Frustration and Microstructure: An Example in Magnetostriction

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Abstract Microstructural properties of materials, especially crystalline solids, are implicated in many of their properties. Vice versa, there are macroscopic environments which limit microstructural configurations. Certain iron/rare earth alloys, eg, $TbDyFe_2$, display both a huge magnetostriction and frustration, i.e., minimum energy not achieved, in which microstructure plays an important, if puzzling, role. We discuss this example in the framework of continuum thermoelasticity theory, where symmetry demands energy densities which are highly degenerate. This leads to novel analytical and computational issues, many of which we have been unable to resolve.

1. Introduction

Crystals are idealized as materials with a high degree of configurational order[1]. 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. The limit deformation alone need not be sufficient to characterize many of the properties of the limit configuration. Martensitic materials, in particular, exhibit fine structure in the form of fine twinned microstructure, often appearing as layers or layers within layers.

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 termed *frustration*, cf. Sethna [62]. Our

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calculations 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. A different mechanism is given by Sethna for the blue phase.

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 [16]. $TbDyFe_2$ (terfenol) solidifies from the melt with a textured microstructure which plays an important, if puzzling, role in its magnetostrictive properies. Our objective in this note is to describe briefly a theory of magnetoelastic interactions based on the micromagnetics of W. F. Brown, Jr. [10,11,12] and the symmetry considerations introduced by Ericksen [23-31]. It has some similarities with Toupin's theory of the elastic dielectric [70]. We shall then illustrate how the equilibrium microstructure of $TbDyFe_2$ is consistent with this theory. Our information about the properties of $TbDyFe_2$ comes primarily from Lord [53].

For relatively rigid materials one may assume the free energy to depend on magnetization alone, [39,40,51]. 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 analysis introduced to study the micromagnetic theory is based on the study of minimizing sequences, or devices used to summarize their oscillatory behavior. This gives a reasonable description of microscopic aspects of domain structure and macroscopic state functions. The particular averaging device used by us is the Young measure, Young [72], and first introduced in partial differential equations by Tartar [68,69]. The Young measure is particularly useful for predicting where in the body fine structure will occur. We refer to Ball [3], Ball and James [4,5], Chipot [14], Chipot and Kinderlehrer [13], Collins and Luskin [17,18,19], Collins, Kinderlehrer, and Luskin [20], Firooze and Kohn [32], Fonseca [33,34,35], James [36,37], James and Kinderlehrer [38], Kinderlehrer [43], Kohn [48,49], Matos [57], Pedregal [58,59], Sverak [64-67], and Zhang [73,74].

In addition to Brown's work, general references to the theory of ferromagnetism and ferromagnetic domain structure include Clark [16], Craik and Tebble [21], Kléman [47], Landau and Lifshitz [50], Landau, Lifshitz and Piatevskii [51], and Lifshitz [52]. Recent mathematical analysis includes Anzellotti, Baldo, and Visintin [1], Brandon and Rogers [9], Rogers [60,61],

and Visintin [71]. Computational aspects of micromagnetics have been studied by Luskin and Ma [54] and Ma [55].

2. Energy of magnetostriction

Equilibrium configurations of the system are interpreted as stationary points of a variational principle which consists of the sum of a stored energy and the induced magnetic field energy. In this section we describe the energy of a configuration and in §3 we discuss a variational principle. The stored energy density of the material will depend on the deformation gradient $F \in \mathbb{M}$, 3×3 matrices, magnetization (per unit mass) $m \in \mathbb{R}^3$, and temperature $\theta \in \mathbb{R}$. We suppose it given by a nonnegative function

$$W(F, m, \theta) \quad F \in D,\ m \in \mathbb{R}^3, \theta \in \mathbb{R}, \tag{2.1}$$

where $D \subset \mathbb{M}$ is a suitable domain of matrices with positive determinant. It is subject to the condition of frame indifference

$$W(QF, mQ^T, \theta) = W(F, m, \theta), \qquad Q \in SO(3), \tag{2.2}$$

and F, m, θ as in (2.1). We also impose a condition of material symmetry which is derived from a Cauchy-Born rule applied to the symmetry imputed to the underlying crystal lattice. This is explained in [41] and relies on the ideas set forth by Ericksen [24]. This symmetry is that

$$W(FP, m, \theta) = W(F, m, \theta), \qquad P \in \mathbb{P}, \tag{2.3}$$

where $\mathbb{P}$ is a crystallographic point group. We are hesitant to impose full magnetic symmetry including invariance under time reversals for reasons explained in [41].

In the spatial configuration, Maxwell's equations hold. Let y denote the spatial variable and B, H, and M denote the magnetic induction, the magnetic field, and the magnetization (dipole moment per unit volume), respectively. Then, for an appropriate choice of units,

$$\begin{aligned} &B = H + M, \\ &\operatorname{div}_y B = 0 \quad \text{and} \quad \operatorname{curl}_y H = 0 \quad \text{in } \mathbb{R}^3. \end{aligned} \tag{2.4}$$

Introducing $U(y)$ for which $H = -\nabla_y U$, we obtain that (2.4) is equivalent to

$$\operatorname{div}_y(-\nabla_y U + M) = 0 \quad \text{in } \mathbb{R}^3. \tag{2.5}$$

The field energy density is given by

$$\tfrac{1}{2}|H|^2 = \tfrac{1}{2}|\nabla_y U|^2.$$

The material is assumed magnetically saturated, leading to the constraint

$$|\frac{M}{\rho}| = f(\theta) \quad \text{in the body,} \tag{2.6}$$

where ρ is the density, cf. Brown [11], James and Müller [42], Landau and Lifschitz [50].

