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Theory of Magnetostriction with
Applications to $Tb_xDy_{1-x}Fe_2$

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Abstract

We present a new approach to magnetostriction that is formulated to describe materials with large magnetostriction. The main idea of the theory is to derive precisely from lattice considerations the potential wells of the anisotropy energy. The theory exhibits frustration in the sense explored by the authors in the rigid case (James and Kinderlehrer [1990]), with fine domains modeled by minimizing sequences. The theory is applied to the material $Tb_xDy_{1-x}Fe_2$. The theory predicts accurately the domain structures observed by Lord[1990] in growth twinned crystals, and suggests a mechanism of magnetostriction involving a switch from a coarse domain structure to a different finer domain structure.

1. Introduction

In this paper we present a new theory of magnetostriction that is particularly well-suited for predicting the microstructure and domain structure of materials that undergo large magnetostriction. We apply the theory to the material $Tb_xDy_{1-x}Fe_2(x \doteq 0.3)$, the material that undergoes the largest known magnetostrictive strain at room temperature. For this material we give detailed predictions of the microstructure that minimizes the energy appropriate to a growth-twinned specimen, and we discuss the implications for the macroscopic behavior of a specimen.

The energy that we write down for $Tb_xDy_{1-x}Fe_2$ exhibits frustration in the sense explored by the authors in an earlier paper [1990]. That is, the minimum value of the energy is not generally attained. This means that there is no deformation or magnetization that minimizes the total energy, but there are sequences of deformations and magnetizations $(\mathbf{y}^{(k)}, \mathbf{m}^{(k)}), k = 1, 2, 3 \ldots$ that drive the total energy to its smallest value as $k \to \infty$. Our point of view in this situation is to study these minimizing sequences and to interpret them as representing the fine microstructures observed in magnetostrictive materials. This kind of theory is appropriate for large bodies, as discussed by DeSimone [1992]. The fact that a sequence is a minimizing sequence is a strong restriction on the nature of its oscillations, which can be quantified by the use of Young measures and H-measures (see James and Kinderlehrer [1989,1990,1991], Tartar [1990,1991], DeSimone [1992]; Ball [1989], Ball and James [1992], Bhattacharya [1991], Chipot and Kinderlehrer [1988], Gerard [1992], James and Müller [1992], Kinderlehrer and Pedregal [1991], Kohn [1991] Pedregal [1992]). In the present paper, in order to make the treatment accessible to a wide audience, we deal with the sequences directly and suppress some technical arguments.

Our main idea in formulating the theory is to focus on the potential wells of the energy. We think that this approach brings a simplicity to the subject that is not obvious in approaches that involve large numbers of magnetoelastic constants and their associated symmetry restrictions. For many aspects of the behavior of $Tb_xDy_{1-x}Fe_2$ most of these

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constants are not essential. The important constants are those that determine the potential wells, so we forget about the constants altogether and focus our effort on a precise specification of these wells. For aspects of domain structure near saturation, we would need to know more than the locations of the potential wells.

The basic theory is given in Sections 1-3 and summarized in Section 4. Readers mainly interested in applications of the theory to $Tb_xDy_{1-x}Fe_2$ can pass to Section 4, then to Remark 5.6 and then on to Section 6.

The specification of the theory for $Tb_xDy_{1-x}Fe_2$ owes much to the interpretations of micrographs of Lord [1990,1992] and to discussions with Savage [1990,1992]. We have essentially taken the deformations and magnetizations observed by Lord and assigned them as minimizers of the anisotropy energy. The full potential-well structure is then determined by the basic theory. The theory for $Tb_xDy_{1-x}Fe_2$ turns out to have some features in common with a theory for martensitic transformations specialized to a cubic-to-trigonal transformation (Section 6a).

We show that the theory (specialized to $Tb_xDy_{1-x}Fe_2$) admits lamellar minimizing sequences with interfaces on {100} and {110}; both of these kinds of laminates are observed by Lord et al. [1988]. The theory as given is appropriate for a single crystal. We rewrite the energy in Section 6c for a crystal with growth twins on (111), since nearly all specimens of $Tb_xDy_{1-x}Fe_2$ have these twins. We model the growth twinned crystal as a coherent composite, and we study its minimizing sequences. We do a complete analysis of all minimizing sequences which are lamellar above and below the growth twin boundary (Sections 6d,e). We find a variety of such sequences, some of which agree accurately with Lord's photomicrograph (Figure 6). Among these sequences we find some that exhibit exact compatibility, or attainment, in the terminology given above.

All of these minimizing sequences found for the growth twinned crystal have a free parameter $\gamma \in [0,1]$, which represents the volume fraction of one of the variants. We calculate in Section 6g the macroscopic strain of a rod oriented along $[-211]$ for all of the

minimizing sequences. As γ passes from 0 to 1, the theory says that the growth twinned rod experiences a macroscopic uniaxial strain that is approximately 8/9 of the theoretical maximum. However, the maximum strain is not achieved by all of the laminates and, in particular, the *attained* minima do not achieve maximum magnetostriction. Going beyond the theory, we are led to speculate on a mechanism for magnetostriction that involves a switch from attained minima to minimizing sequences (Section 6g). Our mechanism is related to, but different from, the "λ-jumping" of Clark, Teter and McMasters [1988].

The theory highlights two features of the potential well structure of $Tb_x Dy_{1-x} Fe_2$. The first is that for minimizing sequences under no applied field, the magnetic domain structure does not have to be much finer than the wavelength of oscillations of distortion. This is explained in Remark 5.4 and the conditons for this to be possible are given in Lemma 6.1. The second feature is that the growth twin planes happen to exactly coincide with planes on which lamellar microstructures can be compatible and, moreover, some of these lamellar microstructures yield a magnetostrictive strain that is very near the theoretical maximum. For this reason we conclude that there will be minimal benefits, with regard to actuator applications, in trying to remove the growth twins in this alloy. On the contrary, our calculations suggest that improvements in large amplitute actuator performance will be gained by trying to eliminate waviness of the growth twin boundaries.

1. Lattice considerations

The form of our energy will be based on a simple and classical lattice picture. A *magnetic Bravais lattice* is a pair $L(e_i, d)$ consisting of an infinite set of points

$$L(e_i) = \left\{ x \in \mathbf{R}^3 : x = \nu^i e_i, \ \nu^k \in Z, \ k = 1, 2, 3 \right\}$$

determined by the three lattice vectors $\{e_1, e_2, e_3\}$ together with a magnetic dipole field

$$d : L(e_i) \to \mathbf{R}^3.$$

Here Z represents the integers and the summation convention is used. As is typical of studies of micromagnetics, we ignore fluctuations of the lattice positions and dipoles associated with nonzero temperature. We regard this as being sufficient to suggest the forms of the terms in the energy and their symmetry restrictions.

The symmetry of a magnetic Bravais lattice is normally treated in the context of point group and time reversal symmetry. The usual treatment is described in terms of linear constitutive relations and is not sufficient for our purpose of treating large magnetostriction. Also, there is not universal agreement on the transformation laws under a time reversal.

In Pauli's treatment of the spin of an electron a time reversal in the time-dependent Schrödinger equation does not affect charge, whereas the electronic spin is reversed. These transformation laws are consistent with the effect of a time reversal in Maxwell's equations if we transform $\rho \to \rho$, $\mathbf{d} \to \mathbf{d}$, $\mathbf{h} \to -\mathbf{h}$, $\mathbf{b} \to -\mathbf{b}$, $\mathbf{e} \to \mathbf{e}$, where ρ is the charge, $\mathbf{d}$ is the electric displacement, $\mathbf{h}$ is the magnetic field, $\mathbf{b}$ is the magnetic induction and $\mathbf{e}$ is the electric field. Equally valid, from the point of view of Maxwell's equations, are the transformation laws $\rho \to -\rho$, $\mathbf{d} \to -\mathbf{d}$, $\mathbf{h} \to \mathbf{h}$, $\mathbf{b} \to \mathbf{b}$, and $\mathbf{e} \to -\mathbf{e}$ under a time reversal. The former point of view, combined with the idea that in equilibrium a quantity and its transform under a time reversal have the same free energy, implies that certain property tensors vanish, leading to various forbidden effects (Birss [1964]). The argument against the conventional viewpoint, mentioned to us by Jerry Ericksen, are the existence of certain materials that exhibit these forbidden effects and prejudices that Maxwell's equations should be transformed according to the second set of rules above. This prejudice stems from the assumption that the four-dimensional formulation of electromagnetism (e.g., Truesdell and Toupin [1960]) should be invariant under tensor transformations of space-time, together with the universally accepted assumption that $\mathbf{b}$ is an axial vector. Putting these together, it is found that under a time reversal $\mathbf{b} \to \mathbf{b}$. For these reasons we adopt in this paper the unconventional viewpoint that free energy functions are *not* necessarily invariant under the transformation $\mathbf{m} \to -\mathbf{m}$.

This issue does not affect the calculations in this paper concerning our application to $Tb_x Dy_{1-x} Fe_2$, because our calculations on $Tb_x Dy_{1-x} Fe_2$ only make use of the energy wells of the free energy function, and these energy wells are necessarily invariant under the transformation $\mathbf{m} \to -\mathbf{m}$ by virtue of the special symmetries of this alloy. However, for the behavior of $Tb_x Dy_{1-x} Fe_2$ under large stress, this point could conceivably become relevant.

Linear transformations of the magnetic Bravais lattice will be sufficient for our purposes. Adopting the viewpoint expressed above for time reversals, we say that the linear transformation $\mathbf{G} \in L(\mathbf{R}^3, \mathbf{R}^3)$ belongs to the *magnetic lattice group* $G(L, \mathbf{d})$ of the magnetic Bravais lattice $(L, \mathbf{d})$ if there is a $\mathbf{c} \in \mathbf{R}^3$ such that

$$L = \mathbf{G}L + \mathbf{c}, \quad \mathbf{d}(\mathbf{Gx} + \mathbf{c}) = \mathbf{d}(\mathbf{x}) \quad \forall \, \mathbf{x} \in L. \tag{2.3}$$

The presence of $\mathbf{c}$ permits translations of the lattice which may be necessary to bring the dipoles into coincidence (The necessity of introducing $\mathbf{c}$ can be appreciated by considering a BCC lattice with $\mathbf{d} = (100)$ at body centers and $\mathbf{d} = (-100)$ at the body corners).

Suppose $L = L(\mathbf{e}_i)$ for some lattice vectors $\{\mathbf{e}_i\}$. It is easily seen that $(2.3)_1$ is satisfied if and only if $\mathbf{c}$ is of the form $n^i \mathbf{e}_i$ for integers n^i and then that $(2.3)_1$ is equivalent to the statement

$$L = \mathbf{G}L. \tag{2.4}$$

The general solution of (2.4) is given by a classical theorem of crystallography (e.g., Ericksen [1977]) which states that for a Bravais lattice $L = L(\mathbf{e}_i)$,

$$L = \mathbf{G}L \quad \Leftrightarrow \quad \mathbf{Ge}_i = \mu_i^j \mathbf{e}_j \text{ where } \mu_i^j \text{ are integers and det } \mu = \pm 1. \tag{2.5}$$

The group specified by (2.5) is too large to serve as an invariance group for the free energy, as it includes the large shears associated with plasticity. Our constitutive equations will not be appropriate for plastic deformations. This issue has been confronted during the development of recent theories of martensitic transformations (*cf.* Ball and James [1992]) and has been resolved by a theorem due to Ericksen [1980] and Pitteri [1984] (for a slight generalization of this theorem see Ball and James [1992], Theorem 2.4). To state the result, we use the notation $\mathbf{Q}N$ for the set $(\mathbf{Qf}_1, \mathbf{Qf}_2, \mathbf{Qf}_3)$, $\mathbf{Q} \in O(3)$, $\{\mathbf{f}_i\} \in N$, N being a set of vector-triples, whereas we denote by $\mu[N]$ the set of all vector-triples of the form $\mu_i^j \mathbf{f}_j$ where μ_i^j is a 3×3 matrix. The theorem says that given any triple of lattice vectors $\{\mathbf{e}_i\}$

there is a bounded open neighborhood $N(\mathbf{e}_i)$ of $\{\mathbf{e}_i\}$ in the space of all vector-triples with the properties

N1 N is frame-indifferent: $\mathbf{Q}N = N \ \forall \ \mathbf{Q} \in O(3)$,

N2 For each $\mu \in G := \left\{ \nu_i^j \in \mathsf{M}^{3 \times 3} : \nu_i^j \text{ are integers and } \det \nu = \pm 1 \right\}$,

$\mu[N] = N$ or $\mu[N] \cap N = \phi$,

N3 If $\mu \in G$ satisfies $\mu[N] = N$, then $\mu_i^j \mathbf{e}_j = \mathbf{Q}\mathbf{e}_j$ for some $\mathbf{Q} \in O(3)$.

Here, $O(3) := \left\{ \mathbf{Q} \in \mathsf{M}^{3x3} : \mathbf{Q}^T \mathbf{Q} = 1 \right\}$ is the group of orthogonal matrices. Briefly, this theorem says that the neighborhood $N(\mathbf{e}_i)$ is frame-indifferent and invariant under the point group of the "central" lattice vectors $\{\mathbf{e}_i\}$, and also that any symmetry transformation for the lattice not in the point group of $\{\mathbf{e}_i\}$ maps the neighborhood far away. The neighborhood will provide a domain for the free energy with a consistent and finite symmetry group. We note that the *point group* $P(\mathbf{e}_i)$ of the lattice $L(\mathbf{e}_i)$ is the set

$$P(\mathbf{e}_i) := \left\{ \mathbf{Q} \in O(3) : \mathbf{Q}\mathbf{e}_i = \mu_i^j \mathbf{e}_i, \ \mu \in G \right\}. \tag{2.6}$$

The point group is a property of the lattice, as indicated by the terminology, i.e., two sets of lattice vectors that generate the same lattice give the same point group.

3. Symmetry restrictions and the passage to continuum theory

In passing from the lattice picture to a continuum theory, we first consider the dipole field $\mathbf{d} : L(\mathbf{e}_i) \to \mathbf{R}^3$. In the classical framework the magnetization arises as a volume average of the dipole field over a sphere that is small relative to the wavelength of oscillations of $\mathbf{d}$ and large relative to the lattice spacing (Lorentz [1909]). This calculation has been examined recently by James and Müller [1992]. Adapting that treatment, we consider a family of scaled lattices $L_\gamma := L(\gamma \mathbf{e}_i)$, $\gamma > 0$, defined for a fixed set of lattice vectors $\{\mathbf{e}_i\}$. Let

$$U := \{\xi^i \mathbf{e}_i : 0 < \xi^i \leq 1, \quad i = 1, 2, 3\} \tag{3.1}$$

be the unit cell of the 1-lattice L_1. We identify macroscopic quantities as limits of corresponding lattice quantities as $\gamma \to 0$. We assume that for each $\gamma > 0$ there is a dipole field $\mathbf{d}_\gamma : L_\gamma \to \mathbf{R}^3$ and a given *background field* $\mathbf{m} \in L^2(\mathbf{R}^3, \mathbf{R}^3)$ with support on a bounded open set Ω' such that

$$\mathbf{d}_\gamma(\mathbf{y}) = \int_{\mathbf{y}+\gamma U} \mathbf{m}(\mathbf{z})d\mathbf{z}, \quad \mathbf{y} \in L_\gamma. \tag{3.2}$$

We identify $\mathbf{m}$ as the (macroscopic) magnetization and Ω' as some deformed configuration of the body.

> More generally, we could allow $\mathbf{m}$ to depend on γ in the formula (3.2), as long as we assume that $\mathbf{m}_\gamma \to \mathbf{m}$ in $L^2(\mathbf{R}^3, \mathbf{R}^3)$. In this case we identify the limit $\mathbf{m}$ as the magnetization and note that the expression (3.6) for the limiting energy continues to be valid (James and Müller [1992]).

> We caution that the assumption of strong convergence of $\mathbf{m}_\gamma$ forbids oscillations on the scale of the lattice that would occur with extremely fine magnetic domains (such as in ferrimagnetism). Oscillations on the scale of the lattice can be modeled by expressions of the form $\mathbf{m}_\gamma(\mathbf{x}) = \mathbf{m}_o(\mathbf{x}/\gamma)\varphi(\mathbf{x})$, where $\mathbf{m}_o$ is say a periodic function on $\mathbf{R}^3$ and φ has compact support on Ω', and correspond to weak convergence of $\mathbf{m}_\gamma$. Expressions for the macroscopic energy in such cases are given by James and Müller [1992] and differ from (3.5).

The expression for the total energy of the dipoles is obtained by summing the work done in bringing each dipole $\mathbf{d}_\gamma(\mathbf{x})$ from ∞ to a point $\mathbf{x}$ on the lattice L_γ. This gives (Brown [1962,1963], Toupin [1956]) the energy

$$e_\gamma := \sum_{\substack{\mathbf{x},\mathbf{y} \in L_\gamma \\ \mathbf{x} \neq \mathbf{y}}} \mathbf{d}_\gamma(\mathbf{x}) \cdot \mathbf{K}(\mathbf{x} - \mathbf{y})\mathbf{d}_\gamma(\mathbf{y}), \tag{3.3}$$

$$\mathbf{K}(\mathbf{z}) := \frac{-1}{4\pi|\mathbf{z}|^3}\left\{1 - 3\frac{\mathbf{z}}{|\mathbf{z}|} \otimes \frac{\mathbf{z}}{|\mathbf{z}|}\right\}, \quad \mathbf{z} \in \mathbf{R}^3. \tag{3.4}$$

Here, $\mathbf{d}_\gamma$ is given by (3.2) and we interpret the limiting value of e_γ as $\gamma \to 0$ as the macroscopic field energy. This limit is (James and Müller [1992])

$$e_\gamma \to \frac{1}{2}\int_{\Omega'}[-\mathbf{m}(\mathbf{y}) \cdot \mathbf{h}(\mathbf{y}) + \mathbf{m}(\mathbf{y}) \cdot \hat{\mathbf{S}}\mathbf{m}(\mathbf{y}) + \frac{1}{3}|\mathbf{m}(\mathbf{y})|^2]dy \tag{3.5}$$

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and this agrees with the classical formula (Brown [1962,1963]). Here, $\mathbf{h} = -\nabla u$ is the unique solution (in $L^2\,(\mathbf{R}^3,\ \mathbf{R}^3)$, see James and Kinderlehrer [1990]) of the equations

$$\mathbf{h} = -\nabla u, \quad \mathrm{div}(\mathbf{h} + \mathbf{m}) = 0, \tag{3.6}$$

and $\hat{\mathbf{S}} = \hat{\mathbf{S}}(\mathbf{e}_i)$ is a spatially constant symmetric matrix that depends on the lattice vectors only, *i.e.*, it does not depend on the arrangement of dipoles on the lattice. We shall use the expression on the right hand side of (3.5) for the field energy. In this expression $\mathbf{h}$ is determined from $\mathbf{m}$ by the equations (3.6).

Turning to the anisotropy energy, we consider a fixed Bravais lattice L^o, termed the *reference lattice*, which is interpreted as the undistorted crystal at the Curie temperature θ_c. Let $L^o = L(\mathbf{e}_i^o)$ for some lattice vectors $\{\mathbf{e}_i^o\}$. The lattice vectors $\{\mathbf{e}_i^o\}$ determine an Ericksen-Pitteri neighborhood $N^o := N(\mathbf{e}_i^o) \subset (\mathbf{R}^3)^3$ satisfying properties N1, N2, N3 listed at the end of Section 2. Let $M \subset (\mathbf{R}^3)^3 \times \mathbf{R}^3 \times \mathbf{R}$ be a set with the property

$$\{(\mathbf{e}_i,\ \mathbf{m},\ \theta) \in M : (\mathbf{m}, \theta) \text{ are fixed}\} = \{N^o, \mathbf{m}, \theta\}\,. \tag{3.7}$$

The assumption (3.7) is formulated to allow for a variety of constraints on the magnetization $\mathbf{m}$ which would model magnetic saturation. We assume M is objective in the sense that if $\{\mathbf{e}_i,\ \mathbf{m},\ \theta\} \in M$ then so does $\{\mathbf{Re}_i,\ \mathbf{Rm},\ \theta\}$ for all $\mathbf{R} \in SO(3)$. Here, $SO(3) := \{\mathbf{R} \in O(3) : \det \mathbf{R} = +1\}$ is the group of 3×3 rotation matrices. We discuss such constraints at the end of this section. We assume the existence of a function $\tilde{\varphi} : M \to \mathbf{R}$ with the interpretation that

$$\tilde{\varphi}(\mathbf{e}_i,\ \mathbf{m},\ \theta) \tag{3.8}$$

represents the free energy per unit volume of a lattice $L(\mathbf{e}_i)$ with magnetization $\mathbf{m}$ at temperature θ.

