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Mathematical Approaches to the Study of Smart Materials

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1. INTRODUCTION

The smartness of a shape-memory material is a consequence of its ability to form a flexible variant structure at one temperature while recognizing only a homogeneous equilibrium at a different temperature[1]. The fine scale morphology or microstructure of this variant structure has a clear role in the macroscopic behavior of the material. To investigate these phenomena, two issues are paramount. First, the presence of several stable variants at a given temperature reflects a complicated potential well structure for the free energy of the material. Second, the presence of spatially oscillatory behavior at the small scale suggests competition between the free energy of the material and loading or other environmental effects. Both of these features represent highly nonlinear processes and thus it is to nonlinear analysis we turn for methods to successfully describe these systems.

In this report we describe in an expository fashion one such technique which has been applied in several instances especially related to certain alloys or other crystalline materials. This is an averaging method, briefly explained in §2 below, which accounts for rapidly spatially varying systems and accomodates 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. These statistics require that interfaces be coherent, either precisely or in the fine phase limit. We illustrate this technique by analyzing the equilibrium configurations of $TbDyFe_2$, Terfenol, an iron/rare earth alloy with the highest known magnetostriction at room temperature. We propose to highlight here exactly the issue of when interfaces are compatible only in the fine phase limit and when they are exactly coherent.

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. This kind of theory is appropriate for large bodies, of the order of a millimeter or larger, and therefore is suitable for many actuator applications, although not for micromachines. Thus fine phase laminar

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[1] To appear in Mathematics in Smart Structures, Proc. Smart Structures and Materials '93

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. More generally, predictions based on the theory may lead to specific recommendations for the improvement of materials for actuators and sensors.

Examples of this sort of analysis served to generalize the crystallographic theory of martensite, Ball and James [3], and to compute the relaxation of energy densities in the presence of symmetry, Chipot and Kinderlehrer [11] and Fonseca [24]. It has subsequently played a role in many discussions related to microstructure, eg, [4,5,6,10,16,17,18,19,20,25,26,28,44,45,47,48]. A treatment of the variational foundations of this method is given in [27,36,37,38]. Kohn [40,41] 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 an example: a theory for highly magnetostrictive iron/rare earth alloys, [28,29,30] and, in particular, [31]. A major impetus for these investigations is to provide a basis for the numerical computation of configurations with complicated microstructure. This subject is covered in several of the articles in this volume and in the articles mentioned above. We cite also [42,43].

2. Local spatial averages; Young measures

We describe the portrayal of microstructure or fine phase 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,

$$f^k: \Omega \to \mathbb{R}^N, \ k = 1,2,..., \tag{2.1}$$

may describe a spatially oscillatory structure or system in the region Ω. For example, if Ω is a cube, f_o a fixed periodic function, and

$$f^k(x) = f_o(kx),$$

the system represents spatial oscillations modulated in some fashion by f_o. A specific one dimensional example is

$$f^k(x) = \sin \pi kx, \quad 0 \le x \le 1, \ k = 1,2,3... \tag{2.2}$$

Another one is given by

$$f_o(x) = \begin{cases} -1 & 0 < x < \frac{1}{2} \\ 1 & \frac{1}{2} \le x \le 1 \end{cases}, \ 0 \le x \le 1, \tag{2.3}$$

extended to the line as periodic of period one.

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 of which smart materials are an important example.

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

$$\bar{f}(a) = \lim_{\rho \to \infty} \lim_{k \to \infty} \frac{1}{|B_\rho|} \int_{B_\rho(a)} f^k \, dx, \tag{2.4}$$

where $|B_\rho|$ stands for the volume of the ball of radius ρ. 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*, or in some circumstances, *weak* convergence*. To overcome this, we calculate generalized moments. Let ψ 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

$$\bar{\psi}(a) = \lim_{\rho \to \infty} \lim_{k \to \infty} \frac{1}{|B_\rho|} \int_{B_\rho(a)} \psi(f^k) \, dx. \tag{2.5}$$

The association

$$\psi \to \bar{\psi}(a)$$

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

$$\bar{\psi}(a) = \int_{R^N} \psi(\lambda) \, d\nu_a(\lambda) \tag{2.6}$$

which has the property

$$\int_E \psi(f^k) \, dx \to \int_E \bar{\psi} \, dx \quad \text{for any subset } E \subset \Omega. \tag{2.7}$$

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 [55] to study control problems. Its first use in differential equations is due to Tartar [50,51] who studied hyperbolic conservation laws and compensated compactness. 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).