Assume now that initially the material occupies a reference configuration $\Omega \subset \mathbb{R}^3$ and has constant density ρ_o. As discussed below, Ω is interpreted as an undistorted single crystal above the Curie temperature. By an abuse of notation, let $y(x)$ denote the deformation of Ω to $y(\Omega)$, assumed for the purposes of discussion to be 1:1. Since $\rho(x) = \rho_o/\det \nabla y(x)$, the magnetization per unit mass previously introduced,

$$m = \frac{1}{\rho_o} \det \nabla y\, M,$$

so the constraint (2.6) assumes the form

$$|m| = f(\theta).$$

For our purposes it suffices to assume that $\rho_o = 1$, $m = m(x)$ and

$$\begin{aligned} &m = 0 \qquad \text{if } \theta > \theta_o \text{ and} \\ &|m| = 1 \qquad \text{in } \Omega \text{ at } \theta < \theta_o, \end{aligned} \tag{2.7}$$

where θ_o is the Curie point (associated with the onset of magnetization) and θ is fixed for our purposes.

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

$$E(y,m) = \int_\Omega W(\nabla y, m, \theta)\, dx + \tfrac{1}{2}\int_{\mathbf{R}^3} |\nabla_y U|^2\, dy \tag{2.8}$$

subject to the constraints, cf. (2.4) and (2.7),

$$\operatorname{div}_y\left(-\nabla_y U + \frac{1}{\det \nabla y}\, m\right) = 0 \quad \text{in } \mathbb{R}^3. \tag{2.9}$$

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

From (2.9), we may also write the energy in the form

$$E(y,m) = \int_\Omega W(\nabla y,m,\theta)\,dx + \frac{1}{2}\int_\Omega \frac{1}{\det \nabla y}\, m\cdot\nabla_y U\, dy \quad . \tag{2.10}$$

To express this in terms of reference variables alone, introduce $u(x) = U(y(x))$, so $\nabla u(x) = \nabla_y U(y(x))F(x)$, $F(x) = \nabla y(x)$. With $C = F^TF$, the constraint equation (2.9) becomes

$$\mathrm{div}(\, -\nabla u\, C^{-1}\det F + mF^{-T}\,) = 0 \quad \text{in } \mathbb{R}^3, \tag{2.11}$$

and the saturation condition is simply

$$|\,m\,| = 1 \quad \text{in } \Omega. \tag{2.12}$$

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

$$E(y,m) = \int_\Omega W(\nabla y,m,\theta)\,dx + \frac{1}{2}\int_{\mathbb{R}^3} \nabla u\, C^{-1}\cdot\nabla u \det F\, dx, \tag{2.13}$$

subject to (2.11) and (2.12). Analogous to (2.10), we may also write (2.13) as

$$E(y,m) = \int_\Omega W(\nabla y,m,\theta)\,dx + \frac{1}{2}\int_{\mathbb{R}^3} \nabla u\cdot mF^{-T}\, dx. \tag{2.14}$$

We wish to note here in a parenthetical fashion that in (2.11), (2.13) and (2.14) we have conveniently ignored the behavior of y outside of the region Ω occupied by the material. Without entering into a complete discussion of this issue, let us consider the most naive point of view. Suppose that y is a 1:1 deformation of Ω defined on all of $\mathbb{R}^3$ and that $y'(x) = y(\eta(x))$ where $\eta(x) = x$ in Ω. The potential $U(y)$ is then independent of the choice of mapping y or y' and so is the expression (2.10). Thus the energy of a configuration does not depend on the particular extension of $y(x)$ if $y_{|\Omega}$ is 1:1.

Moreover, as we shall illustrate shortly, the infimum of $E(y,m)$ depends only on $y_{|\Omega}$ in situations of interest.

The symmetry condition (2.3) induces a potential well structure on W. Our schema for understanding this well structure begins by choosing for $\mathbb{P}$ the symmetry group of a putative high temperature non-magnetic parent phase of the material. For example, in the case we shall consider here, $\mathbb{P}$ is the cubic group of order 24: relative to a cubic basis, these are the proper orthogonal matrices of the form $P = (p_{ij})$, $p_{ij} = \pm 1$ or 0. This is the appropriate assumption for $TbDyFe_2$. For $\theta < \theta_o$, we assume there exists a pair (U_1,m_1) with $|\,m_1\,| = 1$ and $U_1 = U_1^T$ positive definite satisfying

$$W(U_1,m_1,\theta) \le W(F,m,\theta) \quad \text{for } F \in D,\ |\,m\,| = 1. \tag{2.15}$$

Generally, U_1 and m_1 depend on temperature. The conditions (2.7) and (2.8) imply the existence of other minima by (2.9). We shall assume that *the full set of minima is determined by the orbits of* (U_1,m_1) *under these actions.* Thus

$$\inf W = W(RU_1H,m_1R^T) < W(F,m) \quad \text{for } R \in SO(3),\ H \in \mathbb{P} \text{ and } F \in \mathbb{M},\ |m| = 1, \text{ with } (F,m) \neq (RU_1H,m_1R^T). \tag{2.16}$$

The potential wells may be described as

$$\begin{aligned} &(RU_1,m_1R^T), \quad R \in SO(3),\\ &(RU_2,m_2R^T), \quad R \in SO(3),\\ &\quad\vdots\\ &(RU_n,m_nR^T), \quad R \in SO(3), \end{aligned} \tag{2.17}$$

where

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

An orbit of the form (RU_i,m_iR^T), $R \in SO(3)$, will be called a *variant.*

3. A variational principle

We would like to investigate variational principles compatible with minimizing the functional (2.8) or (2.13). A first requirement is that a variational principle be capable of delivering the possible minimum energy configurations determined by the well structure described in the preceding section. We formulate here a requirement for this which is a slight modification of our treatment of the rigid ferromagnet [40]. In this section we suppress the dependence of various quantities on temperature θ.