In (3.8) we have mixed macroscopic quantities $\mathbf{m}$ and θ with the lattice scale quantity $\{\mathbf{e}_i\}$. In an expanded treatment, we would consider a family of reference lattices $L_\gamma^o := \gamma L^o$ and deformations of these lattices $\mathbf{y} : L_\gamma^o \to \mathbf{R}^3$, by analogy with the discussion of

dipoles above. Accounting for short range interactions between atoms, we would then pass to the limit $\gamma \to 0$ to get the internal energy. The temperature dependence might then be treated by statistical mechanics, using a model that allowed small vibrations of atoms and dipoles. Lacking good molecular models of magnetostrictive materials, we are unable to carry out these calculations.

On the other hand, rudimentary calculations of this type do give the form (3.8). We are able to specify details of the form of $\widetilde{\varphi}$ by phenomenological considerations, as described below. As in the discussion of the energy of a lattice of dipoles, if we allow the deformation to depend on γ, $\mathbf{y}_\gamma : L^o_\gamma \to \mathbf{R}^3$, which would be necessary to treat oscillations of deformation on the scale of the lattice, then we would not get (3.8).

Having adopted (3.8), it is clear how to proceed. Any reasonable molecular model will have the property that the dipole moments and the lattice vectors will transform as objective vectors under a change of frame. Hence, the principle of material frame-indifference states that

$$\widetilde{\varphi}(\mathbf{Q}\mathbf{e}_i, \ \mathbf{Q}\mathbf{m}, \ \theta) = \widetilde{\varphi}(\mathbf{e}_i, \ \mathbf{m}, \ \theta) \quad \forall \, \mathbf{Q} \in SO(3), \quad \forall (\mathbf{e}_i, \ \mathbf{m}, \ \theta) \in M. \quad (3.9)$$

The restriction (3.9) makes sense because $SO(3)N^o = N^o$ by N1 and because M has been assumed to be objective. Also, the free energy at a given temperature should only depend on the lattice and the dipole field on that lattice. Hence, if two sets of lattice vectors generate the same lattice via (2.1), then the free energy should be the same, so long as we leave the dipole field unchanged. This gives the restriction

$$\widetilde{\varphi}(\mathbf{e}_i, \ \mathbf{m}, \ \theta) = \widetilde{\varphi}(\hat{\mathbf{e}}_i, \ \mathbf{m}, \ \theta), \ whenever$$

$$(\mathbf{e}_i, \ \mathbf{m}, \ \theta) \ and \ (\hat{\mathbf{e}}_i, \ \mathbf{m}, \ \theta) \ belong \ to \ M \ and \quad (3.10)$$

$$\hat{\mathbf{e}}_i = \mu^j_i \mathbf{e}_i; \ for \ some \ \mu \in G.$$

Note that the domain of the dipole field is $L(\mathbf{e}_i)$ which by (3.10) is the same as $L(\hat{\mathbf{e}}_i)$; hence, it makes sense to keep the magnetization the same in (3.10) (cf. (2.2)).

We shall pass to continuum theory by using the Cauchy-Born rule. This seems to be adequate for $TbDyFe_2$ and works well in the analogous case of martensitic transformations (cf. Ball and James [1992]). Arguing formally, we consider a bounded open set Ω that

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we interpret as the undistorted crystal at θ_c. Deformations of Ω are given by functions $\mathbf{y} : \Omega \rightarrow \mathbf{R}^3$, with gradient $\mathbf{F} = \nabla \mathbf{y}(\mathbf{x})$.

We define for $(\mathbf{Fe}_i^o, \mathbf{m}, \theta) \in M$,

$$\hat{\varphi}(\mathbf{F}, \mathbf{m}, \theta) := \widetilde{\varphi}(\mathbf{Fe}_i^o, \mathbf{m}, \theta) \det \mathbf{F},$$

$$\left(= \widetilde{\varphi}(\mathbf{Fe}_1^o, \mathbf{Fe}_2^o, \mathbf{Fe}_3^o, \mathbf{m}, \theta) \det \mathbf{F} \right). \tag{3.11}$$

Here the factor $\det \mathbf{F}$ serves to make φ the free energy per unit volume in Ω. The Cauchy-Born rule states that the free energy of continuum mechanics is given by

$$\int_\Omega \hat{\varphi}(\nabla \mathbf{y}(\mathbf{x}), \mathbf{m}(\mathbf{y}(\mathbf{x})), \theta) \, d\mathbf{x}. \tag{3.12}$$

We obtain the total free energy by adding (3.12) to the field energy given by the right hand side of (3.5).

The free energy $\hat{\varphi}(\mathbf{F}, \mathbf{m}, \theta)$ inherits certain properties from (3.9), (3.10). First we note that by (3.11) $\hat{\varphi}$ is defined on the domain $\mathcal{M}$, where

$$\mathcal{M} := \left\{ (\mathbf{F}, \mathbf{m}, \theta) \in \mathbf{M}^{3 \times 3} \times \mathbf{R}^3 \times \mathbf{R} : (\mathbf{Fe}_i^o, \mathbf{m}, \theta) \in M \text{ and } \det \mathbf{F} > 0 \right\}. \tag{3.13}$$

We have added the restriction $\det \mathbf{F} > 0$ in (3.13) because, by adopting the Cauchy-Born rule, we are naturally led to restrict attention to deformations that are invertible and orientation preserving, these being the only physically allowable deformations. The domain (3.13) objective by N1 and assumptions on M, and the principle of material frame-indifference (3.9) yields

$$\hat{\varphi}(\mathbf{R}\mathbf{F}, \mathbf{R}\mathbf{m}, \theta) = \hat{\varphi}(\mathbf{F}, \mathbf{m}, \theta) \tag{3.14}$$

for all $\mathbf{R} \in SO(3)$ and for all $(\mathbf{F}, \mathbf{m}, \theta) \in \mathcal{M}$. Standard arguments in continuum mechanics applied to (3.14) show that

$$\hat{\varphi}(\mathbf{F}, \mathbf{m}, \theta) = \bar{\varphi}(\mathbf{F}^T \mathbf{F}, \mathbf{F}^T \mathbf{m}, \theta) \tag{3.15}$$

for some function $\bar{\varphi}$ with domain inherited from (3.15).

Now we turn to the implications of (3.10). Recalling N3, let the Laue group of the lattice $L(\mathbf{e}_i^o)$ be given by

$$P^o := \left\{ \mathbf{Q} \in SO(3) : \mathbf{Q}\mathbf{e}_i^o = \mu_i^j \mathbf{e}_i^o, \ \mu \in G \right\}. \tag{3.16}$$

The restriction (3.16) to $SO(3)$, which restricts the point group $P(\mathbf{e}_i^o)$ to its Laue subgroup, is in anticipation of being restricted to det $\mathbf{F} > 0$ in (3.11) (*cf.* N3, (2.6), (3.13)$_{ff}$ and (3.16)). Expressed in terms of $\hat{\varphi}$, the condition (3.10) becomes

$$\hat{\varphi}(\mathbf{FQ}, \mathbf{m}, \theta) = \hat{\varphi}(\mathbf{F}, \mathbf{m}, \theta) \quad \forall \, \mathbf{Q} \in P^o \quad \forall \, (\mathbf{F}, \mathbf{m}, \theta) \in \mathcal{M}. \tag{3.17}$$

Hence, the governing symmetry group of the energy is the Laue group of the *reference* lattice $L(\mathbf{e}_i^o)$. In $Tb_x Dy_{1-x} Fe_2$ this will mean that, despite the fact that no observed configuration of $Tb_x Dy_{1-x} Fe_2$ for $\theta < \theta_c$ is cubic (because of magnetostriction!), the free energy will be invariant under one of the cubic Laue groups.

At this point it is simplest to combine the free energy $\hat{\varphi}$ with the local contributions to the field energy, *i.e.*, the last two terms of (3.5). To this end, we define the *anisotropy energy* by

$$\varphi(\mathbf{F}, \mathbf{m}, \theta) := \hat{\varphi}(\mathbf{F}, \mathbf{m}, \theta) + (\frac{1}{2}\mathbf{m} \cdot \mathbf{S}(\mathbf{F})\mathbf{m} + \frac{1}{6}|\mathbf{m}|^2) \det \mathbf{F}. \tag{3.18}$$

Here, $\mathbf{S}(\mathbf{F}) := \hat{\mathbf{S}}(\mathbf{Fe}_i^o)$ and the anisotropy energy φ retains the properties (3.14) and (3.17) of $\hat{\varphi}$ (to see this, it is necessary to look at the particular form of $\mathbf{S}(\mathbf{F})$, *cf.* James and Müller [1992]).

Since we observe discontinuities of strain and magnetization in magnetostrictive materials, it is natural to expect that φ has potential wells so that, roughly speaking, the observed discontinuities represent jumps between potential wells. The simplest assumption of this type seems to work well. We assume that there are functions $\mathbf{U}_1 : \mathbf{I} \to \mathbf{M}^{3\times3}$, $\mathbf{m}_1 : \mathbf{I} \to \mathbf{R}^3$, $\mathbf{I}$ being a suitable temperature interval, such that $(\mathbf{U}_1(\theta), \mathbf{m}_1(\theta), \theta) \in \mathcal{M}$ and

$$\varphi(\mathbf{U}_1(\theta), \mathbf{m}_1(\theta), \theta) \leq \varphi(\mathbf{F}, \mathbf{m}, \theta) \quad \forall \, (\mathbf{F}, \mathbf{m}, \theta) \in \mathcal{M}. \tag{3.19}$$

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The pair $(\mathbf{U}_1(\theta), \mathbf{m}_1(\theta))$ represents a pair of easy stretch and corresponding magnetization of the material at the temperature θ. Typically, we will have $\mathbf{U}_1(\theta_c) = \mathbf{1}$ and $\mathbf{m}_1(\theta_c) = 0$, θ_c being the Curie temperature. Without loss of generality (by (3.14) and the polar decomposition theorem) we can take $\mathbf{U}_1$ to be symmetric and positive-definite.

The conditions of frame-indifference (3.14) and material symmetry (3.17) imply immediately that φ necessarily has other minimizers besides $(\mathbf{U}_1, \mathbf{m}_1)$. According to (3.14) and (3.17), the full set of minimizers of φ is given by all pairs of the form $(\mathbf{R}\mathbf{U}_1\mathbf{Q}, \mathbf{R}\mathbf{m}_1)$ where $\mathbf{R} \in SO(3)$ and $\mathbf{Q} \in P^o$. To describe these potential wells, we use the notation

$$SO(3)(\mathbf{A}, \mathbf{m}) := \{(\mathbf{R}\mathbf{A}, \mathbf{R}\mathbf{m}) : \mathbf{R} \in SO(3)\}. \tag{3.20}$$

Note that in this definition both $\mathbf{A}$ and $\mathbf{m}$ are premultiplied by the same rotation. Again using the polar decomposition theorem, it is easy to see that the potential wells (the minimizers of φ) given by (3.14) and (3.17) are

$$SO(3)(\mathbf{U}_1, \mathbf{m}_1),$$

$$SO(3)(\mathbf{U}_2, \mathbf{m}_2),$$

$$\vdots \tag{3.21}$$

$$SO(3)(\mathbf{U}_n, \mathbf{m}_n),$$

where

$$\{(\mathbf{U}_1, \mathbf{m}_1), \ldots, (\mathbf{U}_n, \mathbf{m}_n)\} = \{(\mathbf{Q}\mathbf{U}_1\mathbf{Q}^T, \mathbf{Q}\mathbf{m}_1), \mathbf{Q} \in P^o\} \tag{3.22}$$

By analogy to the theory of martensitic transformations, we call each orbit of the form $SO(3)(\mathbf{U}_1, \mathbf{m}_1)$ a *variant*. By (3.22) the number of variants n is less than or equal to the order of the Laue group P^o, because there can be duplication (In $Tb_xDy_{1-x}Fe_2$ there will be 8 variants, but the order of P^o will be 24). In (3.21) and (3.22) we have suppressed the temperature dependence.

For all the calculations of this paper it will only be necessary to know where the potential wells lie, assuming the φ is otherwise a continuous function on $\mathcal{M}$. The variants

(3.20) represent all minimizers of φ delivered by frame-indifference and symmetry. We assume that (3.20) represents *all* minimizers of φ. That is, if we denote

$$\mathbf{M}(\theta) := SO(3)(\mathbf{U}_1(\theta),\ \mathbf{m}_1(\theta))\ \cup \ldots\ \cup\ SO(3)(\mathbf{U}_n(\theta),\ \mathbf{m}_n(\theta)), \qquad (3.23)$$

then

$$\varphi(\mathbf{F},\ \mathbf{m},\ \theta) = \varphi(\mathbf{U}_1(\theta),\ \mathbf{m}_1(\theta),\ \theta)$$

$$\Updownarrow \qquad\qquad\qquad\qquad (3.24)$$

$$(\mathbf{F},\ \mathbf{m},\ \theta)\ \in\ \mathbf{M}(\theta).$$

It is easy to see that, regardless of the choice $(\mathbf{U}_1,\ \mathbf{m}_1)$, it is possible to assign a smooth function φ with these potential wells.

Finally we discuss conditions of magnetic saturation. The idea used by Brown [1966] is that at constant temperature the magnetic moment *of each atom* has a fixed magnitude, regardless of the deformation. To formulate this constraint, let U_o be a unit cell of the reference lattice $L(\mathbf{e}_i^o)$ so that $U = \mathbf{F}U_o$ is a unit cell for the lattice $L(\mathbf{e}_i)$ where $\mathbf{e}_i = \mathbf{F}\mathbf{e}_i^o$, $i = 1, 2, 3$. Then, the condition that the magnitude of the magnetic moment of each atom is a function of temperature is

$$\lim_{\gamma \to 0}\ \left|\frac{\mathbf{d}_\gamma(\mathbf{y})}{\gamma^3 \mathrm{vol}\ U_o}\right| = g(\theta), \qquad \theta \in \mathbb{I}. \qquad (3.25)$$

Combining (3.25) with (3.2) we get the constraint

$$|(\det \mathbf{F})\mathbf{m}(\mathbf{y})| = g(\theta), \qquad \mathbf{y} \in \mathbf{R}^3. \qquad (3.26)$$

Now using the Cauchy-Born rule in the same way as in (3.11)-(3.12), we get the continuum version of (3.26),

$$|(\det \nabla \mathbf{y}(\mathbf{x}))\mathbf{m}(\mathbf{y}(\mathbf{x}))| = g(\theta), \qquad \mathbf{x} \in \Omega, \qquad \theta \in \mathbb{I}. \qquad (3.27)$$

The constraint (3.27) restricts deformations and magnetizations. It is naturally imposed as part of the definition (3.13) of $\mathcal{M}$.

For materials with large magnetostriction like $Tb_xDy_{1-x}Fe_2$ we are less inclined to believe the reasoning leading to the constraint (3.27). Note also that with our treatment a constraint of the form (3.27) is automatically satisfied on the potential wells:

$$(\mathbf{F}, \mathbf{m}) \in \mathbf{M}(\theta) \quad \Rightarrow \quad |(\det \mathbf{F})\mathbf{m}| = |(\det \mathbf{U}_1(\theta))\mathbf{m}_1(\theta)|, \qquad (3.28)$$

(Hence, to check the constraint experimentally, we expect it would be necessary for example to apply sufficiently large fields on non-easy axes.) Because of the fact that in the applications studied in this paper we only essentially use deformations from the potential wells, the constraint (3.27) is irrelevant anyway. An alternative to this constraint that is perhaps more physically realistic is to impose conditions of rapid growth of φ for deformations and magnetizations that depart from (3.27).

4. The energy of a magnetoelastic configuration

We now summarize and simplify the theory as developed above. We have obtained an anisotropy energy $\varphi(\mathbf{F}, \mathbf{m}, \theta)$ defined on a domain $\mathcal{M}$. A natural choice of $\mathcal{M}$, which includes Brown's condition of saturation, is

$$\mathcal{M} = \{(\mathbf{F}, \mathbf{m}, \theta) : \mathbf{Fe}_i^o \in N_o, \ |(\det \mathbf{F})\mathbf{m}| = g(\theta), \quad \det \mathbf{F} > 0\} . \qquad (4.1)$$

Here, N_o is the Ericksen-Pitteri neighborhood based on the fixed reference lattice vectors $\{\mathbf{e}_i^o\}$, these being interpreted as the lattice vectors for the undistorted crystal at the Curie temperature θ_c. The function g is given with $g(\theta) = 0$ for $\theta \geq \theta_c$. The reference configuration $\Omega \subset \mathbf{R}^3$ is interpreted as the region occupied by the crystal at $\theta = \theta_c$. Deformations of the crystal, including deformations arising from either applied forces or intrinsic magnetostriction, are described by functions $\mathbf{y} : \Omega \rightarrow \mathbf{R}^3$, $\mathbf{m} : \mathbf{R}^3 \rightarrow \mathbf{R}^3$ with $\mathbf{m}(\mathbf{z}) = \mathbf{0}$ for $\mathbf{z} \in \mathbf{R}^3 \backslash \mathbf{y}(\Omega)$. (For the present we omit detailed smoothness assumptions and proceed formally.)

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Combining (3.5), (3.6), (3.12) and (3.18), we arrive at the total energy of a magnetoelastic configuration:

$$E_\theta(\mathbf{y}, \; \mathbf{m}) := \int_\Omega \left\{ \varphi(\nabla\mathbf{y}(\mathbf{x}), \mathbf{m}(\mathbf{y}(\mathbf{x})), \theta) + \frac{1}{2}\mathbf{m}(\mathbf{y}(\mathbf{x})) \cdot \nabla u(\mathbf{y}(\mathbf{x}))(\det \nabla\mathbf{y}(\mathbf{x})) \right\} \; d\mathbf{x}. \quad (4.2)$$

Here $\mathbf{u}$ is determined from $\mathbf{m}$ by the magnetostatic equation

$$\text{div } (-\nabla u + \mathbf{m}) = 0 \quad \text{on} \quad \mathbf{R}^3. \quad (4.3)$$

Stable magnetoelastic configurations are found by minimizing E_θ in a suitable class of pairs of functions $(\mathbf{y}, \mathbf{m})$ and with $\theta = \text{const.}$

The existence theorem for the Ericksen-Pitteri neighborhood shows that a bounded neighborhood can always be chosen which also satisfies

$$\mathbf{Fe}_i^o \in N_o \quad \Rightarrow \quad \det \mathbf{F} > c > 0. \quad (4.4)$$

We shall make this choice. With this assumption any (weakly differentiable) deformation in $\mathcal{M}$ is in $W^{1,\infty}(\Omega, \; \mathbf{R}^3)$. We make the natural additional assumption that $\mathbf{y}$ is $1 - 1$. For technical reasons we assume Ω is bounded and open with a Lipschitz boundary. With these assumptions $\mathbf{y}(\Omega)$ will be bounded, open and have a Lipschitz boundary, which allows us to do various manipulations on the magnetostatic equation (4.3). The natural setting for the magnetostatic equation is $u \in H^1(\mathbf{R}^3)$ and $\mathbf{m} \in L^2(\mathbf{R}^3, \; \mathbf{R}^3)$, with supp $\mathbf{m} \subset \mathbf{y}(\Omega)$ (James and Kinderlehrer [1990]; see also Prop 5.1 below). Putting these assumptions together, we shall minimize E_θ over the space

$$\mathcal{A}_\theta : \{ (\mathbf{y}, \; \mathbf{m}) \in W^{1,\infty}(\Omega, \; \mathbf{R}^3) \times L^2(\mathbf{R}^3, \; \mathbf{R}^3) : \mathbf{y} \text{ is } 1 - 1,$$
$$\text{supp } \mathbf{m} \subset \mathbf{y}(\Omega), \quad (\nabla\mathbf{y}(\mathbf{x}), \; \mathbf{m}(\mathbf{x}), \; \theta) \in \mathcal{M} \text{ on } \Omega \}. \quad (4.5)$$

Assuming $(\mathbf{y}, \mathbf{m}) \in \mathcal{A}_\theta$ we shall interpret the magnetostatic equation (4.3) in the weak sense

$$u \in H^1(\mathbf{R}^3) : \int_{\mathbf{R}^3} (-\nabla u + \mathbf{m}) \cdot \nabla\zeta \, d\mathbf{z} = 0 \quad \forall \zeta \in H^1(\mathbf{R}^3, \mathbf{R}). \quad (4.6)$$

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By James and Kinderlehrer [1990] or Rogers [1991], there exists a unique solution $u \in H^1(\mathbf{R}^3)$ of (4.6), whose properties are described in these references. We can take $\zeta = u$ in (4.6) and then substitute for the second term in (4.2), after having used the change of variables formula. This gives the alternative form for the energy

$$E_\theta(\mathbf{y}, \mathbf{m}) = \int_\Omega \varphi(\nabla \mathbf{y}(\mathbf{x}), \mathbf{m}(\mathbf{y}(\mathbf{x})), \theta) d\mathbf{x} + \frac{1}{2} \int_{\mathbf{R}^3} |\nabla u(\mathbf{z})|^2 d\mathbf{z} \qquad (4.7)$$

The formulae (4.2) and (4.6) can be recast entirely in a referential setting, as in James and Kinderlehrer [1991].