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),

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

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. This is the familiar Young-Zermelo tacking problem, [55]. Let $\varphi(\lambda)$ be a double well potential with wells of equal depth 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 Ω. The result is the generation of oscillations, with a typical minimizing sequence given by u^k with

$$\frac{du^k}{dx} = f^k \quad \text{in } \Omega, \tag{2.11}$$

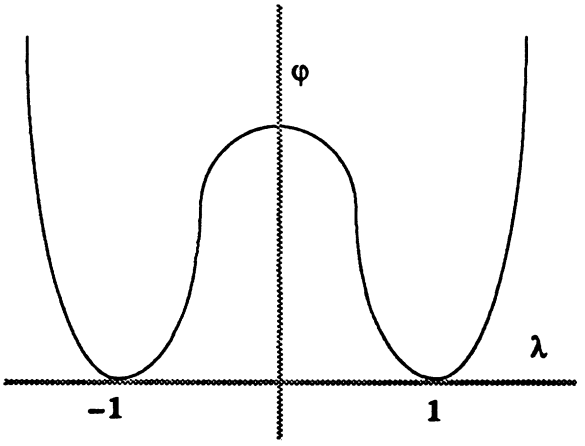

Figure 1 A typical double well potential in one variable.

with the f^k defined in (2.3). The *Young measure solution* of the minimization problem is given by, cf. (2.9),

$$\nu = \tfrac{1}{2}(\delta_{-1} + \delta_{+1}). \tag{2.12}$$

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 kinematic organization of the configuration requires a sufficiently large computational domain as well as certain other features. This issue is under investigation by 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

Certain iron/rare earth alloys display both frustration and a huge magnetostriction. There are cubic Laves phase RFe_2 (R = rare earth) compounds, for example, where magnetically induced strains "overwhelm the conventional thermal expansion of the material", Clark [12]. $TbDyFe_2$ (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 studying this with a theory of magnetoelastic interactions based on the micromagnetics of W. F. Brown, Jr. [7,8,9] and the symmetry considerations introduced by Ericksen [21,22,23]. 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 exhange of stability of mechanical variants under the influence of a change in the magnetic field. This material is the topic of discussion in, for example, [1,2,13,14,15,41].

For relatively rigid materials one may assume the free energy to depend on magnetization alone, [28,29]. 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 relative to the crystal axes, in agreement with observations.

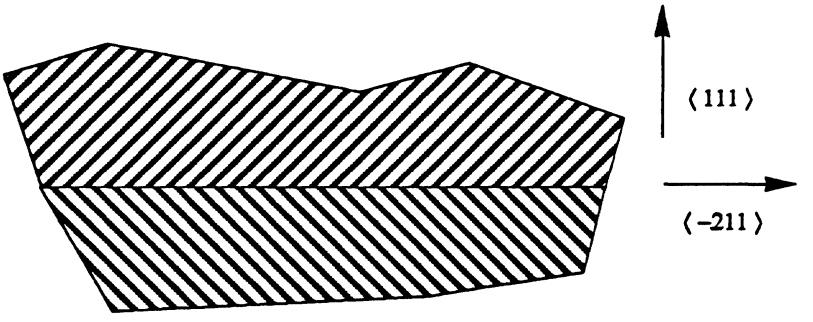

Figure 2. Schematic depiction of the microstructure in a sample of $TbDyFe_2$ illustrating the herringbone structure of two sets of laminar fine structures. Crystallographic directions are with reference to the high temperature nonmagnetic phase.