THEOREM 3.1 *Assume that there exists a pair* (F_o,m_o) *with* $\det F_o > 0$ *and* $|m_o| = 1$ *such that*

$$W(F_o,m_o) = W(F_o,-m_o) = \min W.$$

Then there is a sequence (y^k,m^k) *such that*

$$y^k: \mathbb{R}^3 \to \mathbb{R}^3 \text{ is 1:1 and } m^k: \Omega \to \mathbb{S}^2$$

with $\det \nabla y^k = \det F_o$ *such that*

$$\lim_{k\to\infty} E(y^k,m^k) = \min W\,|\Omega|. \tag{3.1}$$

PROOF. In fact, we choose $y^k(x) = y_o(x) \equiv F_o x$ for all k. Let $n \in \mathbb{S}^2$ satisfy $n \cdot m_o F_o^{-T} = 0$. Set

$$\vartheta(t) = \begin{cases} -1 & 0 \le t < \frac{1}{2} \\ +1 & \frac{1}{2} \le t < 1 \end{cases},$$

and extend ϑ to be periodic of period 1 on $\mathbb{R}$. Define

$$f^k(x) = \vartheta(kn\cdot x)\, m_o F_o^{-T}, \quad k = 1,2,3,\ldots \text{ and}$$

$$m^k(x)F_o^{-T} = \chi_\Omega f^k(x) = \vartheta(kn\cdot x)\,\chi_\Omega m_o F_o^{-T}, \quad k = 1,2,3,\ldots$$

Note that by the choice of ϑ and n,

$$f^k \to 0 \quad \text{in } L^\infty(\mathbb{R}^3;\mathbb{R}^3) \text{ weak*} \quad \text{and} \tag{3.2}$$

$$\operatorname{div} f^k = 0 \quad \text{in } H^{-1}_{loc}(\mathbb{R}^3). \tag{3.3}$$

Now let us note the lemma below, cf. Rogers [61] or [41].

LEMMA 3.2 *If* (f^k) *satisfy* (3.2) *and* (3.3), *then*

$$\operatorname{div} \chi_\Omega f^k \to 0 \quad \textit{in } H^{-1}(\mathbb{R}^3).$$

For the proof of the lemma, we refer to [41]. To continue the proof of the theorem, note that $C_o^{-1} \det F_o$ is positive definite, hence there is a solution

$$u^k \in V:\ \operatorname{div}(-\nabla u^k C_o^{-1} \det F_o + m^k F_o^{-T}) = 0 \quad \text{in } H^{-1}, \text{ where}$$

$$V = \{\, v \in H^1_{loc}(\mathbb{R}^3):\ \nabla v \in L^2(\mathbb{R}^3) \,\},$$

which satisfies

$$\|\nabla u^k\|_{L^2(\mathbb{R}^3)} \le \text{const}\, \|m^k F_o^{-T}\|_{L^2(\mathbb{R}^3)} \le M.$$

Finally,

$$\min W|\Omega| \le E(y^k,m^k) = \min W|\Omega| + \frac{1}{2}\int_{\mathbb{R}^3} \nabla u^k \cdot m^k F_o^{-T}\, dx$$

$$\le \min W|\Omega| + \frac{1}{2}\,\|\nabla u^k\|_{L^2(\mathbb{R}^3)}\,\|\operatorname{div} m^k F_o^{-T}\|_{H^{-1}(\mathbb{R}^3)}$$

$$= \min W|\Omega| + \frac{1}{2}\,\|\nabla u^k\|_{L^2(\mathbb{R}^3)}\,\|\operatorname{div} f^k\chi_\Omega\|_{H^{-1}(\mathbb{R}^3)}.$$

Applying the lemma to the last term,

$$\lim_{k\to\infty} E(y^k,m^k) = \min W|\Omega|. \qquad \text{QED}$$

Since the right hand side of (3.1) is the minimum possible value of E(y,m), the theorem serves us as a criterion in several ways. Any variational principle must recover the infimum of the functional. Also, later on, we can use THEOREM 3.1 to check that a given configuration is of minimum energy.

Rather than survey all the possibilities for minimum principles, let us adopt a point of view convenient for analytical purposes by choosing a reference formulation. In finite elasticity we do not generally require that the admissible deformations be 1:1, although there are occasions where this is feasible to prove (Ball [2], Ciarlet and Necas [15], Fonseca [35]), but we do ask that local orientation be preserved. So one generally imposes the condition that either $\det \nabla y > 0$ for an admissible deformation y or that

$$W(A,m) = \infty \quad \text{when} \quad \det A \le 0.$$

In the present situation, we are also asked to resolve the constraint equation (2.11), which we interpret to mean, cf. LEMMA 3.2,

$$u \in V\colon\ \operatorname{div}(-\nabla u\, C^{-1}\det F + m F^{-T}) = 0 \quad \text{in } H^{-1}(\mathbb{R}^3), \text{ where} \tag{3.4}$$

$$V = \{\, v \in H^1_{loc}(\mathbb{R}^3)\colon\ \nabla v \in L^2(\mathbb{R}^3),\ \int_{\{|x|\le 1\}} v\, dx = 0\,\},$$

when $F = \nabla y$, with y an admissible variation. For this it is convenient to assure that the matrix $C^{-1}\det F$ is positive definite and that the term $\operatorname{div}(m^k F^{-T})$ is in H^{-1}. Our technique is to adopt a van der Waals condition and to assume in addition that y has bounded derivatives. This will permit us to infer, for example, that