Finally, we summarize the important properties of φ. By assumption φ is frame-indifferent

$$\varphi(\mathbf{RF}, \mathbf{Rm}, \theta) = \varphi(\mathbf{F}, \mathbf{m}, \theta) \quad \forall \, (\mathbf{F}, \mathbf{m}, \theta) \in \mathcal{M}, \quad \forall \, \mathbf{R} \in SO(3), \qquad (4.8)$$

and satisfies the condition of material symmetry

$$\varphi(\mathbf{FQ}, \mathbf{m}, \theta) = \varphi(\mathbf{F}, \mathbf{m}, \theta) \quad \forall \, (\mathbf{F}, \mathbf{m}, \theta) \in \mathcal{M}, \quad \forall \, \mathbf{Q} \in P^o, \qquad (4.9)$$

see (3.16). It also has potential wells summarized by

$$\varphi(\mathbf{F}, \mathbf{m}, \theta) \leq \varphi(\mathbf{G}, \mathbf{p}, \theta) \quad \forall \, (\mathbf{G}, \mathbf{p}, \theta) \in \mathcal{M} \quad \forall \, (\mathbf{F}, \mathbf{m}, \theta) \in \mathsf{M}(\theta), \qquad (4.10)$$

where $\mathsf{M}(\theta)$ represents the potential-well minimizers of φ,

$$\mathsf{M}(\theta) = SO(3)(\mathbf{U}_1(\theta), \mathbf{m}_1(\theta)) \cup \ldots \cup SO(3)(\mathbf{U}_n(\theta), \mathbf{m}_n(\theta)). \qquad (4.11)$$

By the assumption (3.27) all minimizers of φ are given by (4.11).

5. Minimizing sequences

As mentioned in the introduction, the problem

$$\inf_{\substack{(\mathbf{y}.\mathbf{m}) \in \mathcal{A}_\theta \\ \mathbf{y} = \mathbf{y}_o \text{ on } (\partial\Omega)_1}} E_\theta(\mathbf{y}, \mathbf{m}), \qquad (5.1)$$

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where $\mathbf{y}_o$ is some assigned function on $(\partial\Omega)_1 \subset \partial\Omega$ is not generally attained. Whether we have attainment or nonattainment depends sensitively on $\mathbf{y}_o$, the constraints embodied in $\mathcal{A}_\theta$ and the detailed structure of φ, especially the location of its potential wells. At present, very little is known of the precise conditions for attainment/nonattainment for the problem (5.1). In this situation our point of view will be to study the minimizing sequences for (5.1), i.e., sequences of pairs $(\mathbf{y}^{(k)}, \mathbf{m}^{(k)}) \in \mathcal{A}_\theta$, $k = 1, 2, 3, \ldots$ with the property

$$E_\theta(\mathbf{y}^{(k)}, \mathbf{m}^{(k)}) \rightarrow \inf_{\ldots} E_\theta \tag{5.2}$$

We argue that for large specimens a great many features of observed microstructures as well as reliable predictions of new structures can be made on this basis.

Since we are holding the temperature fixed throughout, we shall without loss of generality add a suitable constant to φ such that

$$\varphi(\mathbf{U}_1, \mathbf{m}_1, \theta) = 0. \tag{5.3}$$

Below we find minimizing sequences that reduce the total energy E_θ to zero. In various places we suppress the temperature dependence.

In preparation for the construction of these sequences, we record the jump conditions for a surface of discontinuity of $(\nabla\mathbf{y}, \mathbf{m})$. Letting $(\mathbf{F}^+, \mathbf{m}^+)$, $(\mathbf{F}^-, \mathbf{m}^-) \in \mathcal{M}$ denote the limiting values of $(\nabla\mathbf{y}, \mathbf{m})$ at a simple surface of discontinuity, we have

$$\mathbf{F}^+ - \mathbf{F}^- = \mathbf{a} \otimes \mathbf{n}, \quad (\mathbf{m}^+ - \mathbf{m}^-) \cdot \mathbf{n}' = 0, \quad \mathbf{n}' = \frac{(\mathbf{F}^\pm)^{-T}\mathbf{n}}{|(\mathbf{F}^\pm)^{-T}\mathbf{n}|} \tag{5.4}$$

for some $\mathbf{a} \in \mathbf{R}^3$, $\mathbf{n} \in \mathbf{R}^3$, $|\mathbf{n}| = 1$. Equation $(5.4)_1$ expresses the fact that $\mathbf{F}^\pm$ are limiting values of a gradient, and $(5.4)_2$ is the jump condition arising from (5.3) with $\nabla u = 0$, the case of interest with no applied field. The relation $(5.4)_3$ is the standard relation of continuum mechanics relating reference $\mathbf{n}$ and deformed $\mathbf{n}'$ normals.

Recalling that $\mathbf{M}(\theta)$ represents the potential well minima of φ, we note that a common situation is to have

$$(\mathbf{F}, \mathbf{m}) \text{ and } (\mathbf{F}, -\mathbf{m}) \in \mathbf{M}(\theta). \tag{5.5}$$

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In this situation the infimum of E_θ is zero as shown below by a slight variant of our earlier argument (James and Kinderlehrer [1990, Section 3]).

Proposition 5.1. *Let* $(\mathbf{F}, \mathbf{m})$ *and* $(\mathbf{F}, -\mathbf{m})$ *belong to* $\mathsf{M}(\theta)$. *Then*,

$$\inf_{(\mathbf{y}, \mathbf{m}) \in \mathcal{A}_\theta} E_\theta(\mathbf{y}, \mathbf{m}) = 0. \tag{5.6}$$

Proof. Let $\mathbf{y} = \mathbf{F}\mathbf{x}$, $\mathbf{x} \in \Omega$, and let $\xi : \mathbf{R} \to \mathbf{R}$ be periodic of period 1 satisfying

$$\xi(\tau) = \begin{cases} 1, & \tau \in \left[0, \frac{1}{2}\right), \\ -1, & \tau \in \left[\frac{1}{2}, 1\right). \end{cases} \tag{5.7}$$

Choose $\mathbf{p} \in \mathbf{R}^3$ with $\mathbf{p} \cdot \mathbf{m} = 0$, $|\mathbf{p}| = 1$, and let

$$\mathbf{m}^{(k)}(\mathbf{z}) = \begin{cases} \mathbf{m}\, \xi(k\mathbf{p} \cdot \mathbf{z}), & \mathbf{z} \in \mathbf{F}\Omega, \\ 0, & \mathbf{z} \in \mathbf{R}^3 \setminus \mathbf{F}\Omega, \quad k = 1, 2, 3, \ldots \end{cases} \tag{5.8}$$

Since $\mathbf{p} \cdot \mathbf{m} = 0$ then div $\mathbf{m}^{(k)} = 0$ in $\mathbf{F}\Omega$ and in $\mathbf{R}^3 \setminus \mathbf{F}\Omega$, and also the choice of half-and-half domains shows that

$$\mathbf{m}^{(k)} \rightharpoonup 0 \quad \text{in } L^2(\mathbf{R}^3, \mathbf{R}^3). \tag{5.9}$$

We compute the expression

$$E_\theta(\mathbf{y}, \mathbf{m}^{(k)}) = \int_\Omega \varphi(\nabla \mathbf{y}, \mathbf{m}^{(k)})\, d\mathbf{x} + \frac{1}{2} \int_{\mathbf{R}^3} |\nabla u^{(k)}(\mathbf{z})|^2 d\mathbf{z}, \tag{5.10}$$

$$\text{div}(-\nabla u^{(k)} + \mathbf{m}^{(k)}) = 0.$$

By our choice of $\mathbf{y}$ and $\mathbf{m}^{(k)}$, $\varphi(\nabla \mathbf{y}, \mathbf{m}^{(k)}) = 0$. We turn our attention to the field energy. First we recognize that the distribution $T^{(k)} = \text{div } \mathbf{m}^{(k)}$, given by

$$< T^{(k)}, \zeta > = \int_{\mathbf{R}^3} \nabla \zeta \cdot \mathbf{m}^{(k)} d\mathbf{z} \tag{5.11}$$

is a continuous linear functional on $H^1(\mathbf{R}^3)$, that is, $T^{(k)} \in H^{-1}(\mathbf{R}^3)$ with, in fact,

$$\|T^{(k)}\|_{H^{-1}} = \sup_{\|\nabla \zeta\| \leq 1} \int_{\mathbf{R}^3} \nabla \zeta \cdot \mathbf{m}^{(k)}\, d\mathbf{z} = \sup_{\|\nabla \zeta\| \leq 1} \int \nabla u^{(k)} \cdot \nabla \zeta d\mathbf{z} = \|\nabla u^{(k)}\|_{L^2} \tag{5.12}$$

To show that $\|T^{(k)}\| \to 0$ in the H^{-1} norm, we observe that $\mathbf{m}^{(k)} = \chi_D \mathbf{f}^{(k)}$, where $D = \mathbf{F}\Omega$ is bounded, and

$$\mathbf{f}^{(k)} \rightharpoonup 0 \quad \text{in} \quad L^2(\mathbf{R}^3; \mathbf{R}^3),$$

$$\text{div } \mathbf{f}^{(k)} = 0 \quad \text{in} \quad H^{-1}_{loc}(\mathbf{R}^3). \tag{5.13}$$

This is sufficient to prove that $\|T^{(k)}\| \to 0$ by combining the compactness of the injection from L^2 to H^{-1} with an approximation argument.

Hence,

$$E_\theta(\mathbf{y}, \mathbf{m}^{(k)}) \to 0 \quad \text{as } k \to \infty. \tag{5.14} \square$$

For our analysis of domain structures of $Tb_x Dy_{1-x} Fe_2$ below we shall need sequences that have greater flexibility with regard to elastic deformations than those given by Proposition 5.1. The situation encountered in $Tb_x Dy_{1-x} Fe_2$ is that (5.5) is satisfied by certain pairs $(\mathbf{F}^+, \mathbf{m}^+)$ and $(\mathbf{F}^-, \mathbf{m}^-)$, and the pairs also have the property that $\mathbf{F}^+$ and $\mathbf{F}^-$ are compatible.

Theorem 5.2. *Let* $(\mathbf{F}^+, \pm\mathbf{m}^+)$, $(\mathbf{F}^-, \pm\mathbf{m}^-), \in \mathsf{M}(\theta)$ *have the property that for some nonzero vectors* $\mathbf{a}, \mathbf{n} \in \mathbf{R}^3$,

$$\mathbf{F}^+ - \mathbf{F}^- = \mathbf{a} \otimes \mathbf{n}. \tag{5.15}$$

Suppose N_o *contains the line* $\{\mathbf{F}e_i : \mathbf{F} = \delta\mathbf{F}^+ + (1-\delta)\mathbf{F}^-, \ \delta \in [0,1]\}$. *Let*

$$\mathbf{F}_\gamma := \gamma\mathbf{F}^+ + (1-\gamma)\mathbf{F}^-, \quad \gamma \in [0,1]. \tag{5.16}$$

Then

$$\inf_{\substack{\mathbf{y}, \mathbf{m} \in \mathcal{A}_\theta \\ \mathbf{y} = \mathbf{F}_\gamma \mathbf{x} \text{ on } \partial\Omega}} E_\theta(\mathbf{y}, \mathbf{m}) = 0. \tag{5.17}$$

Remark 5.3. To prove this we construct deformations with alternating gradients $\mathbf{F}^+, \mathbf{F}^-$, $\mathbf{F}^+$, $\mathbf{F}^-, \ldots$ on layers of width $\gamma, (1-\gamma), \gamma, (1-\gamma), \ldots$ On each of these layers, we superimpose a domain structure consisting of layers with magnetization $\pm\mathbf{m}^+$ or $\pm\mathbf{m}^-$ at a finer scale. See Figure 1.

Proof. As the case $\gamma = 0, 1$ is covered by Prop. 5.1, let $\gamma \in (0, 1)$. Let $\zeta : \mathbf{R} \rightarrow [0, \gamma(1-\gamma)]$ be the continuous periodic function of period 1 given by

$$\zeta(\tau) = \begin{cases} (1 - \gamma)(\tau + \gamma) & \text{for } -\gamma \leq \tau < 0, \\ -\gamma(\tau - 1 + \gamma) & \text{for } 0 \leq \tau < 1 - \gamma. \end{cases} \tag{5.18}$$

Let

$$\mathbf{y}^{(k)}(\mathbf{x}) := \mathbf{F}_\gamma \mathbf{x} + k^{-1}\zeta(k\mathbf{x} \cdot \mathbf{n})\mathbf{a}, \quad \mathbf{x} \in \Omega. \tag{5.19}$$

Then $\mathbf{y}^{(k)} \in W^{1,\infty}$ and $\nabla\mathbf{y}^{(k)}$ takes the two values $\mathbf{F}^+$ and $\mathbf{F}^-$ on alternating layers. The sequence $\mathbf{y}^{(k)}$ has the property

$$\mathbf{y}^{(k)} \overset{*}{\rightharpoonup} \mathbf{y} \quad \text{in } W^{1,\infty}(\Omega, \mathbf{R}^3), \tag{5.20}$$

where

$$\mathbf{y}(\mathbf{x}) = \mathbf{F}_\gamma \mathbf{x}, \quad \mathbf{x} \in \Omega, \tag{5.21}$$

but it does not quite satisfy the boundary conditions $\mathbf{y}(\mathbf{x}) = \mathbf{F}_\gamma \mathbf{x}$. We therefore alter $\mathbf{y}^{(k)}$ near $\partial\Omega$ using a construction of Chipot and Kinderlehrer [1988, Section 2]. For $\varepsilon > 0$ sufficiently small, let

$$\Omega_\varepsilon = \{\mathbf{x} \in \Omega : \text{dist}(\mathbf{x}, \partial\Omega) > \varepsilon\} \tag{5.22}$$

and let $\xi_\varepsilon \in C^1(\mathbf{R}^3, [0, 1])$ satisfy for each $\varepsilon > 0$

$$\xi_\varepsilon(\mathbf{x}) = \begin{cases} 1 & \text{for } \mathbf{x} \in \Omega_\varepsilon, \\ 0 & \text{for } \mathbf{x} \in \mathbf{R}^3 - \Omega, \end{cases} \tag{5.23}$$

and

$$|\nabla\xi_\varepsilon(\mathbf{x})| < \text{const. } \varepsilon^{-1}, \quad \mathbf{x} \in \mathbf{R}^3. \tag{5.24}$$

Now let

$$\mathbf{y}^{(k,\varepsilon)}(\mathbf{x}) := \xi_\varepsilon(\mathbf{x})\mathbf{y}^{(k)}(\mathbf{x}) + (1 - \xi_\varepsilon(\mathbf{x}))\mathbf{F}_\gamma\mathbf{x}. \tag{5.26}$$

For each sufficiently small $\varepsilon > 0$ $\mathbf{y}^{(k,\varepsilon)}(\mathbf{x}) = \mathbf{F}_\gamma\mathbf{x}$, $\mathbf{x} \in \partial\Omega$, and $\mathbf{y}^{(k,\varepsilon)}(\mathbf{x}) = \mathbf{y}^{(k)}(\mathbf{x}), \mathbf{x} \in \Omega_\varepsilon$. Also,

$$\nabla\mathbf{y}^{(k,\varepsilon)}(\mathbf{x}) = (\mathbf{y}^{(k)}(x) - \mathbf{F}_\gamma\mathbf{x}) \otimes \nabla\xi_\varepsilon + (\xi_\varepsilon\nabla\mathbf{y}^{(k)}(\mathbf{x}) + (1 - \xi_\varepsilon)\mathbf{F}_\gamma), \quad \mathbf{x} \in \Omega. \tag{5.27}$$
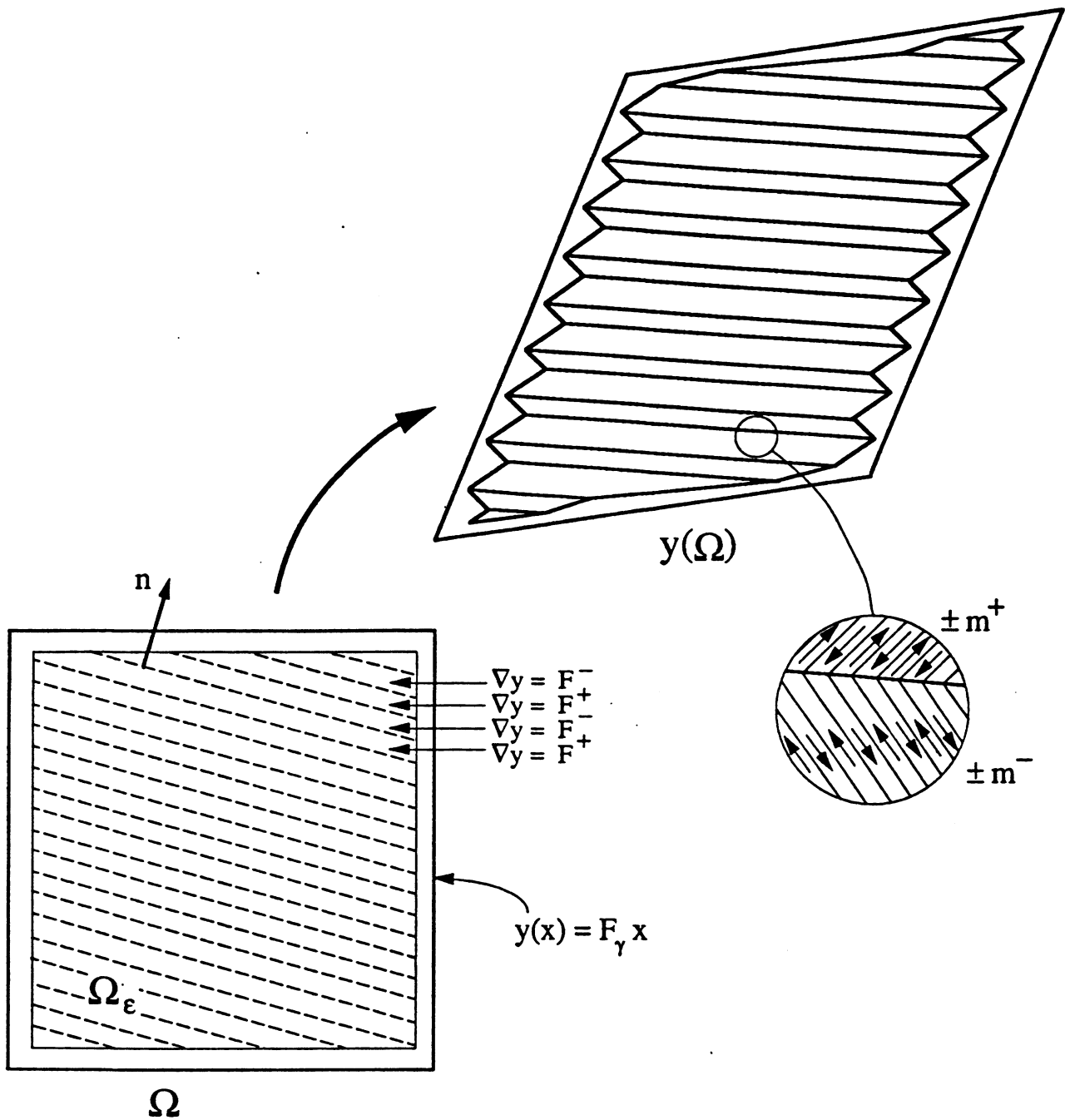
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Figure 1. Microstructure and domain structure used in the proof of Theorem 5.2. The domain structure in the boundary layer $\Omega - \Omega_\epsilon$ is not shown.

