(x,0) = 2x(1-x)$

$u(x,0) = 2.2x(1-x)$

Figure 6  Computation of the solution of (5.6) by a Young measure algorithm.
this is not the case for general initial values $u(x,0)$, although the energy integral is a decreasing function of $t$. We refer also to their article in these proceedings.

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