(i) if $u \in V$ satisfies (3.4), then $\|u\|_V \le$ const. and (3.5)

$$\text{(ii)} \quad \text{if } \frac{1}{2}\int_{\mathbf{R}^3} \nabla u^k\,(C^k)^{-1}\cdot\nabla u^k \det F^k\,dx \;\to\; 0, \text{ then } u^k \;\to\; 0 \quad \text{in } V \tag{3.6}$$

As we have been suggesting, there are many ways to achieve these conditions, but we should like to consider one which has been under discussion for some time, although it may not have appeared explicitly in the literature, and is common in the study of duality theory. Recently it has been taken up by Ball and James [5] and Kinderlehrer and Pedregal [44,45].

We shall assume that there is a subset $D \subset \mathbb{M}$ such that

$$W(A,m) \quad \begin{cases} < \infty & A \in D \\ = +\infty & A \notin D \end{cases} . \tag{3.7}$$

About D we impose these requirements:

$$\Sigma = \{A:\ W(A,m) = \inf W\} \subset D, \tag{3.8}$$

$$D \subset \{A:\ \det A \geq \delta\}, \text{ where } \delta > 0 \text{ is given,} \tag{3.9}$$

$$D\,\mathbb{P} \subset D, \text{ i.e., D is invariant under the symmetry group } \mathbb{P}, \text{ and} \tag{3.10}$$

$$D \text{ is the closure of a bounded open convex set.} \tag{3.11}$$

Let us assume that the symmetry group $\mathbb{P} \subset SO(3)$. Suppose that any A in the potential wells defined by (2.17) satisfies

$$|\,\mathrm{tr}\,(A^TA - 1)\,| \;=\; |\,|A|^2 - 3\,| \;\leq\; r \tag{3.12}$$

with r so small that (3.12) ensures that $\det F \geq \delta > 0$. We let the domain D where W(F,m) is defined as a function of F be determined by (3.12). It is invariant under the action of $\mathbb{P}$ and is convex. Thus all the properties (3.8) - (3.11) are satisfied. (3.9) and (3.11) imply that the constraint equation is well behaved, (3.5) and (3.6). In [5] it is shown how to obtain a D satisfying (3.8) - (3.10) with a general well structure.

A first advantage of (3.12) is that it permits us to understand the relaxation of the energy functional. In general, let K be the closure of a bounded open convex set. Given $\psi \in C(K)$, set

$$\hat{\psi}(A) \;=\; \begin{cases} \psi(A) & A \in K \\ \infty & \text{otherwise} \end{cases} . \tag{3.13}$$

Let

$$\hat{\psi}^{\#}(A) \;=\; \inf_{W^{1,\infty}_{o}(\Omega;\mathbb{R}^3)} \; \frac{1}{|\Omega|}\int_{\Omega} \hat{\psi}(A+\nabla\zeta)\,dx\,, \qquad A \in \mathbb{M} \tag{3.14}$$

Then $\hat{\psi}^{\#}(A) = +\infty$ for $A \notin K$,

$\hat{\psi}^{\#}(A)$ is quasiconvex, and

$$\Psi^{\#}(v) \;=\; \int_{\Omega} \hat{\psi}^{\#}(\nabla v)\,dx, \quad v \in W^{1,\infty}_{o}(\Omega;\mathbb{R}^3),$$

is sequentially weak* lower-semicontinuous [44]. In addition a relaxation result is valid. Suppose that

$$y_o \in W^{1,\infty}(\Omega;\mathbb{R}^3): \; \int_{\Omega} \hat{\psi}(\nabla y_o)\,dx \;<\; +\infty\,.$$

Then

$$\inf_{A} \int_{\Omega} \hat{\psi}(\nabla y)\,dx \;=\; \inf_{A} \int_{\Omega} \hat{\psi}^{\#}(\nabla y)\,dx, \tag{3.15}$$

$$A \;=\; \{y \in W^{1,\infty}(\Omega;\mathbb{R}^3):\; y = y_o \;\text{ on }\; \partial\Omega\}.$$

We have not at present identified the relaxation of a functional of the form

$$\int_{\Omega} \psi(\nabla y, m)\,dx, \qquad y \in W^{1,\infty}(\Omega;\mathbb{R}^3),\; m \in L^{\infty}(\Omega;\mathbb{S}^2)$$

nor of

$$\int_{\Omega} \hat{\psi}(\nabla y, m)\,dx, \qquad y \in W^{1,\infty}(\Omega;\mathbb{R}^3),\; m \in L^{\infty}(\Omega;\mathbb{S}^2).$$

However, it is possible to give the partial result that, for $m \in L^{\infty}(\Omega;\mathbb{S}^2)$ fixed,

$$\inf_{A} \int_{\Omega} \hat{\psi}(\nabla y, m)\,dx \;=\; \inf_{A} \int_{\Omega} \hat{\psi}^{\#}(\nabla y, m)\,dx, \tag{3.16}$$

$$A \;=\; \{y \in W^{1,\infty}(\Omega;\mathbb{R}^3):\; y = y_o \;\text{ on }\; \partial\Omega\},$$

where for each fixed unit vector μ,

$$\hat{\psi}^{\#}(A,\mu) \;=\; \inf_{H_o^{1,\infty}(\Omega;\mathbb{R}^3)} \frac{1}{|\Omega|}\int_{\Omega} \hat{\psi}(A+\nabla\zeta,\mu)\,dx\,, \qquad A \in \mathbb{M}. \tag{3.17}$$

This can be proved by modification of a known method, Marcellini [56], Dacorogna [22].