Since by (5.20) $y^{(k)}(x) \to F_\gamma x$ uniformly on Ω and since N^o is open and contains the line $\{\delta F^+ + (1-\delta)F^-, \delta \in [0,1]\}$, then we can choose k_ε so large that $\nabla y^{(k_\varepsilon,\varepsilon)}(x) \in N_o$ for a.e. $x \in \Omega$ and every sufficiently small $\varepsilon > 0$. It is easily checked that the sequence $y^\varepsilon := y^{(k_\varepsilon,\varepsilon)}$ is 1-1 and maps $\Omega \to F_\gamma \Omega$. Let $x^\varepsilon : F_\gamma \Omega \to \Omega$ be the inverse of y^ε.

Now we construct the magnetization. Let $p^+ \cdot m^+ = 0$, $p^- \cdot m^- = 0$, $p^\pm \in \mathbb{R}^3$, $|p^\pm| = 1$. Let ξ be defined as in (5.7). Recalling the definition (5.18) of ζ, we let

$$
m^{(j,\varepsilon)}(y) := \left\{ \left[\zeta'(k_\varepsilon x^\varepsilon(y) \cdot n) - (1-\gamma) \right] \xi(jp^- \cdot y)m^- \right.
$$
$$
\left. + \left[\zeta'(k_\varepsilon x^\varepsilon(y) \cdot n) + \gamma \right] \xi(jp^+ \cdot y)m^+ \right\} \frac{\det F^\pm}{\det \nabla y^\varepsilon(x^\varepsilon(y))}, \quad y \in F_\gamma \Omega,
\tag{5.28}
$$

and we put $m^{(j,\varepsilon)}(y) = 0$ for $y \in \mathbb{R}^3 \backslash F_\gamma \Omega$. Since ζ' takes only the values $(1-\gamma)$ and $-\gamma$, ξ takes only the values ± 1, and $\det F^+ = \det F^-$ by the definition of $M(\theta)$, we have

$$
|\det \nabla y^\varepsilon(x) m^{(j,\varepsilon)}(y^\varepsilon(x))| = g(\theta), \quad x \in \Omega.
\tag{5.29}
$$

Therefore, for every sufficiently small $\varepsilon > 0$ and every $j = 1, 2, \ldots,$

$$
(y^\varepsilon, m^{(j,\varepsilon)}) \in \mathcal{A}_\theta.
\tag{5.30}
$$

The simple structure of $y^\varepsilon(x)$ on Ω_ε allows us to conclude that

$$
x \in \Omega_\varepsilon^+ := \{x \in \Omega_\varepsilon : \nabla y^\varepsilon(x) = F^+\} \Rightarrow m^{j,\varepsilon}(y^\varepsilon(x)) \in \{\pm m^+\},
$$
$$
x \in \Omega_\varepsilon^- := \{x \in \Omega_\varepsilon : \nabla y^\varepsilon(x) = F^-\} \Rightarrow m^{j,\varepsilon}(y^\varepsilon(x)) \in \{\pm m^-\}.
\tag{5.31}
$$

Since $\Omega_\varepsilon^+ \cup \Omega_\varepsilon^- = \Omega_\varepsilon$ and $F^+ \neq F^-$, we have that

$$
\varphi(\nabla y^\varepsilon(x), m^{j,\varepsilon}(y^\varepsilon(x)), \theta) = 0, \quad x \in \Omega_\varepsilon.
\tag{5.32}
$$

Hence, using the boundedness of φ on $\mathcal{M}$ and (5.32), we have

$$
\int_\Omega \varphi(\nabla y^\varepsilon(x), m^{j,\varepsilon}(y^\varepsilon(x)), \theta) \, dx \to 0 \text{ as } \varepsilon \to 0,
\tag{5.33}
$$

uniformly in j.

It remains to examine the field energy. Fixing ε momentarily, we note that $\mathbf{m}^{(j,\varepsilon)}$ is the sum of three fields

$$\mathbf{m}^{(j,\varepsilon)}(\mathbf{y}) = \mathbf{m}_+^{(j,\varepsilon)}(\mathbf{y}) + \mathbf{m}_-^{(j,\varepsilon)}(\mathbf{y}) + \mathbf{m}_r^{(j,\varepsilon)}(\mathbf{y}), \ \mathbf{y} \in \mathbf{R}^3, \tag{5.34}$$

where

$$\begin{aligned}
\mathbf{m}_+^{(j,\varepsilon)}(\mathbf{y}) &= \ \xi(j\mathbf{p}^+ \cdot \mathbf{y})\mathbf{m}^+ \chi_{\mathbf{y}^\varepsilon(\Omega_\varepsilon^+)}(\mathbf{y}), \\
\mathbf{m}_-^{(j,\varepsilon)}(\mathbf{y}) &= \ \xi(j\mathbf{p}^- \cdot \mathbf{y})\mathbf{m}^- \chi_{\mathbf{y}^\varepsilon(\Omega_\varepsilon^-)}(\mathbf{y}),
\end{aligned} \tag{5.35}$$

and

$$\mathbf{m}_r^{(j,\varepsilon)}(\mathbf{y}) = \ 0 \quad \text{for } \mathbf{x} \in \mathbf{y}^\varepsilon(\Omega_\varepsilon) \cup (\mathbf{R}^3 \backslash \mathbf{F}_\gamma \Omega). \tag{5.36}$$

We apply Proposition 5.1 to each of the fields in (5.35) (see (5.8)-(5.11)) and see that the corresponding potentials satisfy

$$u_+^{(j,\varepsilon)} + u_-^{(j,\varepsilon)} \to 0 \text{ in } L^2(\partial\Omega_\varepsilon^\pm) \text{ as } j \to \infty, \tag{5.37}$$

for each fixed $\varepsilon > 0$. On the other hand, $\mathbf{m}_r^{j,\varepsilon} \to 0$ in $L^2(\mathbf{R}^3, \mathbf{R}^3)$ as $\varepsilon \to 0$, uniformly in j, implying that the corresponding potential satisfies $u_r^{(j,\varepsilon)} \to 0$ in $H^1(\mathbf{R}^3, \mathbf{R})$ as $\varepsilon \to 0$, uniformly in j. Putting these facts together and letting $u^{(j,\varepsilon)}$ be the potential corresponding to $\mathbf{m}^{(j,\varepsilon)}$, we have for the field energy,

$$\begin{aligned}
&\frac{1}{2} \int_\Omega \mathbf{m}^{(j,\varepsilon)}(\mathbf{y}) \cdot \nabla u^{(j,\varepsilon)}(\mathbf{y}) \, d\mathbf{y} \\
&= \frac{1}{2} \int_{\mathbf{y}^\varepsilon(\Omega_\varepsilon)} (\mathbf{m}_+^{(j,\varepsilon)} + \mathbf{m}_-^{(j,\varepsilon)}) \cdot \nabla(u_+^{(j,\varepsilon)} + u_-^{(j,\varepsilon)}) \, d\mathbf{y} \\
&\quad + \frac{1}{2} \int_{\mathbf{y}^\varepsilon(\Omega_\varepsilon)} (\mathbf{m}_+^{(j,\varepsilon)} + \mathbf{m}_-^{(j,\varepsilon)}) \cdot \nabla u_r^{(j,\varepsilon)} \, d\mathbf{y} \\
&\quad + \frac{1}{2} \int_{\mathbf{F}_\gamma\Omega\backslash\mathbf{y}^\varepsilon(\Omega_\varepsilon)} \mathbf{m}_r^{(j,\varepsilon)}(\mathbf{y}) \cdot \nabla u^{(j,\varepsilon)}(\mathbf{y}) \, d\mathbf{y}.
\end{aligned} \tag{5.38}$$

Given ε we may choose j_ε sufficiently large such that the first term on the right hand side of (5.38) is less than ε, by the argument presented in (5.13)$_{2,3}$. The remaining terms tend

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to zero as $\varepsilon \to 0$ uniformly in j, and therefore tend to zero as $\varepsilon \to 0$ with $j = j_\varepsilon$. Therefore, $(\mathbf{y}^\varepsilon, \mathbf{m}^{(j_\varepsilon, \varepsilon)})$ is a minimizing sequence for the total energy. $\square$

Remark 5.4. There are a variety of alternatives to the construction given in Theorem 5.2. Particularly interesting are those constructions which do not require the oscillations of magnetization to be much finer than the oscillations of the deformation gradient. Such is the case when, in addition to the hypotheses of Theorem 5.2, the pairs satisfy (5.4). Then constructions as shown in Figure 2 serve as minimizing sequences.

Generalization 5.5. Theorem 5.2 can be generalized immediately to more complicated constructions involving layers within layers, layers within layers within layers, etc., as long as the appropriate compatibility conditions on the deformation gradient are satisfied. One such generalization follows by combining Theorem 5.2 with Theorem 6.1 of Ball and James [1991]: *Let* $SO(3)$ $(\mathbf{F}^+, \pm\mathbf{m}^+)$ *and* $SO(3)$ $(\mathbf{F}^-, \pm\mathbf{m}^-)$ *belong to* $\mathsf{M}(\theta)$ *and suppose that for some nonzero vectors* $\mathbf{a}, \mathbf{n} \in \mathbb{R}^3, |\mathbf{n}| = 1$,

$$\mathbf{F}^+ = (1 + \mathbf{a} \otimes \mathbf{n})\mathbf{F}^- \tag{5.39}$$

Suppose N_o contains the set

$$\{\mathbf{F}\mathbf{e}_i : \mathbf{F} = (\delta\mathbf{F}^+ + (1-\delta)\mathbf{F}^-) + \mu\mathbf{b} \otimes \mathbf{m}, \ \delta, \ \mu \in [0,1], \ \delta\mathbf{F}^+$$

$$+ (1-\delta)\mathbf{F}^- + \mathbf{b} \otimes \mathbf{m} \in SO(3)\mathbf{F}^+ \cup SO(3)\mathbf{F}^-\}.$$

Then

$$\inf_{\substack{\mathbf{y},\mathbf{m}\in\mathcal{A}_\theta,\mathbf{F}\in\Re \\ \mathbf{y}=\mathbf{F}_\neg\mathbf{x} \text{ on } \partial\Omega}} E_\theta(\mathbf{y},\mathbf{m}) = 0. \tag{5.40}$$

where

$$\Re := \Big\{ \mathbf{G} \in M^{3x3} : \mathbf{G}^T\mathbf{G}\mathbf{e} = (\mathbf{F}^-)^T\mathbf{F}^-\mathbf{e}, \ \mathbf{e} = (\mathbf{F}^-)^{-1}(\mathbf{a} \wedge \mathbf{n}), \ \det \mathbf{G}$$

$$= \det \mathbf{F}^\pm, \ |\mathbf{G}(\mathbf{F}^-)^{-1}(\mathbf{n} - \frac{1}{2}\mathbf{a})|^2 \leq 1 + \frac{1}{4}|\mathbf{a}|^2, \ |\mathbf{G}(\mathbf{F}^-)^{-1}\mathbf{a}|^2 \leq |\mathbf{a}|^2 \Big\} \tag{5.41}$$

In fact the set $\Re$ represents *all* macroscopically linear deformations that can be obtained by using energy minimizing microstructures involving just the four variants $SO(3)(\mathbf{F}^+, \pm\mathbf{m}^+)$,
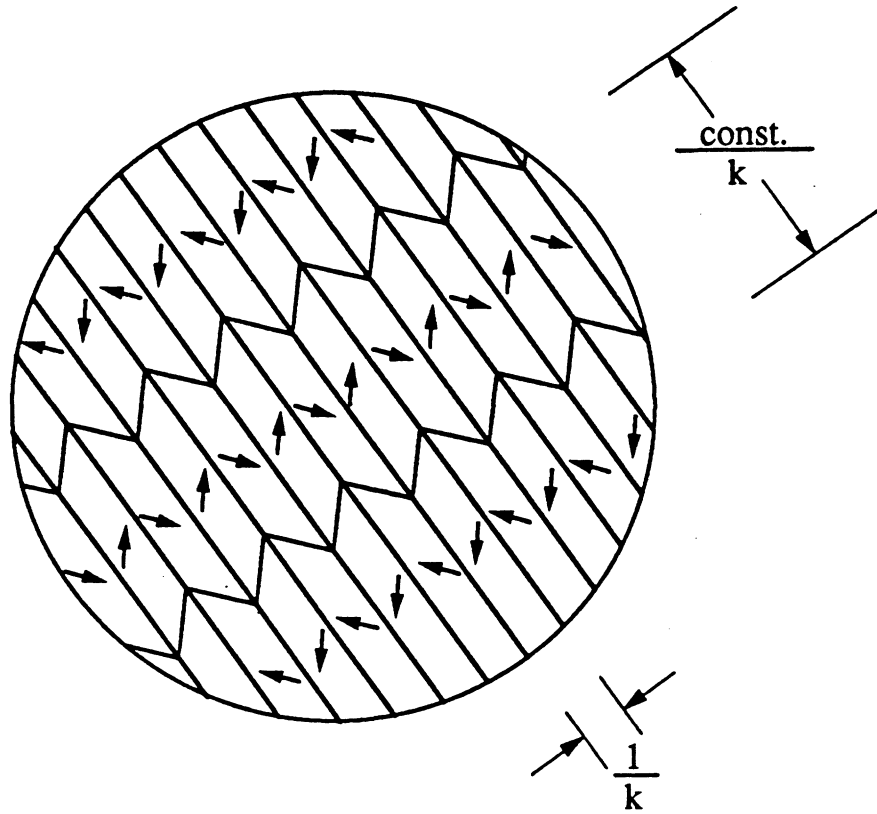
Figure 2. A minimizing sequence involving only one scale which is possible under the condition (5.4) and the hypotheses of Theorem 5.2.

$SO(3)(\mathbf{F}^-, \pm\mathbf{m}^-)$. Descriptively, the set $\Re$ represents the "easy deformations" of the material using four variants of the given type. Since all boundary conditions $\mathbf{y}(\mathbf{x}) = \mathbf{F}\mathbf{x}$, $\mathbf{x} \in \Omega$, $\mathbf{F} \in \Re$ have the same energy, it should be possible by applying slight forces to deform the specimen while staying in this set. Further remarks along these lines are given below in the context of the material $Tb_x Dy_{1-x} Fe_2$.

Remark 5.6 In our study of $Tb_x Dy_{1-x} Fe_2$ we shall need a result which is closely related to Theorem 5.2 but involves four deformation gradients. This will be used in a polycrystalline generalization of our theory and for this reason cannot be stated in the form of Theorem 5.2. *Suppose $0 \in \Omega$ and let $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ be four 3×3 matrices satisfying for some vectors $\mathbf{a}$, $\mathbf{n}$, $\mathbf{a}'$, $\mathbf{n}' \in \mathbb{R}^3$ the conditions*

$$\mathbf{B} - \mathbf{A} = \mathbf{a} \otimes \mathbf{n}, \quad \mathbf{D} - \mathbf{C} = \mathbf{a}' \otimes \mathbf{n}'. \tag{5.42}$$

Suppose also that there are scalars γ, $\delta \in [0, 1]$ and vectors $\mathbf{b}$, $\mathbf{m} \in \mathbb{R}^3$ such that

$$(\gamma \mathbf{B} + (1 - \gamma)\mathbf{A}) - (\delta \mathbf{D} + (1 - \delta)\mathbf{C}) = \mathbf{b} \otimes \mathbf{m}. \tag{5.43}$$

Then, there is a sequence $\mathbf{y}^{(k)} : \Omega \to \mathbb{R}^3$ ($\mathbf{y}^{(k)} \in W^{1,\infty}$) $k = 1, 2, 3, \ldots$, such that

$$\begin{aligned}
\nabla \mathbf{y}^{(k)}(\mathbf{x}) &\in \{\mathbf{A}, \ \mathbf{B}\} \quad \text{for } \mathbf{x} \cdot \mathbf{m} > \frac{1}{k}, \ \mathbf{x} \in \Omega, \\
\nabla \mathbf{y}^{(k)}(\mathbf{x}) &\in \{\mathbf{C}, \ \mathbf{D}\} \quad \text{for } \mathbf{x} \cdot \mathbf{m} < -\frac{1}{k}, \mathbf{x} \in \Omega,
\end{aligned} \tag{5.44}$$

and

$$|\nabla \mathbf{y}^{(k)}(\mathbf{x})| < \text{ const. on } \Omega, \tag{5.45}$$

where the constant is independent of k.

To construct this sequence, we simply apply the proof of Theorem 5.2 back-to-back. That is, we use Theorem 5.2 to construct a sequence on $\{\mathbf{x} \in \Omega : \mathbf{x} \cdot \mathbf{m} > 0\}$ which takes gradients $\mathbf{A}$ and $\mathbf{B}$ in the proportion $(1 - \gamma)/\gamma$. We then apply Theorem 5.2 again to the region $\{\mathbf{x} \in \Omega : \mathbf{x} \cdot \mathbf{m} < 0\}$ using the gradients $\mathbf{C}$ and $\mathbf{D}$ in the proportion $(1 - \delta)/\delta$. It

is then found that (5.43) implies that the boundary values of $\mathbf{y}^{(k)}$ on $\{\mathbf{x} \in \Omega : \mathbf{x} \cdot \mathbf{m} = 0\}$ given by the two constructions agree, completing the proof.

If **A**, **B**, **C**, **D** belong to the potential wells of an anisotropy energy (having a sufficiently large domain and invariance under $\mathbf{m} \to -\mathbf{m}$), then a suitable sequence $(\mathbf{y}^k, \mathbf{m}^k)$ with $\mathbf{m}^k$ as above can be constructed which would be a minimizing sequence for the total energy.

Remark 5.7 The Generalization 5.6 also has a converse, which roughly states that if we assume (5.42) and there is *some* sequence $\mathbf{y}^{(k)} \in W^{1,\infty}(\Omega, \mathbf{R}^3)$ satisfying $\nabla \mathbf{y}^{(k)} \in \{\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}\}$, except on regions whose volume tends to zero as $k \to \infty$, then (5.43) holds. This can be established by a variant of the arguments given by James and Kinderlehrer [1989]. This kind of result is best stated using the Young measure and is omitted from the present treatment.

6. Specialization to $Tb_x Dy_{1-x} Fe_2$

In this section we specialize the theory given above to the alloy $Tb_x Dy_{1-x} Fe_2 (x \doteq 0.3)$ and we compare the predicted microstructures with those observed by Lord [1990,1992].

a) *Structure of the potential wells*

According to (3.19)-(3.23), we will have specified the potential wells of the anisotropy energy φ once we give a pair $(\mathbf{U}_1, \mathbf{m}_1)$ and a Laue group P^o.