We assign to the material a stored energy density which depends on the deformation gradient $F \in \mathbb{M}$, 3×3 matrices, magnetization (per unit mass) $m \in \mathbb{R}^3$, and temperature $\theta \in \mathbb{R}$. In what follows, dependence on temperature will be depressed. We suppose it given by a nonnegative function

$$W(F, m), \qquad F \in \mathbb{M},\ m \in \mathbb{R}^3, \tag{3.1}$$

subject to the condition of frame indifference

$$W(QF,mQ^T) = W(F, m), \quad Q \in SO(3), \tag{3.2}$$

and a condition of material symmetry

$$W(FP, m) = W(F, m), \qquad P \in \mathbf{P}, \tag{3.3}$$

where $\mathbf{P}$ is an appropriate crystallographic point group. The saturation constraint, for our purposes, leads to the constraint

$$|\,m\,| = f(\theta) = 1 \quad \text{in the body.} \tag{3.4}$$

Requiring W to depend on the deformation gradient $F = \nabla y$ and magnetization m but not on $\nabla^2 y$ and ∇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.

In Terfenol-D, onset of ferromagnetism is associated with a stretch of the high temperature unit cell along a main diagonal parallel to the magnetization. W achieves its minimum energy on the eight pairs $(U_i, \pm m_i)$,

$$U_i = \eta_1 1 + (\eta_2 - \eta_1)\, m_i \otimes m_i, \; 1 = 1,2,3,4, \text{ and}$$

$$m_1 = \frac{1}{\sqrt{3}}(1,1,1),\; m_2 = \frac{1}{\sqrt{3}}(1,-1,-1),\; m_3 = \frac{1}{\sqrt{3}}(-1,1,-1),\; m_4 = \frac{1}{\sqrt{3}}(-1,-1,1). \tag{3.5}$$

From Al-Jiboory and Lord [1], we deduce that $\eta_1 = 0.9992\ (\pm 0.0001)$ and $\eta_2 = 1.0016\ (\pm 0.0002)$.

According to the frame indifference, W also achieves its minimum on the eight potential wells

$$(RU_i, m_i R^T),\; (RU_i, -m_i R^T),\; R \in SO(3),\; i = 1,2,3,4. \tag{3.6}$$

An orbit of the form $(RU_i, m_i R^T)$, $R \in SO(3)$, will be called a *variant* by analogy to martensitic transformations. We regard the coordinates chosen so that this represents the upper laminate in Figure 1.

The typical configuration of $TbDyFe_2$ rods consists of parallel growth twins. To model these, we assume that the entire rod is a composite for which we must introduce an inhomogeneous energy $W(F,m,x)$, $x \in \Omega$, cf. [32]. The lower lamellar structure arises from a rotation of $180°$ about the $m_1 = \frac{1}{\sqrt{3}}(1,1,1)$ axis of the original upper lattice. Denoting by R_o this rotation, the energy of the lower portion is given by $W(FR_o,m)$. Assuming coordinates to have been arranged so that the two regimes are separated by $x \cdot m_1 = 0$, we arrive at an energy density for the composite given by