We next wish to investigate the limit configurations available to the energy E(y,m). These are given by the posssible minimizing sequences in terms of the Young measures they define. Suppose that (y^k,m^k), $\nabla y^k = F^k$, is a minimizing sequence with the property

$$(y^k,m^k) \;\to\; (y,\bar{m}) \quad \text{in } H^{1,\infty}(\mathbb{R}^3;\mathbb{R}^3)\times L^{\infty}(\Omega;\mathbb{S}^2) \text{ weak*}. \tag{3.18}$$

Then there is a family $\nu = (\nu_x)_{x\in\mathbb{R}^3}$ of probability measures such that whenever $\psi \in C(\mathbb{M}\times\mathbb{S}^2)$,

$$\psi(F^k,m^k) \;\to\; \bar{\psi} \text{ in } L^{\infty}(\mathbb{M}\times\mathbb{S}^2;\mathbb{R}) \text{ weak*, where}$$

$$\bar{\psi}(x) \;=\; \int_{\mathbb{M}\times\mathbb{S}^2} \psi(A,\mu)\,d\nu_x(A,\mu) \text{ in } \mathbb{R}^3 \text{ a.e.}$$

Let us isolate several basic features of the variational principle in this context. Since

$$\lim_{k\to\infty} E(y,m) \;=\; |\Omega| \min W,$$

it is immediate that

$$\bar{W}(x) \;=\; \min W \quad \text{and} \quad \operatorname{supp} \nu_{|\Omega} \subset \{(A,\mu):\, W(A,\mu) = \min W\} \equiv \Sigma. \tag{3.19}$$

i.e., the support of ν is in the energy wells, and, since we have already constructed one sequence for which the field energy tends to zero,

$$\frac{1}{2}\int_{\mathbb{R}^3} \nabla u^k\,(C^k)^{-1}.\nabla u^k \det F^k\,dx \;\to\; 0, \tag{3.20}$$

whence $u^k \to 0$ in V.

The limit deformation y(x) has gradient

$$F(x) \;=\; \int_{\mathbb{M}\times\mathbb{S}^2} A\,d\nu_x(A,\mu) \text{ in } \mathbb{R}^3 \text{ a.e. and}$$

$$F(x) = \int_{\Sigma \times S^2} A \, d\nu_x(A,\mu) \quad \text{in } \Omega \text{ a.e.} \tag{3.21}$$

so that

$$F(x) \in \text{convex hull } \Sigma \subset D. \tag{3.22}$$

This suggests several questions. First consider any gradient Young measure $\nu = (\nu_x)_{x \in \Omega}$ with $\text{supp } \nu \subset \Sigma$. Is it true that there is a sequence (u^k) with

$$\text{range } \nabla u^k \subset D \tag{3.23}$$

such that (∇u^k) generates ν ? What is known is that there is such a sequence with

$$\text{range } \nabla u^k \subset t\Sigma, \tag{3.24}$$

where $t \geq 1$ depends only on the well structure, [44]. It has also been established that if Σ consists of two variants, then any $F(x)$ satifying (3.21) may be achieved by a ν which consists of a convex combination of 3 ([5]) or 4 ([46]) Dirac masses. The associated sequences (u^k) satisfy (3.24) with $t = 1 + \varepsilon$, for ε chosen arbitrarily small. Also in some interesting cases of self-accomodation, (3.23) may be shown to hold, Bhattacharya [7]. A general open question is whether any function y whose gradient satisfies (3.21) is a limit of finite rank laminates with support in D.

Let us now consider briefly the magnetostatic energy. In the limit, this term vanishes according to (3.20). It follows that

$$m^k F^{k-T} \rightarrow \alpha \quad \text{in } L^\infty(\mathbb{R}^3;\mathbb{R}^3) \text{ weak*}, \quad \alpha = 0 \text{ for } x \notin \Omega, \text{ and}$$

$$\text{div } (m^k F^{k-T}) \rightarrow 0 \quad \text{in } H^{-1}_{\text{loc}}(\mathbb{R}^3). \tag{3.25}$$

Thus

$$\text{div } \alpha = 0 \quad \text{in } H^{-1}(\mathbb{R}^3). \tag{3.26}$$

It need not be true in general that $\alpha = 0$. We briefly inquire about the relationship between α and

$$\bar{m} = \int_{\Sigma \times S^2} \mu \, d\nu_x(A,\mu) \quad .$$

To a product of the form

$$\beta \nabla y^T = (\beta \cdot \nabla y_1, \beta \cdot \nabla y_2, \beta \cdot \nabla y_3)$$

we may seek to apply the div-curl lemma [68] provided β is the limit of quantities β^k with div β^k compact in H^{-1}. In our situation, $\beta^k = m^k F^{k-T}$ satisfies this condition, (3.25), so

$$\beta^k \cdot \nabla y_i^k \rightarrow \alpha \cdot \nabla y_i \text{ in } \mathcal{D}'.$$

Since $(m^k F^{k-T})$ and (∇y^k) are bounded,

$$\bar{m} = \alpha F^T \text{ or } \alpha = \bar{m} F^{-T}. \tag{3.27}$$

We shall use this relation in the next section to illustrate the necessity of magnetic fine structure in certain configurations.