We begin by specifying P^o. $Tb_x Dy_{1-x} Fe_2$ (for values of x of interest and for $\theta \geq \theta_c$) is a cubic Laves phase of the type $MgCu_2$, the Mg sites being occupied by Tb or Dy. Work of Simha [1991] shows that this lattice structure can be described as the union of six interpenetrating FCC Bravais lattices. Fe atoms lie on four of the lattices, while Tb and Dy form a solid solution on the remaining two. We shall make the hypothesis that the lattice model of Section 2 refers to one of these FCC lattices, and displacements among the other FCC lattices are free to adjust themselves to secure equilibrium. See Zanzotto
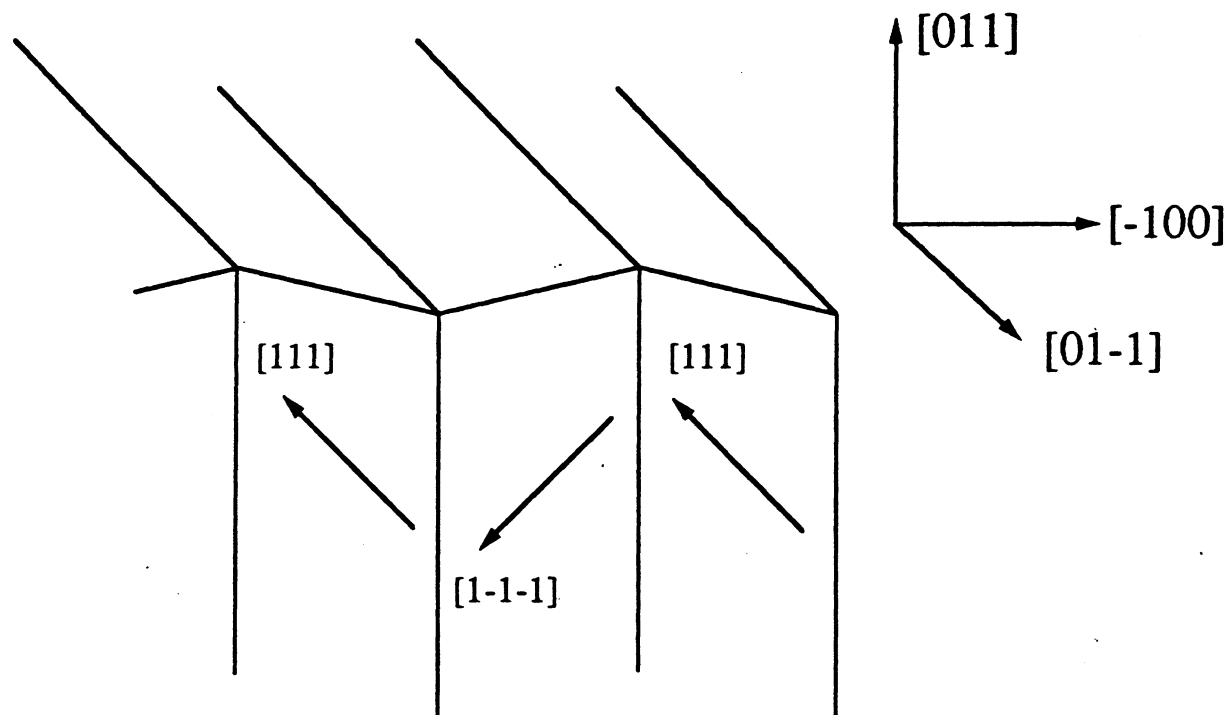
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Figure 3. Lord's interpretation [1990,1992] of magnetostriction in $Tb_xDy_{1-x}Fe_2$.

[1992] for a discussion of the validity of this kind of hypothesis. This gives $P^o = (432)$, the cubic Laue group of order 24, which also agrees with the macroscopic Laue group symmetry of $Tb_xDy_{1-x}Fe_2$ for $\theta \geq \theta_c$.

To assign $(\mathbf{U}_1, \mathbf{m}_1)$, we consider Lord's interpretation [1990,1992] of magnetostriction in $Tb_xDy_{1-x}Fe_2$ summarized by Figure 3. Lord's picture suggests that we should take $\mathbf{m}_1$ in a [111] direction, while $\mathbf{U}_1$ should represent a stretch in the $\mathbf{m}_1$ direction. We shall make the simplest assumption consistent with this observation:

$$\mathbf{m}_1 = \frac{\alpha}{\sqrt{3}}[111]_c$$

$$\mathbf{U}_1 = \eta_1 \mathbf{1} + (\eta_2 - \eta_1)\hat{\mathbf{m}}_1 \otimes \hat{\mathbf{m}}_1, \quad \hat{\mathbf{m}}_1 = \frac{\hat{\mathbf{m}}_1}{|\hat{\mathbf{m}}_1|} = \frac{1}{\sqrt{3}}[111]_c.$$

(6.1)

Here, $[\ \dots\ ]_c$ represents components relative to an orthonormal basis coincident with the cubic axes (at θ_c). The parameters α, η, and η_2 depend upon temperature but we have suppressed this dependence (For the record, $g(\theta)$ in (4.1) is given by $g(\theta) = \eta_1^2 \, \eta_2 \alpha$).

The full set of variants is now determined by (6.1) and the choice of P^o. Referring to (3.21), (3.22), we calculate that the theory delivers the 8 variants

$$SO(3)(\mathbf{U}_1, \mathbf{m}_1), \qquad\qquad SO(3)(\mathbf{U}_1, -\mathbf{m}_1),$$

$$SO(3)(\mathbf{U}_2, \mathbf{m}_2), \qquad\qquad SO(3)(\mathbf{U}_2, -\mathbf{m}_2),$$

$$SO(3)(\mathbf{U}_3, \mathbf{m}_3), \qquad\qquad SO(3)(\mathbf{U}_3, -\mathbf{m}_3),$$

$$SO(3)(\mathbf{U}_4, \mathbf{m}_4), \qquad\qquad SO(3)(\mathbf{U}_4, -\mathbf{m}_4),$$

(6.2)

where

$$\mathbf{m}_1 = \frac{\alpha}{\sqrt{3}}[111]_c,$$

$$\mathbf{m}_2 = \frac{\alpha}{\sqrt{3}}[-111]_c,$$

$$\mathbf{m}_3 = \frac{\alpha}{\sqrt{3}}[1-11]_c,$$

$$\mathbf{m}_4 = \frac{\alpha}{\sqrt{3}}[11-1]_c,$$

(6.3)

and $\mathbf{U}_i := \eta_1 \mathbf{1} + (\eta_2 - \eta_1)\hat{\mathbf{m}}_i \otimes \hat{\mathbf{m}}_i$, $\hat{\mathbf{m}}_i = \hat{\mathbf{m}}_i/|\hat{\mathbf{m}}_i|$, $i = 1,\dots,4$. The energy wells are represented schematically in Figure 4. Specializing the notation, we let $\mathbf{M}$ denote the union

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of the sets given in (6.2). We postpone the evaluation of η_1 and η_2 from measurements to Section 6b.

The potential well structure given above has something in common with energies for cubic-to-trigonal martensitic transformations as constructed using methods of Ball and James [1991, Section 2]. The origin of this remark is the observation that

$$\{\mathbf{R} \in P^o : \mathbf{R}\mathbf{U}_1\mathbf{R}^T = \mathbf{U}_1\} \tag{6.4}$$

is a representation of the trigonal Laue group (32). Such energies would have only 4 variants, as the magnetization would be missing, but much of what we say below would carry over to the martensitic case, including the normals to planes of discontinuity of ∇y and various results on macroscopic deformations. An example of a cubic-to-trigonal martensitic transformation is the R-phase transformation in near equiatomic TiNi (Miyazaki and Wayman [1988]), Miyazaki, Kimura and Otsuka [1988]).

b) *Lamellar microstructures*

We can construct various minimizing sequences for $Tb_x Dy_{1-x} Fe_2$ using the results of Section 5 if we can satisfy certain jump conditions for pairs $(\mathbf{F}^+, \pm\mathbf{m}^+)$ and $(\mathbf{F}^-, \pm\mathbf{m}^-)$ belonging to different variants. Here, we work out these conditions.

The condition of interest is (5.15), since the variants for $Tb_x Dy_{1-x} Fe_2$ already have the property $(\mathbf{F}, \mathbf{m}) \in \mathsf{M} \Rightarrow (\mathbf{F}, -\mathbf{m}) \in \mathsf{M}$. Note that

$$\mathbf{F}^+ - \mathbf{F}^- = \mathbf{a} \otimes \mathbf{n} \quad \Rightarrow \quad \mathbf{R}\mathbf{F}^+\mathbf{Q} - \mathbf{R}\mathbf{F}^-\mathbf{Q} = \mathbf{R}\mathbf{a} \otimes \mathbf{Q}^T\mathbf{n} \quad \forall \, \mathbf{R} \in SO(3),$$
$$\forall \, \mathbf{Q} \in P^o. \tag{6.5}$$

By (6.5) it is only necessary to look at one pair of variants; that is, given $i, j \in \{1, \dots, 4\}$ there is a $\mathbf{Q} \in P^o$ such that

$$\mathbf{Q}^T\mathbf{U}_i\mathbf{Q} = \mathbf{U}_1, \quad \mathbf{Q}^T\mathbf{U}_j\mathbf{Q} = \mathbf{U}_2, \tag{6.6}$$

for example. This is easily checked by looking at the various cases. Hence, using suitable choices of $\mathbf{Q} \in P^o$ and $\mathbf{R} \in SO(3)$ in (6.5), we find that it is only necessary to consider
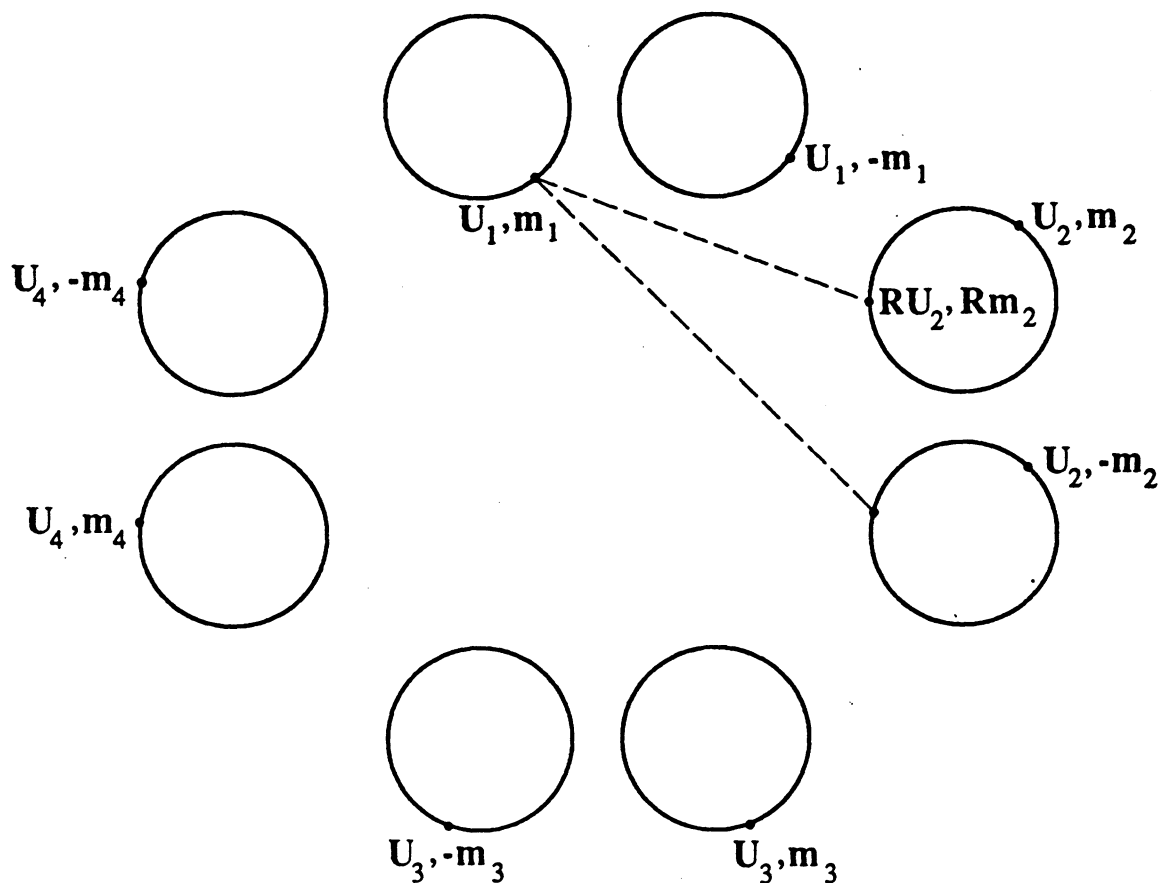
Figure 4. Minimizers of the anisotropy energy φ in the model of $Tb_xDy_{1-x}Fe_2$. Each circle represents a set of the form $(QU, \; Qm)$, $Q \in SO(3)$, with (U, m) assuming the indicated values. The pairs $(U_i \pm m_i)$ are given by (6.2) and (6.3). Dashed lines connect compatible pairs (Section 6b).

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the case

$$RU_2 - U_1 = a \otimes n. \tag{6.7}$$

Here U_2 and U_1 are given in (6.2)-(6.3) and we seek solutions (R, a, n) of (6.7) with $R \in SO(3)$.

The equation (6.7) is the *twinning equation* that arises in the study of martensitic transformations. While the general solution is known for any U_1, U_2 (Ball and James [1987]), it is easier in the present case to calculate directly. Introduce the orthonormal basis

$$\hat{e}_1 = [100]_c, \quad \hat{e}_2 = \frac{1}{\sqrt{2}}[011]_c, \quad \hat{e}_3 = \frac{1}{\sqrt{2}}[0-11]_c, \tag{6.8}$$

and note that

$$
\begin{aligned}
\hat{m}_1 &= \frac{1}{\sqrt{3}}(\hat{e}_1 + \sqrt{2}\hat{e}_2), \\
\hat{m}_2 &= \frac{1}{\sqrt{3}}(-\hat{e}_1 + \sqrt{2}\hat{e}_2), \\
U_1 &= \eta_1 1 + \frac{1}{3}(\eta_2 - \eta_1)[\hat{e}_1 \otimes \hat{e}_1 + 2\hat{e}_2 \otimes \hat{e}_2 + \sqrt{2}(\hat{e}_1 \otimes \hat{e}_2 + \hat{e}_2 \otimes \hat{e}_1)], \\
U_2 &= \eta_1 1 + \frac{1}{3}(\eta_2 - \eta_1)[\hat{e}_1 \otimes \hat{e}_1 + 2\hat{e}_2 \otimes \hat{e}_2 - \sqrt{2}(\hat{e}_1 \otimes \hat{e}_2 + \hat{e}_2 \otimes \hat{e}_1)].
\end{aligned}
\tag{6.9}
$$

Thus,

$$U_1\hat{e}_3 = U_2\hat{e}_3 = \eta_1\hat{e}_3 \quad \text{and} \quad |U_1\hat{e}_2| = |U_2\hat{e}_2|. \tag{6.10}$$

The conditions $(6.10)_{1,2}$ imply that there is a unique $R^+ \in SO(3)$ such that $R^+\hat{e}_3 = \hat{e}_3$ and $R^+U_2\hat{e}_2 = U_1\hat{e}_2$, *i.e.*,

$$(R^+U_2 - U_1)\hat{e}_3 = 0 \quad \text{and} \quad (R^+U_2 - U_1)\hat{e}_2 = 0. \tag{6.11}$$

Hence, there exists $a^+ \in R^3$ such that

$$R^+U_2 - U_1 = a^+ \otimes \hat{e}_1 \quad \text{(twin)}, \tag{6.12}$$

giving us one solution. The $(100)_c$ planes emerge as planes of discontinuity and a^+ is given by the formula

$$a^+ = \left(\frac{2\sqrt{2}}{3}\right)\left(\frac{\eta_1^2 - \eta_2^2}{2\eta_2^2 + \eta_1^2}\right)\left[\sqrt{2}(\eta_2 - \eta_1)\hat{e}_1 + (\eta_1 + 2\eta_2)\hat{e}_2\right]. \tag{6.13}$$

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To calculate (6.13), it is helpful to notice the identities

$$\det \mathbf{U}_2 = \det \mathbf{R}^+\mathbf{U}_2$$

$$= \det (\mathbf{1} + \mathbf{a}^+ \otimes \mathbf{U}_1^{-1}\hat{\mathbf{e}}_1)(\det \mathbf{U}_1)$$

$$= (1 + \mathbf{a}^+ \cdot \mathbf{U}_1^{-1}\hat{\mathbf{e}}_1)(\det \mathbf{U}_1), \tag{6.14}$$

$$\text{and} \quad \hat{\mathbf{e}}_2\mathbf{U}_2^2 \cdot \hat{\mathbf{e}}_1 - \hat{\mathbf{e}}_2 \cdot \mathbf{U}_1^2\hat{\mathbf{e}}_1 = \mathbf{a}^+ \cdot \mathbf{U}_1\hat{\mathbf{e}}_2.$$

The second of these follows by operating (6.12) on $\hat{\mathbf{e}}_1$, then dotting by $\mathbf{U}_1\hat{\mathbf{e}}_2$ and using the relation $(\mathbf{R}^+)^T\mathbf{U}_1\hat{\mathbf{e}}_2 = \mathbf{U}_2\hat{\mathbf{e}}_2$.

The theory of (6.7) says that it has exactly one other solution that we now calculate. By $(6.9)_{3,4}$

$$|\mathbf{U}_1\hat{\mathbf{e}}_1| = |\mathbf{U}_2\hat{\mathbf{e}}_1|. \tag{6.15}$$

Hence, there is a unique $\mathbf{R}^- \in SO(3)$ such that $\mathbf{R}^-\hat{\mathbf{e}}_3 = \hat{\mathbf{e}}_3$ and $\mathbf{R}^-\mathbf{U}_2\hat{\mathbf{e}}_1 = \mathbf{U}_1\hat{\mathbf{e}}_1$, and we therefore have the existence of $\mathbf{a}^- \in \mathbb{R}^3$ such that

$$\mathbf{R}^-\mathbf{U}_2 - \mathbf{U}_1 = \mathbf{a}^- \otimes \hat{\mathbf{e}}_2 \quad \text{(reciprocal twin)}. \tag{6.16}$$

In this case the planes of discontinuity are the $(011)_c$ planes and $\mathbf{a}^-$ is given by

$$\mathbf{a}^- = \frac{2\sqrt{2}}{3}\left(\frac{\eta_1^2 - \eta_2^2}{2\eta_1^2 + \eta_2^2}\right)\left[(2\eta_1 + \eta_2)\hat{\mathbf{e}}_1 + \sqrt{2}(\eta_2 - \eta_1)\hat{\mathbf{e}}_2\right]. \tag{6.17}$$

These results allow us to construct various minimizing sequences using the results of Section 5. The most interesting cases are those that do not require the magnetic domains to be at a much finer scale than the domains of distortion. As mentioned in Remark 5.4 this is possible when the additional jump conditions

$$(\mathbf{m}^+ - \mathbf{m}^-) \cdot \mathbf{n}' = 0, \quad \mathbf{n}' = \frac{(\mathbf{F}^+)^{-T}\mathbf{n}}{|(\mathbf{F}^+)^{-T}\mathbf{n}|}, \tag{6.18}$$

are satisfied. It is a feature of the potential-well structure of $Tb_xDy_{1-x}Fe_2$ that (6.18) can also be satisfied. Using the terminology in (6.12) and (6.16), we need to show that

$$(\pm\mathbf{R}^+\mathbf{m}_2 - \mathbf{m}_1) \cdot \mathbf{U}_1^{-T}\hat{\mathbf{e}}_1 = 0 \quad \text{(for the twin)},$$

$$(\pm\mathbf{R}^-\mathbf{m}_2 - \mathbf{m}_1) \cdot \mathbf{U}_1^{-T}\hat{\mathbf{e}}_2 = 0 \quad \text{(for the reciprocal twin)}, \tag{6.19}$$

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for an appropriate choice of $\pm$. The "accident" that (6.19) holds is really a consequence of compatibility, the constancy of the determinant of the deformation gradient for the variants, and the fact that m_i is an eigenvector of U_1 in the present case, as shown below.