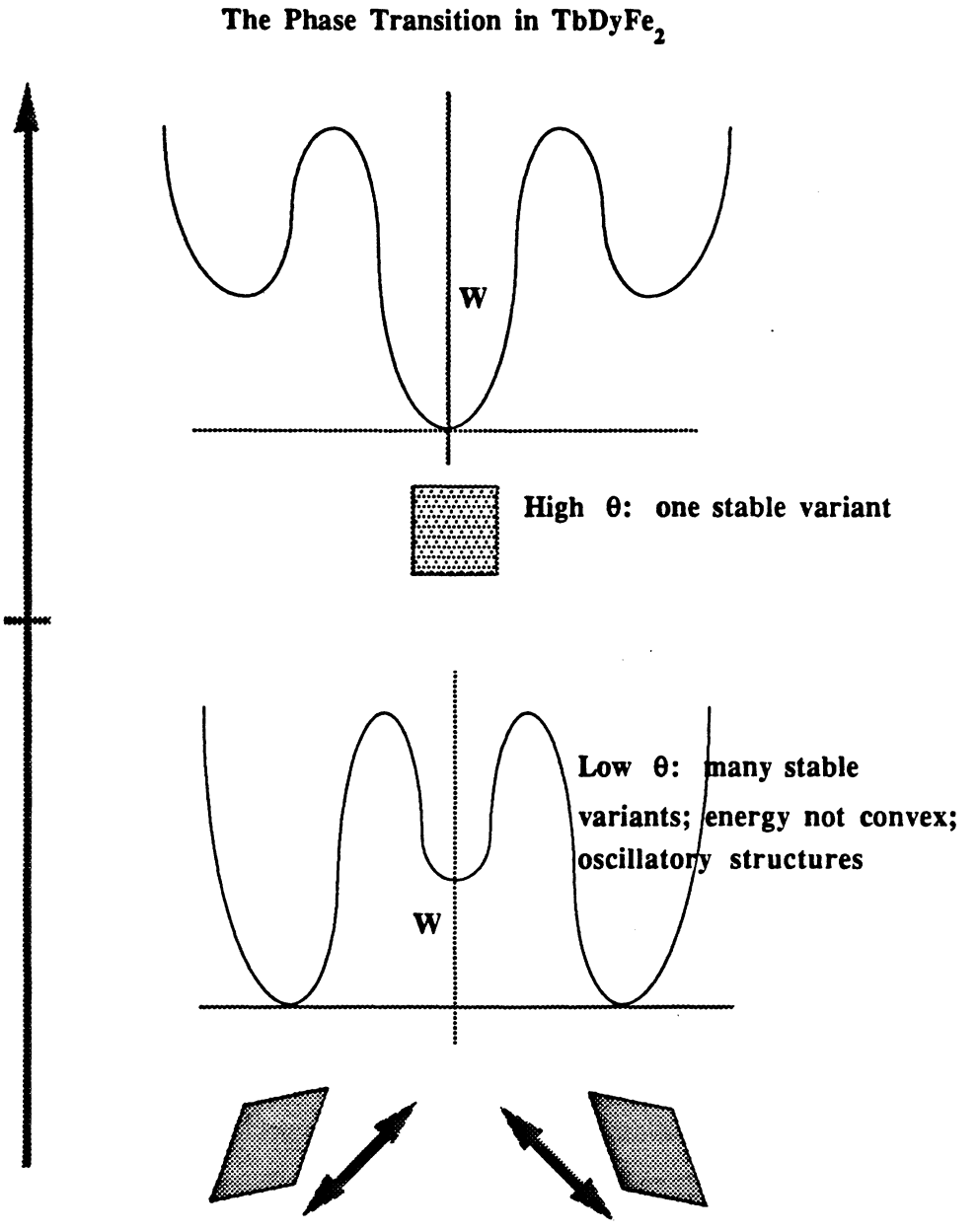

Figure 3 The phase transition in terfenol.

$$W(F,m,x) = \begin{cases} W(F,m) & x\cdot m_1 > 0 \\ W(FR_o,m) & x\cdot m_1 < 0 \end{cases} . \qquad (3.7)$$

Note that R_o is not a symmetry operation of the original energy and, although holding invariant the well of (U_1,m_1), gives a different set of wells with transformation strains and magnetizations

$$U_i' = \eta_1 1 + (\eta_2 - \eta_1)\, m_i' \otimes m_i', \ \pm m_i', \text{ with } m_i' = m_i R_o, \ 1 = 1,2,3,4. \tag{3.8}$$

Maxwell's Equations are introduced into this framework by

$$\operatorname{div}_y (-\nabla_y v + \frac{1}{\det \nabla y}\, m) = 0 \quad \text{in } \mathbf{R}^3. \tag{3.9}$$

where v is a potential for the magnetic field.