4. Description of the equilibrium microstructure

The magnetostrictive material $Tb_xDy_{1-x}Fe_2$, $x \approx .27$, in equilibrium exhibits a herringbone configuration, with two sets of laminar fine structures separated by a (111) plane[2], cf. Figure 1. We shall focus attention on a single set of lamellae, eg., that below the indicated plane of separation in the region labelled Ω^-. Ignoring dependence on temperature, as usual, we assume that $W(F,m)$ is invariant under the group $\mathbb{P}$, the cubic group of order 24. As we have noted

$$\mathbb{P} = \{ P \in SO(3): P = (p_{ij}),\ p_{ij} = \pm 1 \text{ or } 0 \}. \tag{4.1}$$

We choose the pair (U_1, m_1) with

$$U_1 = 1 + \varepsilon m_1 \otimes m_1, \quad m_1 = \frac{1}{\sqrt{3}}(1,1,1),\ |\varepsilon| \text{ small}. \tag{4.2}$$

---

2 Crystallographic directions are referred to the putative high temperature cubic configuration.

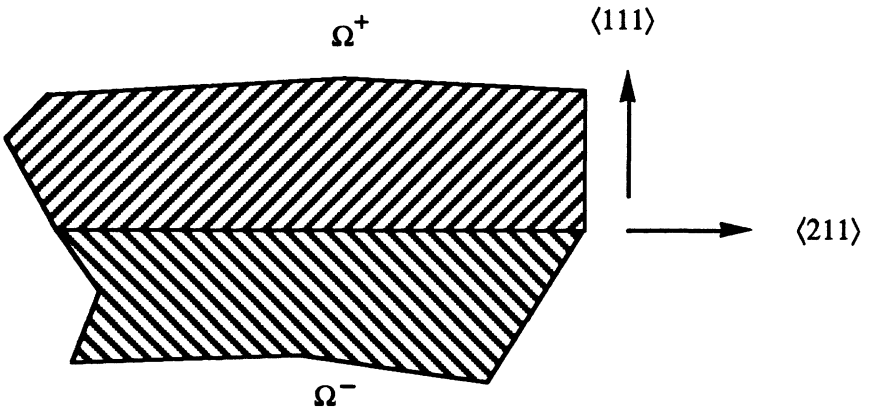

Figure 1 Schematic diagram of microstructure in $TbDyFe_2$, illustrating herringbone structure of two sets of laminar fine structures. Crystallographic directions are indicated.

Here we have made a special choice of reference configuration (see [41] for details.)Thus the low temperature phase derives from the high temperature phase by a stretch or contraction along a principal diagonal. One may easily calculate that there are eight potential wells. With

$$m_2 = \frac{1}{\sqrt{3}}(1,-1,-1), \quad m_3 = \frac{1}{\sqrt{3}}(1,-1,1), \quad m_4 = \frac{1}{\sqrt{3}}(-1,-1,1), \tag{4.3}$$

these are given by the SO(3) orbits of

$$(U_i,m_i) \text{ and } (U_i,-m_i), \quad U_i = 1 + \varepsilon m_i \otimes m_i, \; i = 1,\ldots,4, \tag{4.4}$$

according to (2.17). The conclusion of Theorem 3.1 obviously holds in this situation. We now consider the variant structure, for which we prove a special case of [4], Theorem 7. To understand the statement of this theorem, we recall a few terms. Two orbits $SO(3)M_1$ and $SO(3)M_2$ are *mechanically compatible*, or simply, *compatible*, provided there is at least one matrix $F_1 \in SO(3)M_1$ and one matrix $F_2 \in SO(3)M_2$ such that $F_2 - F_1$ is rank one. If $F_2 - F_1 = a \otimes n$, then there is a continuous piecewise affine deformation $y(x)$ such that

$$\nabla y(x) = \begin{cases} F_1 & n\cdot x < \gamma \\ F_2 & n\cdot x > \gamma \end{cases}, \text{ for any given } \gamma.$$

In fact, if for one F_1 there is one F_2, there are two such F_2's and this property holds for every $F_1 \in SO(3)M_1$. The pairs (F_1,m_1) and (F_2,m_2) are *mechanically and magnetically compatible* provided that $F_2 - F_1 = a \otimes n$, as before, and

$$(m_2 F_2^{-T} - m_1 F_1^{-T}) \cdot n = 0.$$

This means that the vector field

$$\alpha(x) = \begin{cases} m_1 F_1^{-T} & n \cdot x < \gamma \\ m_2 F_2^{-T} & n \cdot x > \gamma \end{cases},$$

satisfies

$$\operatorname{div} \alpha = 0 \text{ in } H^{-1}(\mathbb{R}^3),$$

and, does not induce any field energy in the functional E, and is a first step toward constructing a minimizing sequence. The compatibility of the minimum energy wells of W is assured by the result below, cf. [41].

THEOREM 4.1 *Suppose that*

$$U_1 = 1 + \varepsilon m_1 \otimes m_1 \text{ and } U_2 = 1 + \varepsilon m_2 \otimes m_2, \tag{4.5}$$

$$|m_i| = 1 \text{ and } m_1, m_2 \text{ independent.}$$

Then

$SO(3)U_1$ *and* $SO(3)U_2$ *are compatible wells.*

There are rotations $R^{\pm}$ *with axis* $p = m_1 \wedge m_2$ *such that*

$$U_1 = R^{\pm} U_2 (1 + a^{\pm} \otimes n^{\pm}), \tag{4.6}$$

with $n^+ \parallel p \wedge (m_1 - m_2)$, $n^- \parallel p \wedge (m_1 + m_2)$, *and* $a^{\pm} \cdot n^{\pm} = 0$.