Lemma 6.1. *Suppose* U_1 *and* U_2 *are symmetric* 3×3 *matrices with* $\det U_1 = \det U_2 \neq 0$, *and assume there is an* $R \in SO(3)$ *and vectors* $a, n \in \mathbf{R}^3$ *such that*

$$RU_2 - U_1 = a \otimes n. \tag{6.20}$$

Suppose $m_1, m_2 \in \mathbf{R}^3$ *satisfy* $U_1 m_1 = \gamma m_1, U_2 m_2 = \gamma m_2$ *for some nonzero* $\gamma \in \mathbf{R}$. *Then*

$$(Rm_2 - m_1) \cdot n' = 0 \quad \Longleftrightarrow \quad (m_2 - m_1) \cdot n = 0, \tag{6.21}$$

where $n' = U_1^{-1} n$.

Proof. If we premultiply (6.20) by U_1^{-1} and take its determinant, using $\det U_1 = \det U_2 \neq 0$, we get

$$U_1^{-1} a \cdot n = 0. \tag{6.22}$$

We now multiply (6.21)$_1$ by γ, use $\gamma m_i = U_i m_i$, and then substitute (6.20) to show that (6.21)$_1$ yields

$$(U_1 m_2 + a(n \cdot m_2) - U_1 m_1) \cdot U_1^{-1} n = 0. \tag{6.23}$$

Using (6.22), the middle term vanishes, so we get

$$(m_2 - m_1) \cdot n = 0. \tag{6.24}$$

The converse is proved by reversing the argument. $\quad \square$

We apply the lemma to (6.19) and get the equivalent equations

$$\begin{aligned}
(\pm m_2 - m_1) \cdot \hat{e}_1 &= 0 \quad \text{(for the twin)}, \\
(\pm m_2 - m_1) \cdot \hat{e}_2 &= 0 \quad \text{(for the reciprocal twin)}.
\end{aligned} \tag{6.25}$$

It follows immediately from (6.9)$_{1,2}$ we can satisfy (6.25) if we take $-$ for the twin and $+$ for the reciprocal twin.
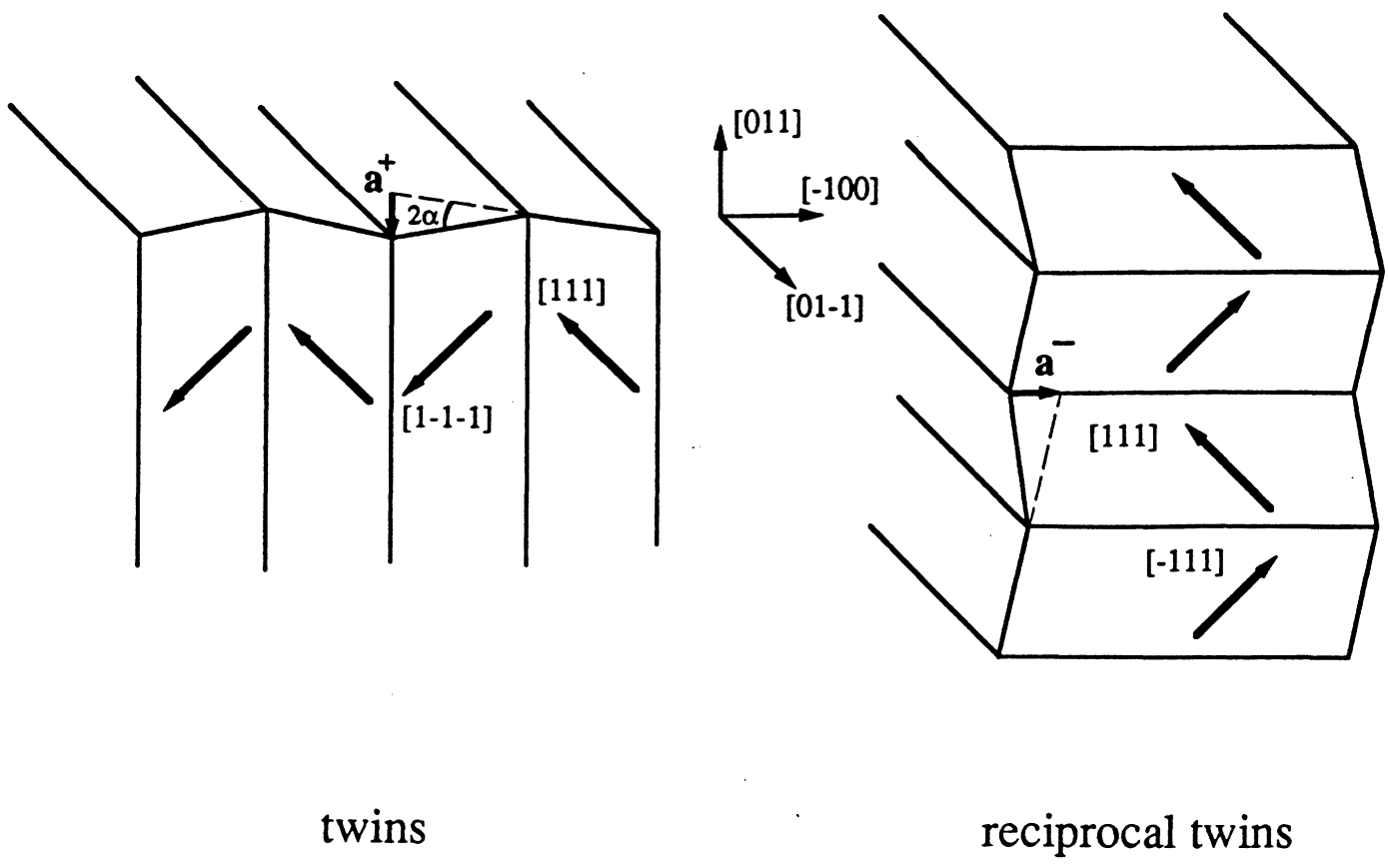
Figure 5. Pictures of the two families of solutions (6.12) and (6.16).

Combining these results with those of Section 5, we get various minimizing sequences. We shall not pursue the mathematical description of these sequences or the ones implied by the Generalization 5.5.

We now evaluate η_1 and η_2. The theory, as set up above, has as reference configuration the undistorted single crystal at the Curie temperature θ_c. This is a little inconvenient at this stage, since we would have to follow the deformation of line elements from θ_c down to room temperature; this is further complicated by the fact that the thermal expansion data in the literature does not appear to be consistent. The theory retains its present form if the reference configuration is allowed to be any configuration that is related by a pure dilation to the undistorted single crystal at θ_c. This dilation scales η_1 and η_2 uniformly. We shall make the convenient choice that at room temperature, there is no stretch along $< 100 >$, i.e.,

$$|\mathbf{U}_1 \ \hat{\mathbf{e}}_1| = 1. \tag{6.26}$$

The assumption (6.26) also remains closely satisfied as the temperature is changed. The equation (6.26) implies that

$$\eta_2^2 + 2\eta_1^2 = 3. \tag{6.27}$$

A measurement is necessary to establish another relation between η_1 and η_2. We prefer a direct measurement, rather than evaluating η_1 and η_2 by forcing a correspondence with linear theory. Such a direct measurement is given by Al-Jiboory and Lord [1990] who measure the angle α shown in Figure 5. Using the results (6.8)-(6.13), we have the relation

$$\cos 2\alpha = \mathbf{U}_1 \ \hat{\mathbf{e}}_1 \cdot \mathbf{R}^+\mathbf{U}_2 \ \hat{\mathbf{e}}_1 \ / \ |\mathbf{U}_1 \ \hat{\mathbf{e}}_1||\mathbf{U}_2 \ \hat{\mathbf{e}}_1|, \tag{6.28}$$

which yields

$$\cos 2\alpha = 1 - \frac{4(\eta_2^2 - \eta_1^2)^2}{(2\eta_2^2 + \eta_1^2)(2\eta_1^2 + \eta_2^2)}. \tag{6.29}$$

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Combining (6.27) and (6.29) with the value $\alpha = \sqrt{2}(1.6 \pm 0.2) \times 10^{-3}$ given by Al-Jiboory and Lord, we get (at room temperature)

$$\eta_1 = 0.9992 \ (\pm 0.0001),$$
$$\eta_2 = 1.0016 \ (\pm 0.0002). \tag{6.30}$$

There is another solution corresponding to $\eta_1 > \eta_2$ which we have discarded. We now turn attention to modifications of the theory for growth-twinned specimens.

c) *Energy of a composite crystal with growth twins on* (111)

Typical specimens of $Tb_x Dy_{1-x} Fe_2$ are not single crystals but rather contain growth twins on a family of parallel {111} planes. A photograph taken by Donald Lord of the microstructure with no applied field on a (0-11) plane is shown in Figure 6. The horizontal boundaries in this picture are the growth twins.

Since these growth twins are created at high temperature during growth of the rod from the melt, we shall model these as material surfaces. Lord [1990,1992] makes a distinction between the plane horizontal boundaries in Figure 6 and the slightly curved ones, referring to the latter as grain boundaries, but we ignore this distinction here and treat them all as twin boundaries. The crystallography of these twins has been discussed by Lord [1990,1992] and analyzed by Simha [1991], and is a typical growth twin for $MgCu_2$ structures. These analyses show that these are type I twins; the crystal structure of the twin is obtained from that of the parent by rotation of 180° about $\mathbf{m}_1$. Let $\mathbf{R}_o$ be such a rotation,

$$\mathbf{R}_o = -1 + 2\hat{\mathbf{m}}_1 \otimes \hat{\mathbf{m}}_1 = \mathbf{R}_o^T, \tag{6.31}$$

and consider for simplicity two regions

$$\Omega_1 := \{\mathbf{x} \in \Omega : \mathbf{x} \cdot \mathbf{m}_1 \geq 0\}, \quad \Omega_2 = \{\mathbf{x} \in \Omega : \mathbf{x} \cdot \mathbf{m}_1 < 0\} \tag{6.32}$$

On Ω_1 we use the energy already described above with the potential-well structure given in (6.2) and (6.3). Modeling the growth twinned crystal as a coherent composite, we use standard continuum mechanical arguments (*e.g.* James [1984]) to show that the energy of
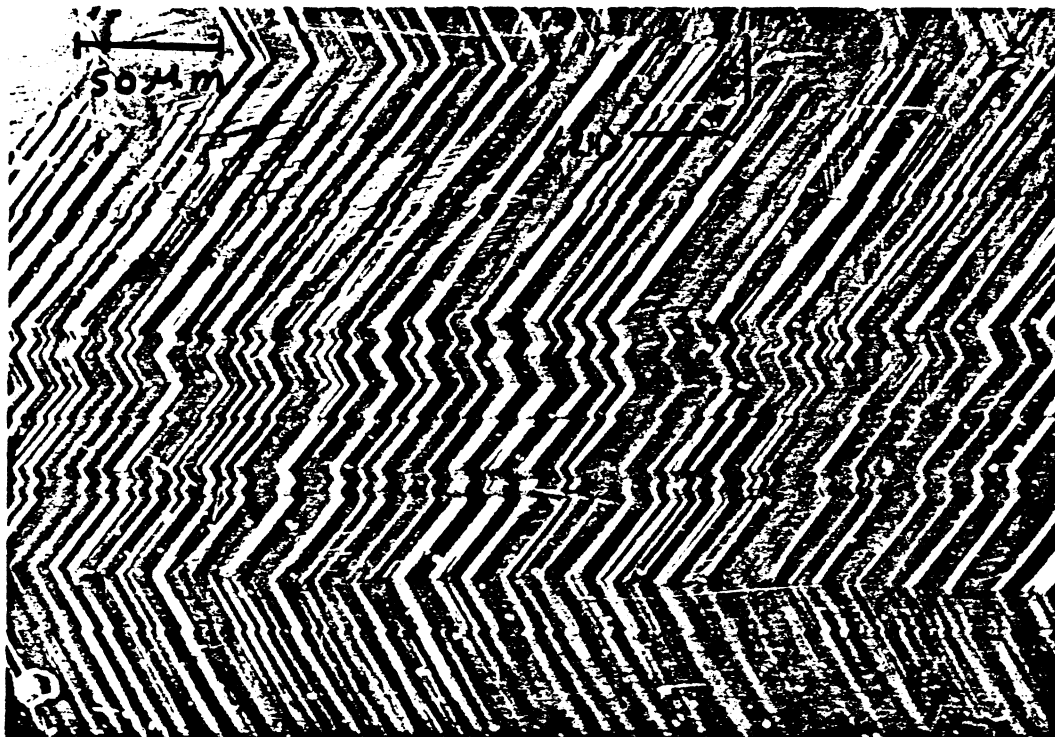
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Figure 6. Distortion of $Tb_x Dy_{1-x} Fe_2$ on a (0-11) plane. The photograph taken with DIC microscopy to show distortion of the surface but not the magnetic domain structure. Photograph courtesy of D. Lord.

Ω_2 is

$$\int_{\Omega_2} \varphi(\nabla \mathbf{y}(\mathbf{x})\mathbf{R}_o, \ \mathbf{m}(\mathbf{y}(\mathbf{x}))) \, d\mathbf{x} \tag{6.33}$$

The total energy for the growth twinned crystal is therefore

$$
\begin{aligned}
E_{gt}(\mathbf{y}, \mathbf{m}) = & \int_{\Omega_1} \varphi(\nabla \mathbf{y}(\mathbf{x}), \mathbf{m}(\mathbf{y}(\mathbf{x}))) \, d\mathbf{x} \\
& + \int_{\Omega_2} \varphi(\nabla \mathbf{y}(\mathbf{x})\mathbf{R}_o, \ \mathbf{m}(\mathbf{y}(\mathbf{x}))) \, d\mathbf{x} \\
& + \frac{1}{2} \int_{\mathbf{R}^3} |\nabla u(\mathbf{z})|^2 \, d\mathbf{z},
\end{aligned}
\tag{6.34}
$$

where, as before,

$$\operatorname{div} \ (-\nabla u + \mathbf{m}) = 0 \quad \text{on } \mathbf{R}^3. \tag{6.35}$$

In this formulation $\mathbf{y}(\mathbf{x})$ is the actual deformation of $\Omega = \Omega_1 \cup \Omega_2$, and therefore we shall still assume $(\mathbf{y}, \mathbf{m}) \in \mathcal{A}_\theta$ (*cf.* (4.5)) with the obvious adjustment to $\mathcal{M}$. We have suppressed the θ-dependence in (6.34). We have also considered only two regions Ω_1 and Ω_2. However, the arguments leading to (6.34) apply to the case of many twinned layers as well; we may simply allow Ω_1 to be a disconnected set of disjoint parallel layers and let $\Omega_2 = \Omega - \Omega_1$.

The key observation concerning (6.34) is that the energy density $\varphi(\mathbf{F}\mathbf{R}_o, \mathbf{m})$ does not have the same potential wells as $\varphi(\mathbf{F}, \mathbf{m})$. For later use we calculate the potential-well minima of $\varphi'(\mathbf{F}, \mathbf{m}) := \varphi(\mathbf{F}\mathbf{R}_o, \mathbf{m})$. It follows directly from the definition of φ' that these are given by

$$
\begin{array}{ll}
SO(3)(\mathbf{U}_1', \ \mathbf{m}_1'), & SO(3)(\mathbf{U}_1', \ -\mathbf{m}_1'), \\[4pt]
SO(3)(\mathbf{U}_2', \ \mathbf{m}_2'), & SO(3)(\mathbf{U}_2', \ -\mathbf{m}_2'), \\[4pt]
SO(3)(\mathbf{U}_3', \ \mathbf{m}_3'), & SO(3)(\mathbf{U}_3', \ -\mathbf{m}_3'), \\[4pt]
SO(3)(\mathbf{U}_4', \ \mathbf{m}_4'), & SO(3)(\mathbf{U}_4', \ -\mathbf{m}_4'),
\end{array}
\tag{6.36}
$$

where

$$
\begin{aligned}
\mathbf{m}_i' &= \mathbf{R}_o \mathbf{m}_i, \\
\mathbf{U}_i' &= \mathbf{R}_o \mathbf{U}_i \mathbf{R}_o^T = \eta_1 \mathbf{1} + (\eta_2 - \eta_1)\hat{\mathbf{m}}_i' \otimes \hat{\mathbf{m}}_i', \quad i = 1, \ldots, 4,
\end{aligned}
\tag{6.37}
$$

and $\hat{\mathbf{m}}'_i = \mathbf{m}'_i/|\mathbf{m}'_i|$, $i = 1,\ldots,4$. Note that one of the variants remains the same, $\mathbf{U}'_1 = \mathbf{U}_1$, $\mathbf{m}'_1 = \mathbf{m}_1$, but all the others change. Extending the notation, we let $\mathbf{M}'$ denote the union of the sets given in (6.36).

For the rest of this paper all indices $< a\ b\ c >$ of vectors are referred to the cubic axes of the "parent," *i.e.*, the cubic axes of P^o.

d) *Energy minimizing microstructures for the growth twinned crystal*

Now we minimize the energy (6.13) appropriate to the growth twinned crystal. To minimize energy, we would like to place $(\nabla\mathbf{y}(\mathbf{x}), \mathbf{m}(\mathbf{y}(\mathbf{x}))) \in \mathbf{M}$ for $\mathbf{x} \in \Omega_1$ and $(\nabla\mathbf{y}(\mathbf{x}), \mathbf{m}(\mathbf{y}(\mathbf{x}))) \in \mathbf{M}'$ for $\mathbf{x} \in \Omega_2$, but there is the obvious problem of compatibility at the growth twin boundary (*i.e.*, $\mathbf{y}$ is a continuous function).

Motivated by Lord's picture (Figure 6), we shall look for minimizing sequences in which $\nabla\mathbf{y}^{(k)}$ is a laminate in Ω_1 and another laminate in Ω_2, together with a suitable magnetic domain structure. Sequences of this kind are governed by Remark 5.6. Combining this remark with the potential-well structures $\mathbf{M}$ and $\mathbf{M}'$, we can construct minimizing sequences $(\mathbf{y}^k, \mathbf{m}^k)$ for the energy E_{gt} (6.34) if we can satisfy the equations

$$\mathbf{B} - \mathbf{A} = \mathbf{a} \otimes \mathbf{n},$$

$$\mathbf{B}' - \mathbf{A}' = \mathbf{a}' \otimes \mathbf{n}',$$

$$(\gamma\mathbf{B} + (1-\gamma)\mathbf{A}) - (\delta\mathbf{B}' + (1-\delta)\mathbf{A}') = \mathbf{b} \otimes \mathbf{m}_1, \qquad (6.38)$$

$$(\mathbf{A}, \,^{\pm}\mathbf{p}), (\mathbf{B}, \,^{\pm}\mathbf{q}') \in \mathbf{M},$$

$$(\mathbf{A}', \,^{\pm}\mathbf{p}'), (\mathbf{B}', \,^{\pm}\mathbf{q}') \in \mathbf{M}',$$

for some $\gamma \in [0,1]$, $\delta \in [0,1]$, $\mathbf{a}$, $\mathbf{a}'$, $\mathbf{n}$, $\mathbf{n}'$, $\mathbf{b}$, $\mathbf{p}$, $\mathbf{p}'$, $\mathbf{q}$, $\mathbf{q}' \in \mathbb{R}^3$, and for some 3×3 matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{A}'$, $\mathbf{B}'$. Here, $\mathbf{M}$ is the union of the orbits in (6.2) and $\mathbf{M}'$ is the union of the orbits in (6.36). Note that the vectors $\mathbf{p}$, $\mathbf{p}'$, $\mathbf{q}$, $\mathbf{q}'$ can always be chosen to satisfy (6.38)$_{3,4}$ because both $\mathbf{M}$ and $\mathbf{M}'$ exhibit the invariance $(\mathbf{F}, \mathbf{m}) \to (\mathbf{F}, -\mathbf{m})$. Hence, these vectors play no further role in the analysis of (6.38).