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

$$E(y,m) = \int_\Omega W(\nabla y, m, x)\, dx + \frac{1}{2} \int_{\mathbf{R}^3} |\nabla_y v|^2\, dy \tag{3.10}$$

subject to the constraints,

$$\operatorname{div}_y (-\nabla_y v + \frac{1}{\det \nabla y}\, m) = 0 \quad \text{in } \mathbf{R}^3. \tag{3.11}$$

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

From (3.9), we may also write the energy in the form

$$E(y,m) = \int_\Omega W(\nabla y, m, x)\, dx + \frac{1}{2} \int_{y(\Omega)} \frac{1}{\det \nabla y}\, m \cdot \nabla_y v\, dy \ . \tag{3.12}$$

Both for computational and analytical reasons, it is useful to express this in terms of reference variables alone. For this, introduce $u(x) = v(y(x))$, so $\nabla u(x) = \nabla_y v(y(x))F(x)$, $F(x) = \nabla y(x)$. With $C = F^T F$, the constraint equation (3.9) becomes

$$\operatorname{div}(-\nabla u\, C^{-1} \det F + m F^{-T}) = 0 \quad \text{in } \mathbf{R}^3. \tag{3.13}$$

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

$$E(y,m) = \int_\Omega W(\nabla y, m, x)\, dx + \frac{1}{2} \int_{\mathbf{R}^3} \nabla u\, C^{-1} \cdot \nabla u \det F\, dx, \tag{3.14}$$

subject to (3.10) and (3.11). Analogous to (3.12), we may also write (3.14) as

$$E(y,m) = \int_\Omega W(\nabla y, m, x)\, dx + \frac{1}{2} \int_{\mathbf{R}^3} \nabla u \cdot m F^{-T}\, dx. \tag{3.15}$$

Our idea of a variational principle is to find a pair (y,m) such that

$$E(y,m) = \inf \{ E(\eta,\mu): (\eta,\mu) \text{ subject to (3.11)} \}.$$

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:

$$\inf E = \min W |\Omega|. \tag{3.16}$$

4. THE VARIATIONAL CONTEXT

4.1 The variational context: energetics

Consider the minimization question associated to (3.16) subject to (3.11). By choosing a special sequence of magnetizations, one may show that

$$\inf E(y,m) = \min W |\Omega|, \tag{4.1}$$

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

$$E(y^*,m^*) = \min W |\Omega|. \tag{4.2}$$

We are led in this manner to consider a sequence of deformation fields and magnetizations (y^k,m^k) subject to (3.9) for which

$$E(y^k,m^k) \to \min W |\Omega|, \quad \nabla y^k \to \nabla \bar{y} \quad \text{and} \quad m^k \to \bar{m}, \tag{4.3}$$

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

The only way for (4.3) to occur is if

$$W(y^k,m^k) \to \min W \quad \text{and} \quad \frac{1}{2} \int_{R^3} |\nabla_y v^k|^2 \, dy \to 0. \tag{4.4}$$

Since

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

$$\bar{W}(x) = \int_{M \times S^2} W(A,\mu) \, d\nu_x(A,\mu),$$

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

$$\operatorname{supp} \nu \subset \{(A,\mu): W(A,\mu) = \min W \} = \Sigma. \tag{4.5}$$

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

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

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

4.2 The variational context: kinematics

The minors of ∇y^k are special functions $\psi(A)$ which are continuous with respect to weak 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

$$\nabla\bar{y}(x) = \int_\Sigma A \, d\nu_x(A,\mu) , \tag{4.7}$$

$$\operatorname{adj} \nabla\bar{y}(x) = \int_\Sigma \operatorname{adj} A \, d\nu_x(A,\mu) \text{ , and} \tag{4.8}$$

$$\det \nabla\bar{y}(x) = \int_\Sigma \det A \, d\nu_x(A,\mu) , \tag{4.9}$$

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*. They are among the most useful tools in analyzing microstructure.

Analogous formulas hold for any problem in thermoelasticity, but in magnetostriction we also have a relation about magnetization owing to (4.6). This relation is most useful in reference coordinates. Recall that

$$\bar{m}(x) = \int_\Sigma \mu \, d\nu_x(A,\mu) . \tag{4.10}$$

The new relation is that

$$\bar{m}(x)\nabla\bar{y}(x)^{-T} = \int_\Sigma \mu A^{-T} \, d\nu_x(A,\mu) , \tag{4.11}$$

with

$$\operatorname{div} (\bar{m}(\nabla\bar{y})^{-T}) = 0 \quad \text{in } \mathbb{R}^3. \tag{4.12}$$

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.