The pairs

$$\{(U_1, m_1), (R^{\pm} U_2, \pm m_2 (R^{\pm})^T\}$$

are mechanically and magnetically compatible across planes $n^{\pm} \cdot x = \gamma$.

For example, with m_1 and m_2 given above, $n^+ = \langle 100 \rangle$ and $n^- = \langle 011 \rangle$, in agreement with the data of D. Lord. The Theorem applies to other transitions as well; m_i could be $\langle 100 \rangle$ or $\langle 110 \rangle$ directions and the result specifies the twin planes for more common cubic/tetragonal, etc., transitions.

We now exhibit a minimizing sequence which has Young measure

$$\nu_x = \tfrac{1}{2}(1-\lambda)(\delta_{(U_1,m_1)} + \delta_{(U_1,-m_1)}) + \tfrac{1}{2}\lambda(\delta_{(R^+U_2,m_2(R^+)^T)} + \delta_{(R^+U_2,-m_2(R^+)^T)}),\ x \in \Omega^-. \tag{4.7}$$

where $0 \le \lambda \le 1$. For convenience of notation, denote by $\Omega \subset \mathbb{R}^3$ be the region occupied by the material, instead of Ω^-, and suppose it has a sufficiently regular boundary. Set $n = n^+$ and $R = R^+$ and define the functions

$$\vartheta(t) = \begin{cases} -1 & 0 \le t < \frac{1}{2} \\ +1 & \frac{1}{2} \le t < 1 \end{cases}, \text{ and}$$

$$\eta(t) = \begin{cases} 1 & 0 \le t < \lambda \\ 0 & \lambda \le t < 1 \end{cases},$$

and extend ϑ and η to be periodic of period 1 on $\mathbb{R}$. Define $y^k(x)$ by $y^k(0) = 0$ and

$$\nabla y^k = F^k = (1-\eta(kx\cdot n))U_1 + \eta(kx\cdot n)RU_2,\ x \in \mathbb{R}^3. \tag{4.9}$$

Now in each layer where $F^k = U_1$, say, $j+\lambda \le kx\cdot n \le j+1$, define

$$m^k(x) = \vartheta(kp\cdot x)m_1,$$

and in each layer where $F^k = RU_2$, define

$$m^k(x) = \vartheta(kp\cdot x)m_2R^T.$$

Hence,

$$m^k(x) = \vartheta(kp\cdot x)((1-\eta(kx\cdot n))m_1 + \eta(kx\cdot n)m_2),\quad x \in \mathbb{R}^3. \tag{4.10}$$

According to this construction,

$$f^k(x) = m^k(x)\,F^k(x)^{-T} = \frac{\vartheta(kp\cdot x)}{1+\varepsilon}((1-\eta(kx\cdot n))m_1 + \eta(kx\cdot n)m_2),\quad x \in \mathbb{R}^3, \tag{4.11}$$

satisfies

$$\operatorname{div} f^k = 0 \text{ in } H^{-1}(\mathbb{R}^3) \text{ and } f^k \to 0 \text{ in } L^\infty(\mathbb{R}^3) \text{ weak*}.$$

Hence by Lemma 3.2,

$$\operatorname{div} \chi_\Omega f^k \to 0 \text{ in } H^{-1}(\mathbb{R}^3).$$

Since $W(F^k,m^k) = \min W$, we have that for this sequnce (y^k,m^k),

$$\lim_{k\to\infty} E(y^k,m^k) = |\Omega| \min W.$$

It is not necessary to be so precise in the construction of the minimizing sequence. It is possible to have a "slow" deformation variable and a "fast" magnetization variable, for example, and to exploit Lemma 3.2 in such a way that the magnetic compatibility across planes $x \cdot n = \text{const.}$ is not used.

5. Magnetic fine structure

Using (3.27), we can investigate the magnetization distribution associated with specific mechanical microstructures. We give two illustrations of this. We shall show that (4.7) is the unique Young measure whose underlying deformation gradient is the constant matrix

$$F = (1-\lambda)U_1 + \lambda RU_2 \quad \text{in } \Omega, \tag{5.1}$$

where $R = R^+$ and whose support is given by (5.3) below. Consequently, any equilibrium configuration of the form described by Ω^- in Figure 1 necessarily has magnetic fine structure. We then extend this to the composite $\Omega^+ \cup \Omega^-$. Indeed, in both cases our objective is to show that

$$\bar{m} = 0 \quad \text{in } \Omega. \tag{5.2}$$

Let us assume that $\nu = (\nu_x)_{x\in\Omega}$ is a Young measure generated by a minimizing sequence (y^k,m^k) of the functional E with the properties

$$\text{supp } \nu \subset X = \{(A,\mu): A = QU_i, \mu = m_iQ^T, Q \in SO(3), i = 1,2\} \tag{5.3}$$

where

$$U_i = 1 + \varepsilon m_i\otimes m_i, \ |m_i| = 1, i = 1,2, \text{ with } m_1, m_2 \text{ independent.} \tag{5.4}$$