The equations (6.38)$_{1,4}$ have already been solved in (6.12), (6.13), (6.16), (6.17). From these explicit solutions all crystallographically equivalent solutions can be read off using

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the method explained in (6.5)-(6.7). In fact, we have also secretly solved $(6.38)_{2,5}$. This follows because, by the construction of M' from M, any solution $(\mathbf{B}, \mathbf{A}, \mathbf{a}, \mathbf{n})$ of $(6.38)_{1,4}$ yields a solution

$$(\mathbf{R}_o\mathbf{B}\mathbf{R}_o^T, \ \mathbf{R}_o\mathbf{A}\mathbf{R}_o^T, \ \mathbf{R}_o\mathbf{a}, \ \mathbf{R}_o\mathbf{n}) \tag{6.39}$$

of $(6.38)_{2,5}$ and conversely. Alternatively, all solutions of $(6.38)_2$ are crystallographically equivalent (via the group $\mathbf{R}_o P^o \mathbf{R}_o^T$) to the pair of solutions

$$\bar{\mathbf{R}}^{\pm}\mathbf{U}_2' - \mathbf{U}_1' = (\mathbf{a}')^{\pm} \otimes (\mathbf{n}')^{\pm}, \tag{6.40}$$

where

$$(\mathbf{a}')^+ = \mathbf{R}_o\mathbf{a}^+ = \left(\frac{2\sqrt{2}}{3}\right)\left(\frac{\eta_1^2 - \eta_2^2}{2\eta_2^2 + \eta_1^2}\right)\left(\sqrt{2}(\eta_1 - \eta_2)\hat{\mathbf{e}}_1 - (\eta_1 + 2\eta_2)\hat{\mathbf{e}}_2 + \frac{6\sqrt{2}}{\sqrt{3}}\eta_2\hat{\mathbf{m}}_1\right)$$

$$(\mathbf{n}')^+ = \mathbf{R}_o\hat{\mathbf{e}}_1 = -\hat{\mathbf{e}}_1 + \frac{2}{\sqrt{3}}\hat{\mathbf{m}}_1$$

$$\tag{6.41}$$

$$(\mathbf{a}')^- = \mathbf{R}_o\mathbf{a}^- = \left(\frac{2\sqrt{2}}{3}\right)\left(\frac{\eta_1^2 - \eta_2^2}{2\eta_1^2 + \eta_2^2}\right)\left(-(2\eta_1 + \eta_2)\hat{\mathbf{e}}_1 + \sqrt{2}(\eta_1 - \eta_2)\hat{\mathbf{e}}_2 + \frac{6}{\sqrt{2}}\eta_2\hat{\mathbf{m}}_1\right)$$

$$(\mathbf{n}')^- = \mathbf{R}_o\hat{\mathbf{e}}_2 = -\hat{\mathbf{e}}_2 + \frac{2\sqrt{2}}{\sqrt{3}}\hat{\mathbf{m}}_1$$

To complete the analysis, we take all pairs $(\mathbf{A}, \mathbf{B})$ and $(\mathbf{A}', \mathbf{B}')$ of solutions of $(6.38)_{1,4,2,5}$ and check to see if they satisfy $(6.38)_3$. Counting all combinations of twins and reciprocal twins, we have 144 possibilities to check. There are certain crystallographic equivalences that reduce this number, but crystallographic equivalence is now less useful because the vector $\mathbf{m}_1$ in $(6.38)_3$ is given. We summarize the equivalence below:

a. We can premultiply (6.38) by a constant rotation matrix and get another solution. This allows us to make one of the matrices $(\mathbf{A}, \mathbf{B}, \mathbf{A}'$ or $\mathbf{B}')$ symmetric.

b. If $\mathbf{Q} \in P^o \cap (\mathbf{R}_o P^o \mathbf{R}_o)$ and $\mathbf{Q}\mathbf{m}_1 = \mathbf{m}_1$ we can premultiply $(6.38)_3$ by $\mathbf{Q}$ and postmultiply by $\mathbf{Q}^T$ to get another solution. The matrices $\mathbf{Q}$ satisfying these conditions are

$$\mathbf{Q} \in \left\{\mathbf{1}, \ \hat{\mathbf{Q}}, \ \hat{\mathbf{Q}}^2\right\}, \tag{6.42}$$

where $\mathbf{Q}[a\ b\ c] = [c\ a\ b]$ in the cubic basis.

c. If $\mathbf{Q} \in P^o \cap (\mathbf{R}_o P^o \mathbf{R}_o)$ and $\mathbf{Q}\mathbf{m}_1 = -\mathbf{m}_1$ we can premultiply $(6.38)_3$ by $\mathbf{Q}$ and post-multiply by $\mathbf{Q}^T$ to get another solution. The matrices $\mathbf{Q}$ satisfying these conditions are

$$\mathbf{Q} \in \{\mathbf{Q}_1,\ \mathbf{Q}_2,\ \mathbf{Q}_3\} \tag{6.43}$$

where $\mathbf{Q}_1\ [a\ b\ c] = [-a\ -c\ -b]$, $\mathbf{Q}_2\ [a\ b\ c] = [-c\ -b\ -a]$, $\mathbf{Q}_3\ [a\ b\ c] = [-b\ -a\ -c]$, all in the cubic basis.

To describe the reduced number of possibilities, we shall use the following notation. We let

$$\frac{ij}{k'l'} \tag{6.44}$$

denote the set of four calculations using variants i and j above the plane $\{\mathbf{x} \cdot \mathbf{m}_1 = 0\}$ and variants k' and l' below this plane, that is, the special cases of (6.38) in which $\mathbf{A} = \mathbf{R}_1\mathbf{U}_i$, $\mathbf{B} = \mathbf{R}_2\mathbf{U}_j$, $\mathbf{A}' = \mathbf{R}_3\mathbf{U}'_k$, $\mathbf{B}' = \mathbf{R}_4\mathbf{U}'_l$. There are four calculations represented by (6.44), as we can use either twins or reciprocal twins above the plane and twins or reciprocal twins below. Accounting for the invariance listed in a, b, c above, the 144 calculations represented by (6.38) can be reduced to the 24 calculations

$$\frac{1\ 2}{1'\ 2'},\ \frac{1\ 2}{1'\ 3'},\ \frac{1\ 2}{2'\ 3'},\ \frac{1\ 2}{3'\ 4'},\ \frac{2\ 3}{2'\ 3'},\ \frac{2\ 3}{2'\ 4'}. \tag{6.45}$$

We have examined each of these cases in detail. Assuming here and below the mild conditions $\eta_1 \neq \eta_2$, $\eta_1 > 0$, $\eta_2 > 0$, $\eta_1 < 2\eta_2$, $\eta_2 < 2\eta_1$, we find after lengthy calculations that the only solutions of (6.38) are found among the 8 problems

$$\frac{1\ 2}{1'\ 2'},\ \frac{2\ 3}{2'\ 3'}. \tag{6.46}$$

In executing the computations whose results are reported below, we employed several principles which we review now. Returning to (6.38), we write

$$\mathbf{F} = (1 - \gamma)\mathbf{A} + \gamma\mathbf{B},\ \mathbf{F}' = (1 - \delta)\mathbf{A}' + \delta\mathbf{B}',\ \mathbf{C} = \mathbf{F}^T\mathbf{F},\ \text{and}\ \mathbf{C}' = \mathbf{F}^T\mathbf{F}, \tag{6.47}$$

where $\mathbf{A}, \mathbf{B}, \mathbf{A}'$, and $\mathbf{B}'$ determine a $\frac{ij}{k'l'}$ growth twin laminate as described above. Given $\mathbf{F}$, we seek $\mathbf{F}'$ so that

$$\mathbf{F}' - \mathbf{F} = \mathbf{b} \otimes \mathbf{m}_1. \qquad (6.48)$$

The following consequences of compatibility are given by, *e.g.*, Ball and James [1987], Ericksen [1991].

(1) If $\mathbf{C} = \mathbf{F}^{\mathbf{T}}\mathbf{F}$, and $\mathbf{C}' = \mathbf{F}'^{\mathbf{T}}\mathbf{F}'$ are two symmetric, positive-definite 3×3 matrices satisfying

$$\mathbf{C}' - \mathbf{C} = \mathbf{g} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{g}, \quad |\mathbf{m}| = 1, \qquad (6.49)$$

then the two wells are compatible with normal $\mathbf{m}$, that is, there is a rotation $\mathbf{R} \in SO(3)$ and $\mathbf{a} \in \mathbb{R}^3$ such that

$$\mathbf{R}\mathbf{F}' = \mathbf{F} + \mathbf{a} \otimes \mathbf{m}. \qquad (6.50)$$

On the other hand, *any* Cauchy Green strain is compatible with its 180° rotation about an axis:

(2) If $\mathbf{C}$ and $\mathbf{C}'$ above are related by $\mathbf{C}' = \mathbf{P}\mathbf{C}\mathbf{P}, \mathbf{P}$ a 180° rotation about the axis $\mathbf{m}$, then there is a 180° rotation with axis $\mathbf{Q} \| \mathbf{F}^{-\mathbf{T}}\mathbf{m}$ such that

$$\mathbf{Q}\mathbf{F}\mathbf{P} = \mathbf{F} + \mathbf{a} \otimes \mathbf{m}. \qquad (6.51)$$

Finally, in the special case where $\mathbf{F}$ and $\mathbf{F}'$ are essentially stretches in given directions, it is easy to compute the normals and amplitudes.

(3) If $\mathbf{C}_i = \eta_1 \mathbf{U}_i^2, \mathbf{U}_i = 1 + (\eta_2 - \eta_1)\,\mathbf{g}_i \otimes \mathbf{g}_i, |\mathbf{g}_i| = 1, i = 1, 2$, then

$$\mathbf{R}\mathbf{U}_2 = \mathbf{U}_1(1 + \mathbf{a} \otimes \mathbf{n}) \qquad (6.52)$$

for two choices of $(\mathbf{a}, \mathbf{n})$ which satisfy $\mathbf{n} \| \mathbf{g}_1 + \mathbf{g}_2, \mathbf{a} \| \mathbf{g}_1 - \mathbf{g}_2$ and $\mathbf{n} \| \mathbf{g}_1 - \mathbf{g}_2, \mathbf{a} \| \mathbf{g}_1 + \mathbf{g}_2$. In both cases the axis of $\mathbf{R}$ is parallel to $\mathbf{g}_1 \wedge \mathbf{g}_2$.

We find immediately that if we have solutions of the form (6.46) only in the case that twins are used above and below or reciprocal twins are used above and below, for otherwise the appropriate $\mathbf{C}$ and $\mathbf{C}'$ satisfy rank $(\mathbf{C}' - \mathbf{C}) = 3$, violating (6.49) above.

Examining the well structure in (6.36), (6.37) we see that

$$\mathbf{C}' - \mathbf{C} = \mathbf{g} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{g}, \quad |\mathbf{m}| = 1, \tag{6.53}$$

with $\mathbf{m} = \mathbf{m}_1$ only when $\delta = \gamma$. But, there are planes with normals near $\mathbf{m}_1$ at which we have compatible laminates when δ is close to γ. We are, at present, uncertain of the implications of this. It may possibly add to the ability of the material to have certain low energy, compatible domain structures when the growth twin boundaries are slightly wavy.

We now describe the four solutions given by (6.46).

I. $12/1'2'$. In this case the explicit solutions of $(6.38)_{1,2}$ are given by (6.12), (6.13), (6.16), (6.17), (6.40), (6.41). We insert these equations into $(6.38)_3$ and use a) above to get

$$\left(\gamma \mathbf{R} \left\{ \begin{matrix} \mathbf{R}^+ \mathbf{U}_2 \\ \mathbf{R}^- \mathbf{U}_2 \end{matrix} \right\} + (1 - \gamma) \mathbf{R} \mathbf{U}_1 \right) - \left(\delta \left\{ \begin{matrix} \bar{\mathbf{R}}^+ \mathbf{U}_2' \\ \bar{\mathbf{R}}^- \mathbf{U}_1' \end{matrix} \right\} + (1 - \delta) \mathbf{U}_1 \right) = \mathbf{b} \otimes \mathbf{m}_1 \tag{6.54}$$

which is to be solved for $\mathbf{R} \in SO(3)$, $\mathbf{b} \in \mathbb{R}^3$, γ, $\delta \in [0,1]$.

Equation (6.54) is equivalent to the equation

$$\left[\mathbf{R}_o \mathbf{R} \left[\mathbf{U}_1 + \gamma \left\{ \begin{matrix} \mathbf{a}^+ \otimes \hat{\mathbf{e}}_1 \\ \mathbf{a}^- \otimes \hat{\mathbf{e}}_2 \end{matrix} \right\} \right] + \left[\mathbf{U}_1 + \delta \left\{ \begin{matrix} \mathbf{a}^+ \otimes \hat{\mathbf{e}}_1 \\ \mathbf{a}^- \otimes \hat{\mathbf{e}}_2 \end{matrix} \right\} \right] \right] \mathbf{g} = 0 \quad \forall \mathbf{g} \cdot \mathbf{m}_1 = 0, \tag{6.55}$$

which is a little more useful. As mentioned above, (6.47) has solutions if and only if we use $+$ throughout or $-$ throughout. All solutions have the important property that

$$\delta = \gamma, \tag{6.56}$$

and we obtain exactly two solutions (corresponding to $+$ and $-$) for each $\gamma \in [0,1]$. For each $\gamma \in [0,1]$, the two solutions have $\mathbf{R} = \mathbf{R}_o(-1 + 2\mathbf{f} \otimes \mathbf{f})$ where $\mathbf{f}$ satisfies, respectively,

$$\hat{\mathbf{e}}_3 \cdot \mathbf{f} = 0, \quad \left[2\eta_1 \mathbf{e} + 2\gamma \left\{ \begin{matrix} -2 \, \mathbf{a}^+ \\ \sqrt{2} \, \mathbf{a}^- \end{matrix} \right\} \right] \cdot \mathbf{f} = 0, \tag{6.57}$$

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and $e = [-211]$. The vector $\mathbf{b}$ may be obtained by operating (6.54) on $\hat{e}_1$.

II. 2 3/2′ 3′. In this case we first must obtain the solutions of $(6.38)_{1,2}$. These are found by first letting $\mathbf{Q} \in P^o$ be given by $\mathbf{Q}[a\ b\ c] = [-c\ b\ a]$ and then observing that

$$\mathbf{Q}\mathbf{U}_1\mathbf{Q}^T = \mathbf{U}_2, \quad \mathbf{Q}\mathbf{U}_2\mathbf{Q}^T = \mathbf{U}_3. \tag{6.58}$$

Operating $\mathbf{Q} \ldots \mathbf{Q}^T$ on (6.12), (6.13), (6.16), (6.17), we get

$$\begin{Bmatrix} \mathbf{R}_1^+ \\ \mathbf{R}_1^- \end{Bmatrix} \mathbf{U}_3 - \mathbf{U}_2 = \begin{Bmatrix} \mathbf{Q}a^+ \otimes \mathbf{Q}\hat{e}_1 \\ \mathbf{Q}a^- \otimes \mathbf{Q}\hat{e}_2 \end{Bmatrix}, \tag{6.59}$$

where $\mathbf{R}_1^\pm = \mathbf{Q}\mathbf{R}^\pm\mathbf{Q}^T$. Now we operate $\mathbf{R}_o \ldots \mathbf{R}_o^T$ on (6.59) to get the solutions of $(6.38)_2$,

$$\begin{Bmatrix} \bar{\mathbf{R}}_1^+ \\ \bar{\mathbf{R}}_1^- \end{Bmatrix} \mathbf{U}_3' - \mathbf{U}_2' = \begin{Bmatrix} \mathbf{R}_o\mathbf{Q}a^+ \otimes \mathbf{R}_o\mathbf{Q}\hat{e}_1 \\ \mathbf{R}_o\mathbf{Q}a^- \otimes \mathbf{R}_o\mathbf{Q}\hat{e}_2 \end{Bmatrix}, \tag{6.60}$$

where $\bar{\mathbf{R}}_1^\pm = \mathbf{R}_o\mathbf{R}_1^\pm\mathbf{R}_o$. The explicit forms are easily calculated but we do not give them here. The remaining equation $(6.38)_3$ becomes

$$\left(\gamma\mathbf{R} \begin{Bmatrix} \mathbf{R}_1^+\mathbf{U}_3 \\ \mathbf{R}_1^-\mathbf{U}_3 \end{Bmatrix} + (1-\gamma)\mathbf{R}\mathbf{U}_2 \right) - \left(\delta \begin{Bmatrix} \bar{\mathbf{R}}_1^+\mathbf{U}_3' \\ \bar{\mathbf{R}}_1^-\mathbf{U}_3' \end{Bmatrix} + (1-\delta)\mathbf{U}_2 \right) = \mathbf{b} \otimes \mathbf{m}_1, \tag{6.61}$$

which is to be solved for $\mathbf{R} \in SO(3)$, $\mathbf{b} \in \mathbb{R}^3$, $\gamma, \delta \in [0,1]$. Equation (6.61) can also be recast in a form similar to (6.55). All solutions of (6.61) are obtained with $+$ throughout or $-$ throughout and all have the property that

$$\delta = \gamma. \tag{6.62}$$

For each $\gamma \in [0,1]$ the two solutions of (6.61) have $\mathbf{R} = \mathbf{R}_o(-1 + 2\mathbf{f} \otimes \mathbf{f})$ where $\mathbf{f}$ satisfies, respectively,

$$\begin{Bmatrix} \mathbf{Q}^T\hat{e}_2 \\ \mathbf{U}_2\mathbf{e} \end{Bmatrix} \cdot \mathbf{f} = 0, \quad \begin{Bmatrix} \mathbf{U}_2\mathbf{e} - 2\gamma\mathbf{Q}a^+ \\ \mathbf{U}_2\mathbf{Q}e_2 + \gamma\mathbf{Q}a^- \end{Bmatrix} \cdot \mathbf{f} = 0, \tag{6.63}$$

where $e = [11-2]$. In fact, $\mathbf{m}_1$ is the only possible vector that can appear in (6.61), at least for $|\gamma - \delta|$ sufficiently small.

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Before closing this subsection, we retrace the reduction from all laminates to the 24 represented by (6.45). We find that *all* solutions of (6.38), not accounting for crystallographic equivalence, are given by

$$\frac{1\ 2}{1'\ 2'} \sim \frac{1\ 3}{1'\ 3'} \sim \frac{1\ 4}{1'\ 4'},$$
$$\frac{2\ 3}{2'\ 3'} \sim \frac{3\ 4}{3'\ 4'} \sim \frac{2\ 4}{2'\ 4'}. \tag{6.64}$$

Here, $\sim$ means that the problems are related by the equivalence given in a), b) or c) above. The solutions for the crystallographically equivalent cases can be read off immediately. A comparison of these solutions and Figure 6 will be given below in Section 6f.

The fact that there are solutions of (6.38) of the form $ij/i'j'$ and with equal volume fraction is not surprising, as can be seen from the following argument. This argument is a direct application of (6.51) above. Let $\mathbf{A}$ and $\mathbf{B}$ be as in (6.38) and let $\mathbf{F}_\gamma = \gamma\mathbf{B} + (1-\gamma)\mathbf{A}$. Set $\mathbf{F}'_\gamma = \mathbf{F}_\gamma\mathbf{R}_o$. It is easily verified that if we let $\mathbf{Q}_\gamma$ be the 180° rotation with axis parallel to $\mathbf{F}_\gamma^{-T}\mathbf{m}_1$, then $\mathbf{Q}_\gamma\mathbf{F}'_\gamma - \mathbf{F}_\gamma = \mathbf{b}_\gamma \odot \mathbf{m}_1$ for some $\mathbf{b}_\gamma \in \mathbb{R}^3$. Clearly $\mathbf{F}'_\gamma = \gamma\mathbf{B}' + (1-\gamma)\mathbf{A}'$ for some $\mathbf{B}'$ and $\mathbf{A}'$ satisfying (6.38)$_5$ by our construction, so in fact we have solved (6.38). The miracle of the structure of $Tb_xDy_{1-x}Fe_2$ is that, because it is constructed from growth twins, $\mathbf{B}' = \mathbf{B}\mathbf{R}_o$ and $\mathbf{A}' = \mathbf{A}\mathbf{R}_o$ lie on the energy wells $\mathbf{M}'$ of the growth twin whenever $\mathbf{A}$ and $\mathbf{B}$ lie on the energy wells $\mathbf{M}$ of the parent, which makes this procedure of "twinning the whole laminate" possible.

e) *Exact compatibility at the growth twin boundary*

The minimizing sequences found in Section 6f all have the property that by refining the laminates on either side of this boundary ($k \to \infty$), the energy in the transition layer at the growth twin boundary can be reduced to zero. It remains possible, and is permitted by the analysis given above, that this layer can be made to vanish at a finite value of k. This is the case of exact compatibility of two laminates at the growth twin boundary. We examine this possibility here.