5. EQUILIBRIUM STRUCTURES IN TERFENOL

To ascertain the equilibrium configurations of Terfenol, we describe how deformation gradients chosen from the potential wells (3.5) and (3.8) give rise to coherent fine phase and exactly coherent minimum energy laminates and composites. At the conclusion of this section we report on the implications of these configurations for the magnetostrictive properties of Terfenol. We focus, for brevity, on the mechanical deformation. We refer to [30,32] where magnetic domains and the role of (4.12) are discussed. A deformation y with gradient ∇y which assumes exactly two values in some domain Ω, say,

$$\nabla y(x) = M_1 \text{ or } M_2 \text{ in } \Omega,$$

M_1 and M_2 3×3 matrices, must have the property

$$M_2 - M_1 = a \otimes n = \text{rank one.} \tag{5.1}$$

In addition, there is a function $f(t)$ which assumes only the values 0 and 1 such that

$$\nabla y(x) = M_1 + f(x \cdot n)\, a \otimes n = (1 - f(x \cdot n))M_1 + f(x \cdot n)M_2.$$

We refer to y as a (coherent) laminate. The $\{ M_i \}$ may represent the deformation gradients of twin related variants with normal n.

Similarly, if a sequence (y^k) of deformations with $y^k \to y$ weakly generates a Young measure $\nu = (\nu_x)_{x \in \Omega}$ such that

$$\bar{\psi}(x) = \int_{\Sigma} \psi(A)\, d\nu_x(A,\mu) = (1 - \theta((x))\, \psi(M_1) + \theta(x)\, \psi(M_2), \tag{5.2}$$

where $0 \le \theta(x) \le 1$, the minors relations imply that

$$M_2 - M_1 = a \otimes n = M_1 a \otimes n = \text{rank one,} \tag{5.3}$$

and there is a function $f(t)$ such that

$$\theta(x) = f(x \cdot n).$$

The average or limit deformation gradient is

$$\nabla y(x) = (1 - \theta((x))M_1 + \theta(x)\, M_2 = M_1 + \theta(x)\, a \otimes n. \tag{5.4}$$

We consider ν to determine a fine phase laminate.

We may construct a sequence (y^k) which gives rise to (4.14), for example, in the case of constant $\theta \in (0,1)$ by setting

$$\nabla y^k(x) = (1 - f^k(x \cdot n))M_1 + f^k(x \cdot n)\, M_2 , \quad x \in \Omega, \tag{5.5}$$

where $f^k(t) = f_o(kt)$ and

$$f_o(z) = \begin{cases} 1 & 0 < z < \theta \\ 0 & \theta < z < 1 \end{cases}$$

and is extended periodically on the line. Specifically,

$$\nabla y(x) = F = (1-\theta)M_1 + \theta M_2 \tag{5.6}$$

When M_i lie in minimum energy wells for an energy $W(F)$, then y^k is a sequence of minimum energy laminates whose limit is the fine phase laminate Young measure ν of (5.2). If we require the sequence y^k to satisfy a boundary condition or, as will occur in the present situation, a matching sequence of deformations defined in an adjacent region, a small transition layer will generally arise in which the ∇y^k will have small but not minimum energy.

Neglecting for the present the role of magnetization, we show how minimum energy laminates may be found. Laminates and fine phase laminates may be constructed from any pair of energy wells $SO(3)\tilde{U}_i$ where $|\varepsilon| < 1$ and

$$\tilde{U}_1 = 1 + \varepsilon\, \xi_1 \otimes \xi_1 \quad \text{and} \quad \tilde{U}_2 = 1 + \varepsilon\, \xi_2 \otimes \xi_2, \; |\xi_i| = 1, \; \xi_1 \text{ and } \xi_2 \text{ independent.} \tag{5.7}$$