We further assume that the underlying deformation gradient is given by (5.1) in a neighborhood Ω. In addition, we assume that $|\varepsilon|$ is small. First of all, it is known ([5],[46]) and easily shown that under the conditions of (4.8), (4.9) the deformation portion of the Young measure whose support is given by (5.3) is unique and given by a convex combination of Dirac masses. Hence in view of the restriction on the support of ν given by (5.3),

$$\nu_x = (1-\lambda)\{(1-\gamma_1(x))\,\delta_{U_1}\otimes\delta_{m_1} + \gamma_1(x)\,\delta_{U_1}\otimes\delta_{-m_1}\} +$$

$$\lambda\{(1-\gamma_2(x))\,\delta_{RU_2}\otimes\delta_{m_2R^T} + \gamma_2(x)\,\delta_{RU_2}\otimes\delta_{-m_2R^T}\}, \qquad (5.5)$$

where $0 \le \gamma_i(x) \le 1$. Now

$$\bar{m}(x) = \int_X \mu\, d\nu_x(A,\mu) \quad \text{in } \Omega \text{ a.e. and} \qquad (5.6)$$

$$\alpha(x) = \int_X \mu A^{-T}\, d\nu_x(A,\mu) \quad \text{in } \Omega \text{ a.e..} \qquad (5.7)$$

Thus

$$\bar{m} = ((1-\lambda)(1-2\gamma_1)m_1 + \lambda(1-2\gamma_2)m_2R^T)\chi_\Omega \qquad (5.8)$$

while on the other hand

$$\alpha = (1-\lambda)\{(1-\gamma_1)\,m_1U_1^{-T} - \gamma_1 m_1U_1^{-T}\}\chi_\Omega +$$

$$\lambda\{(1-\gamma_2)\,m_2R^T(RU_2)^{-T} - \gamma_2\,m_2R^T(RU_2)^{-T}\}\chi_\Omega$$

Since $U_i^{-T} = U_i^{-1}$, the above simplifies to

$$\alpha = \{(1-\lambda)(1-2\gamma_1)\,m_1U_1^{-1} + \lambda(1-2\gamma_2)\,m_2U_2^{-1}\}\chi_\Omega \qquad (5.9)$$

We now seek to identify the quantities in the expression $\bar{m} = \alpha F^T$, cf. (3.27). Setting $\beta_i = (1-2\gamma_i)$,

$$\alpha F^T = \{(1-\lambda)\beta_1\,m_1U_1^{-1} + \lambda\beta_1\,m_2U_2^{-1}\}\{(1-\lambda)U_1 + \lambda U_2R^T\} \quad \text{in } \Omega.$$

Since this expression must equal (5.9),

$$\lambda(1-\lambda)\{\beta_1m_1\,(1 - U_1^{-1}U_2R^T) + \beta_2m_2\,(R^T - U_2^{-1}U_1)\} = 0. \qquad (5.10)$$

The only case of interest is $0 < \lambda < 1$. If the two (constant) vectors

$$q_1 = m_1\,(1 - U_1^{-1}U_2R^T) \text{ and } q_2 = m_2\,(R^T - U_2^{-1}U_1) \qquad (5.11)$$

are independent, then $\beta_1 = \beta_2 = 0$. If they are dependent, then the functions $\beta_i(x)$ are proportional: there is a scalar $c \in \mathbb{R}$ for which

$$\beta_2(x) = c\,\beta_1(x) \quad \text{or } \beta_1(x) = 0 \quad \text{in } \Omega, \tag{5.12}$$

Hence, since $m_i U_i^{-1} = \frac{1}{1+\varepsilon} m_i$,

$$\alpha = \frac{\beta_1}{1+\varepsilon}((1-\lambda)m_1 + \lambda c m_2)\,\chi_\Omega. \tag{5.13}$$

Suppose at this point that (5.1) is satisfied in the entire region occupied by the material, Ω. Thus α has constant direction and satisfies

$$\operatorname{div} \alpha = 0 \text{ in } H^{-1}(\mathbb{R}^3).$$

This implies that $\alpha = 0$. In fact any mapping of the form

$$\zeta \to \int_{\mathbb{R}^3} f \nabla \zeta \, dx$$

where $f \in L^2(\mathbb{R}^3)$ has compact support either has full rank or f vanishes identically, cf. [40] Lemma 4.1. By (5.13),

$$\int_{\mathbb{R}^3} \frac{\beta_1}{1+\varepsilon} \chi_\Omega \nabla \zeta \, dx \cdot ((1-\lambda)m_1 + \lambda c m_2) = 0,$$

so

$$f = \frac{\beta_1(x)}{1+\varepsilon} = 0.$$

Consequently, $\beta_1 = \beta_2 = 0$ which implies that $\gamma_1 = \gamma_2 = \frac{1}{2}$. This verifies (5.2).

In fact, q_1 and q_2 of (5.11) are always dependent. Manipulation of equation (5.10) reveals that it is equivalent to

$$(\beta_1 m_1 U_1^{-1} - \beta_2 m_2 U_2^{-1})(U_1 - U_2 R^T) = 0,$$

or

$$\frac{1}{1+\varepsilon}(\beta_1 m_1 - \beta_2 m_2)(U_1 - U_2 R^T) = 0. \tag{5.14}$$

Now

$$U_1 - U_2 R^T = n \otimes R U_2 a$$

is a rank one matrix. Since m_1 and m_2 are independent, it is always possible to find β_i such that (5.14) holds. In fact, some additional algebra shows that $\beta_1 + \beta_2 = 0$.

Let us now consider the composite material described in Figure 1, assuming that the variant proportion is constant in the top and the bottom. An expression for the deformation identical to (5.1) holds in each of Ω^+ and Ω^-. We find by the preceding reasoning that α has constant direction in each of Ω^- and Ω^+. Arguing in a manner similar to the single laminate case, we conclude again that $\alpha = 0$.

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