The twins and reciprocal twins have normals

$$n^+ = \frac{1}{\sqrt{2}}(\xi_1 + \xi_2) \quad \text{and} \quad n^- = \frac{1}{\sqrt{2}}(\xi_1 - \xi_2).$$

There are rotations $R^{\pm}(\varepsilon)$ with common axis parallel to $\xi_1 \wedge \xi_2$ and vectors $a^{\pm}(\varepsilon)$ with

$$\tilde{U}_1 = R^{\pm}\tilde{U}_2 (1 + a^{\pm} \otimes n^{\pm}) \tag{5.8}$$

A coherent laminate, as depicted in Figure 4 may be constructed from the deformation gradients $M_1 = \tilde{U}_1$ and $M_2 = R^+\tilde{U}_2$ or from the deformation gradients $\tilde{U}_1$ and $R^-\tilde{U}_2$, cf. also (3.16) - (3.19). Finally, we may select $\tilde{U}_1 = U_i$ and $\tilde{U}_2 = U_j$ for any pair of the transformation strains described in (3.5). In this situation, we may construct a compatible sequence of magnetizations m^k with $m^k = \pm m_i$ in the U_i regions and $m^k = \pm m_j(R^+)^T$ in the R^+U_j regions with the property that the limit average $\bar{m} = 0$, but we omit the details of this, so that

$$\lim E(y^k,m^k) = \min W\,|\,\Omega\,|.$$

Table 1 describes the twins and reciprocal twins obtained in this way.

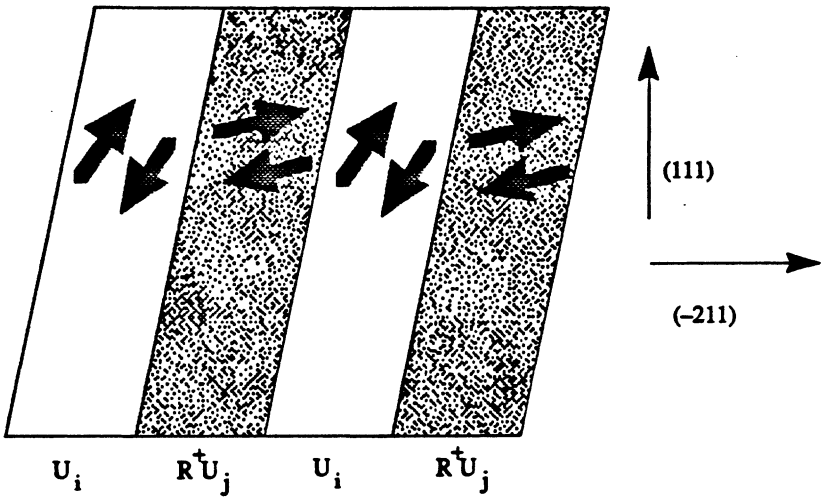

Figure 4. The equilibrium microstructure of a laminate with parameters predicted by the theory. The gray arrows represent directions of the magnetization within the mechanical layers. In the U_i layers they are $\pm m_i$ and in the shaded layers they are $\pm m_j(R^+)^T$.

Next, we describe how homogeneous deformations can be kinematically compatible with rotated energy wells, and hence can form composite laminates. Suppose that $y(x) = Fx$ is a homogeneous deformation defined in an upper region $\Omega_1 = \{ x \in \Omega: x \cdot m > 0 \}$, $|m| = 1$. Let R denote a rotation by 180° about the axis m. Then there is a 180° rotation Q with axis mF^{-1} such that

$$QFR = F(1 + c \otimes m). \tag{5.9}$$

Thus there is a laminate with deformation gradient $M_1 = F$ and $M_2 = QFR$ which has normal m. In particular, we may choose F of the form (5.6) to obtain a twinned herringbone structure like that depicted in Figure 2.

However it is only under special circumstances that this is possible with (5.9) valid for each ∇y^k, for this requires simultaneously choosing the same Q for both $F = M_1$ and $F = M_2$ in (5.9). In general, a small transition layer is necessary in order that the sequence remain coherent. In [32] we determined the condition for exact coherence, which is, in the notations of (5.3) and (5.9), that

$$a \cdot m = 0. \tag{5.10}$$

This condition is fulfilled when $m = m_1$ as long as U_1 is not among the choice of wells comprising the laminate. It then becomes possible to have a more flexible structure. A depiction of some of the possible

variants	*twin planes*	*intersection of twin plane with* (0–11)
1 2	(100) twin	⟨011⟩
	(011) reciprocal	⟨100⟩
1 3	(010) twin	⟨100⟩
	(101) reciprocal	⟨–111⟩
14	(001) twin	⟨100⟩
	(110) reciprocal	⟨–111⟩
23	(001) twin	⟨100⟩
	(110) reciprocal	⟨111⟩
34	(–100) twin	⟨011⟩
	(01–1) reciprocal	parallel to ⟨01–1⟩
24	(0–10) twin	⟨100⟩
	(10–1) reciprocal	⟨111⟩

Table 1. Twinning data for the compatible variants. The third column gives the intersection of the twin plane with the (0–11) plane of observation

configurations is in Figure 6. They are both observed, cf. [2,41]. Zhang and Soffa [56] report on domain structures in FePt and FePd which, by our condition (5.10) can occur only as fine phase laminate configurations.

To conclude this note, we wish to offer a few remarks about magnetostriction. Our computations suggest that the fine phase laminate 12/1'2' has the largest magnetostriction and one which is approximately 90% of maximum strain experienced by a line segment. This suggests a transition between the possibly coarser exactly coherent configuration and the fine phase configuration which is explained in [32].

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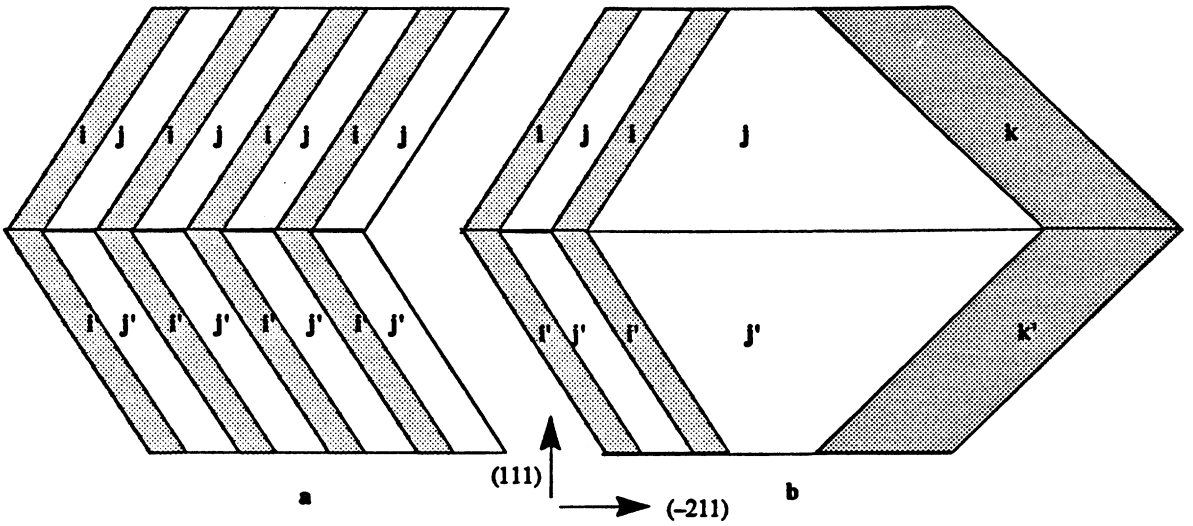

Figure 6. Comparison of fine phase and exact coherence of predicted laminates as viewed on the (0–11) plane. **i, j, k, i', j' k'** denote the potential wells from which the laminate is constructed, cf. (3.5) and (3.8). **a** may be **12/1'2'** fine phase or **34/3'4'** exactly coherent. **b**, with three variants, must be **342/3'4'2'** or **432/4'3'2'** exactly coherent. Both **a** and **b** are observed, [41] and [2] respectively.

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