If two variants $(\mathbf{A}, \mathbf{p}) \in \mathbf{M}$ and $(\mathbf{A}', \mathbf{p}') \in \mathbf{M}'$ meet at the growth twin boundary at

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finite k, we have for some $\mathbf{x}_o \cdot \mathbf{m}_1 = 0$, $r > 0$,

$$\nabla \mathbf{y}^{(k)}(\mathbf{x}) = \begin{cases} \mathbf{A}, & \mathbf{x} \in \Omega \cap B(\mathbf{x}_o, r), \\ \mathbf{A}', & \mathbf{x} \in \Omega \cap B(\mathbf{x}_o, r), \end{cases} \tag{6.65}$$

where $B(\mathbf{x}_o, r)$ is the ball centered at $\mathbf{x}_o$ of radius r (see Figure 7). As usual, necessary and sufficient conditions for (6.65) are that

$$\mathbf{A} - \mathbf{A}' = \mathbf{s} \otimes \mathbf{m}_1, \tag{6.66}$$

or, more explicitly,

$$\widetilde{\mathbf{R}} \mathbf{U}_i - \mathbf{U}'_j = \mathbf{s} \otimes \mathbf{m}_1. \tag{6.67}$$

Here, we have premultiplied (6.66) by a suitable rotation matrix without loss of generality. It is easy to see, using $\mathbf{U}'_j = \mathbf{R}_o \mathbf{U}_j \mathbf{R}_o$ and the explicit forms of $\mathbf{U}_i$ and $\mathbf{U}_j$, that (6.67) has a solution $(i, j, \widetilde{\mathbf{R}} \in SO(3), \mathbf{s} \in \mathbb{R}^3)$ if and only if $i = j$. In this case the solution is

$$\widetilde{\mathbf{R}} = \mathbf{R}_o \left(-1 + 2\mathbf{v} \otimes \mathbf{v} \right), \quad \mathbf{v} = \frac{\mathbf{U}_i^{-1} \mathbf{m}_1}{|\mathbf{U}_i^{-1} \mathbf{m}_1|}, \tag{6.68}$$

with $\mathbf{s}$ obtained from (6.67).

This result covers trivially the cases $\gamma = 0, 1$ of I and II above, but leaves open the interesting possibility that the whole laminate is also exactly compatible with variants i and i' and j and j', respectively, meeting at parts of the growth twin plane. We now examine this. The relevant microstructure is pictured in Figure 7, and we have, as usual, premultiplied by a constant rotation matrix to eliminate the rotation matrix in front of $\mathbf{U}'_j$. The matrices shown in Figure 7 embody the restriction found from (6.67). In addition, we found in Section 6d that if we have a compatible microstructure of the type shown in Figure 7, we must have twins paired with twins or reciprocal twins paired with reciprocal twins; from this result, the matrices shown in Figure 7 satisfy

$$\mathbf{R} \mathbf{U}_i - \mathbf{U}_j = \mathbf{a} \otimes \mathbf{n},$$
$$\mathbf{R}' \mathbf{U}'_i - \mathbf{U}'_j = \mathbf{a}' \otimes \mathbf{n}', \tag{6.69}$$

where $\mathbf{R}' = \mathbf{R}_o\mathbf{R}\mathbf{R}_o^T$, $\mathbf{a}' = \mathbf{R}_o\mathbf{a}$, $\mathbf{n}' = \mathbf{R}_o\mathbf{n}$, for suitable $\mathbf{a}$, $\mathbf{n} \in \mathbb{R}^3$, $\mathbf{R} \in SO(3)$. There is a continuous function $\mathbf{y}^{(k)}$ whose gradients assume the values shown in Figure 7 (with $\mathbf{n} \neq \mathbf{m}_1$) on the indicated domains if and only if (6.69) holds together with the conditions

$$\hat{\mathbf{R}}\mathbf{R}\mathbf{U}_i - \mathbf{R}'\mathbf{U}_i' = \mathbf{b}_i \otimes \mathbf{m}_1,$$

$$\hat{\mathbf{R}}\mathbf{U}_j - \mathbf{U}_j' = \mathbf{b}_j' \otimes \mathbf{m}_1. \qquad (6.70)$$

(In this statement we have ruled out the possibility that $\mathbf{n}\|\mathbf{m}_1$. If $\mathbf{n}\|\mathbf{m}_1$, then the analysis of (6.68) clearly applies. In fact, $\mathbf{n}\|\mathbf{m}_1$, does occur for the paired reciprocal twins of variants 2 3 and 2 4.)

It is straightforward to analyze (6.69) and (6.70). To do this we solve (6.70) by the method given in (6.67)-(6.68), then combine with $(6.69)_{ff}$. The result is that there is a solution $(i, j, \hat{\mathbf{R}} \in SO(3), \mathbf{b}_j \in \mathbb{R}^3, \mathbf{b}_j' \in \mathbb{R}^3)$ of (6.69), (6.70) with $\mathbf{n} \neq \mathbf{m}_1$ if and only if

$$\mathbf{U}_j^{-1}\mathbf{a} \cdot \mathbf{m}_1 = 0. \qquad (6.71)$$

A laborious examination of (6.71) for all variants shows that it is satisfied for exactly the twins (but not the reciprocal twins) of the variants

$$2\ 3, \quad 3\ 4, \quad 2\ 4. \qquad (6.72)$$

(Note that $\mathbf{a}$ depends on the choice of i and j via (6.69).) We discuss possible implications of these results for the magnetostrictive behavior of $Tb_xDy_{1-x}Fe_2$ in Section 6g. This section concerned the exact compatibility of laminates at the growth twin boundary. It is conceivable that more complicated arrangements of variants (*e.g.* those shown by Ball and James [1987]) could be exactly compatible at this boundary. For further remarks in this direction in a model that includes exchange energy, see Kohn and Müller [1992].

f) *Comparison of predicted and observed microstructures*

So as to correspond to Lord's picture (Figure 6), we now fix the plane on which the domains are observed to be the (0-11) plane. The growth twins are on $\mathbf{m}_1$ planes,

$$\nabla y = \quad \hat{R}RU_i \quad \hat{R}U_j \quad \hat{R}RU_i \quad \hat{R}U_j$$

$\hat{R}RU_i$

(111)

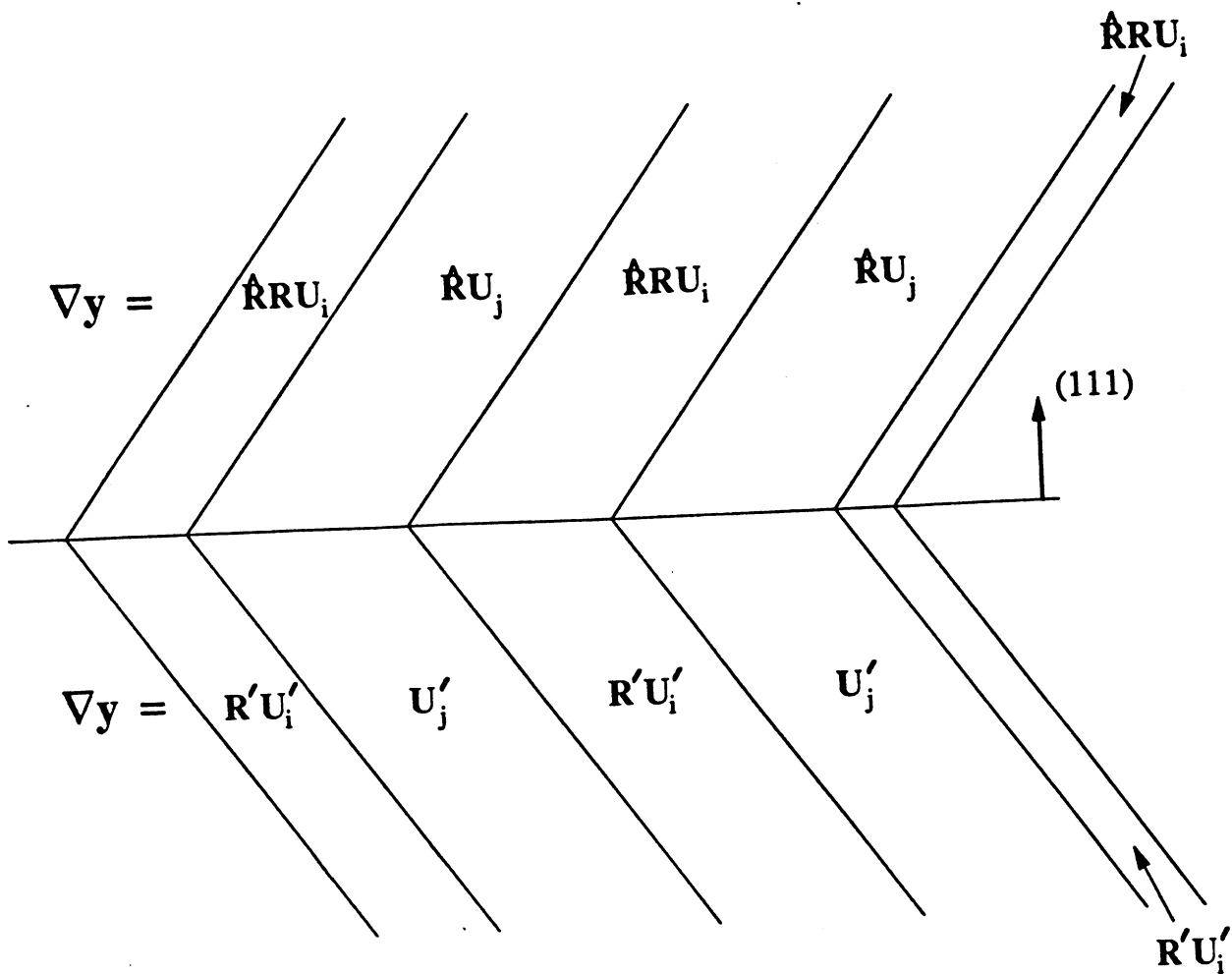$$\nabla y = \quad R'U_i' \quad U_j' \quad R'U_i' \quad U_j'$$

$R'U_i'$

Figure 7. Exact compatibility of two laminates at the growth twin boundary.

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which intersect (0-11) on [−211] lines. Having fixed these planes, we have lost all crystallographic equivalence so we must examine all the compatible variants.

Summarizing the results of Sections 6d and 6e, we found that there are minimizing sequences for the growth twinned crystal. These consist of twinned laminates above and below the growth twin plane $\{x : x \cdot m_1 = 0\}$. All these sequences have the property that twins (reciprocal twins) above the plane are paired with twins (reciprocal twins, respectively) below. They also have the property that the volume fraction γ of a variant i above equals the volume fraction of variant i' below, but we have a minimizing sequence for each $\gamma \in [0,1]$. The combinations of variants that give compatible microstructures are

$$
\frac{1\ 2}{1'\ 2'} \ , \quad \frac{1\ 3}{1'\ 3'} \ , \quad \frac{1\ 4}{1'\ 4'},
$$
$$
\frac{2\ 3}{2'\ 3'} \ , \quad \frac{3\ 4}{3'\ 4'} \ , \quad \frac{2\ 4}{2'\ 4'}. \tag{6.73}
$$

Some of these give also exact compatibility; these are the variants in the second row of (6.73), omitting the pairs of variants that are reciprocally twinned.

We first compare the geometry of the minimizing sequences with Lord's picture. Using the results of Section 6d, we find that twin planes for the different variants are given in Table 1, together with the lines of intersection of these twin planes with the (0-11) plane. Data for the region Ω_2 (the primed variants) is obtained by rotating all the data in Table 1 by R_o. It is seen from Lord's picture that the trace of the twin planes on the (0-11) plane are very nearly [011] directions. The combinations of variants giving this geometry are

$$
\left(\frac{1\ 2}{1'\ 2'} \right)_t , \quad \left(\frac{3\ 4}{3'\ 4'} \right)_t . \tag{6.74}
$$

Here the subscripts r and t mean that we take only the solution corresponding to the reciprocal twin and twin, respectively. A picture of one of these minimizing sequences, drawn with accurate geometry and $\gamma = \frac{1}{2}$, is shown in Figure 8. The general appearance is quite similar to Lord's picture. The general appearance of all the minimizing sequences is shown in Figure 9.

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]
1 4	(001) twin	[100]
	(110) reciprocal	[−111]
2 3	(00-1) twin	[100]
	(1-10) reciprocal	[111]
3 4	(-100) twin	[011]
	(01-1) reciprocal	parallel to $[01 - 1]$
2 4	(0-10) twin	[100]
	(10-1) reciprocal	[111]

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

It is possible that Lord's picture (Figure 6) actually represents the solution $\left(\begin{smallmatrix} 3 & 4 \\ 3' & 4' \end{smallmatrix}\right)_t$, since this solution has the correct geometry and is exactly compatible. Lord's picture suggests exact compatibility to us because of the sharp changes of darkness on crossing the growth twin boundary and because of the variability of the volume fraction as one moves along this boundary.

g) *Macroscopic magnetostriction in a $Tb_xDy_{1-x}Fe_2$ rod*

We have found a surprisingly large variety of minimizing sequences above. Each of these sequences is parameterized by $\gamma \in [0,1]$, and each is a minimizing sequence with no external forces or applied field. Since they are all minimizing sequences, they all have the same limiting energy. Hence, it would seem possible with small forces or small applied fields to easily shift the material from one of these sequences to another. In particular, we expect that it is quite easy with small fields or loads (of suitable orientation) to easily shift γ from 0 to 1.

With this in mind, it becomes interesting to calculate the macroscopic magnetostriction obtainable using each of the minimizing sequences we have found. For this purpose we choose a particular rod axis to be $e := [-211]/\sqrt{6}$. A line segment embedded in the material in the direction e in the reference configuration will become a zig-zag line segment at room temperature, if we consider any of the minimizing sequences constructed above at finite k. However, its end-to-end length will converge to a definite value as $k \to \infty$, and it is natural to identify this length as relating to the macroscopic magnetostriction (this identification is the natural interpretation supplied by the Young measure of the sequence, *cf.* James and Kinderlehrer [1990]). This limiting length is given by

$$\text{length} = |\mathbf{R}(\mathbf{A} + \gamma\mathbf{a} \otimes \mathbf{n})\mathbf{e}| = |(\mathbf{A} + \gamma\mathbf{a} \otimes \mathbf{n})\mathbf{e}|,$$
$$\mathbf{e} = [-211]/\sqrt{6},$$

(6.75)

where $\mathbf{A} = \mathbf{U}_i$, $\mathbf{A} + \mathbf{a} \otimes \mathbf{n} = \hat{\mathbf{R}}\mathbf{U}_j$, $\hat{\mathbf{R}} \in SO(3)$ for the chosen pair of variants ij. Equation (6.75) is the limiting length obtained by embedding the line segment in Ω_1; of course, the
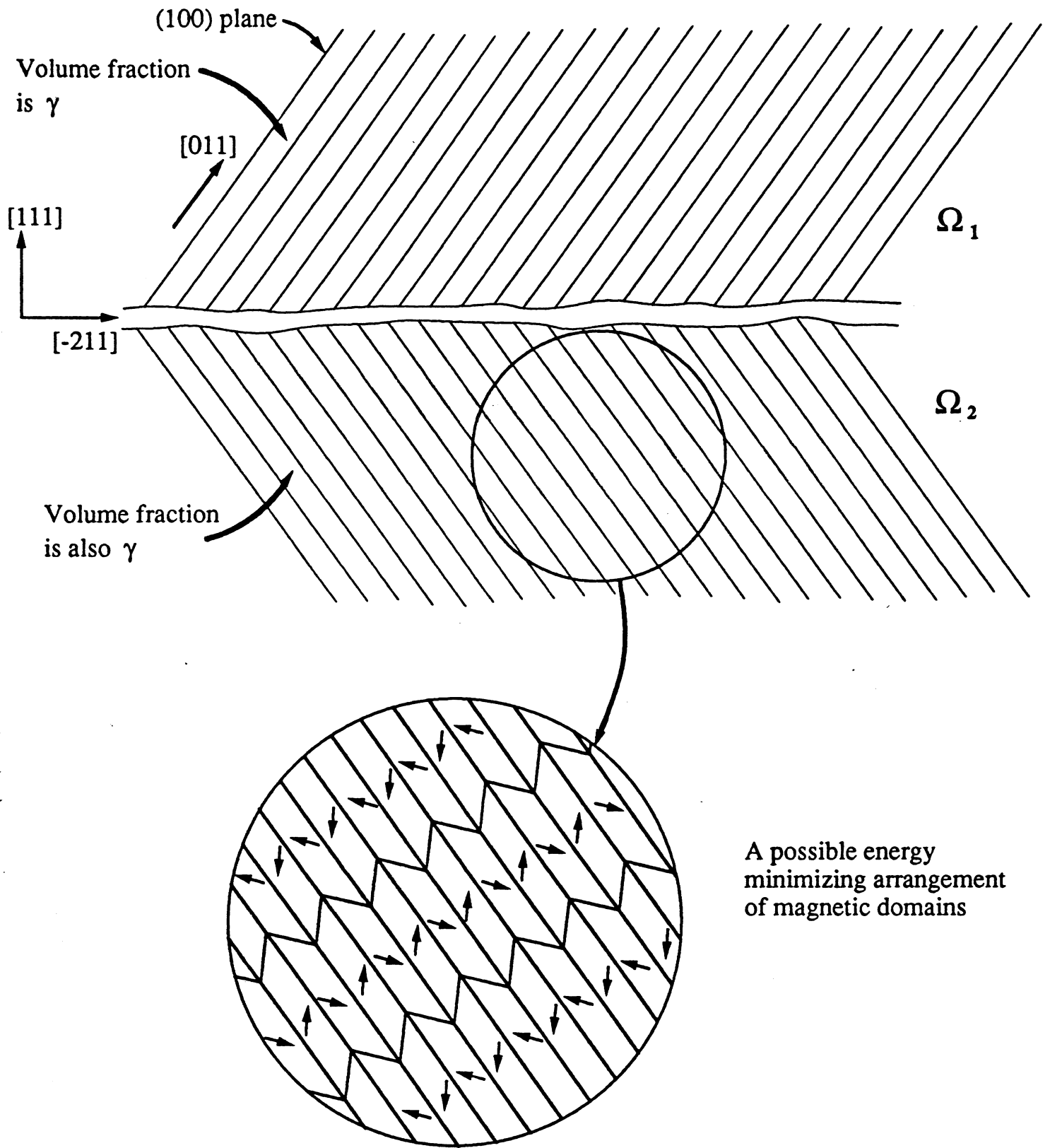
54

Figure 8. Compatible minimizing sequences of the variants listed in (6.67). The inset shows a possible minimizing arrangement of magnetic domains.

$$\left(\frac{1\,2}{1'\,2'}\right)_t \qquad \left(\frac{3\,4}{3'\,4'}\right)_t$$

(cf. Figure 6)

$$\left(\frac{1\,2}{1'\,2'}\right)_r \qquad \left(\frac{1\,3}{1'\,3'}\right)_t \qquad \left(\frac{1\,4}{1'\,4'}\right)_t$$

$$\left(\frac{2\,3}{2'\,3'}\right)_t \qquad \left(\frac{2\,4}{2'\,4'}\right)_t$$

$$\left(\frac{1\,3}{1'\,3'}\right)_r \qquad \left(\frac{1\,4}{1'\,4'}\right)_r$$

$$\left(\frac{2\,3}{2'\,3'}\right)_r \qquad \left(\frac{2\,4}{2'\,4'}\right)_r$$
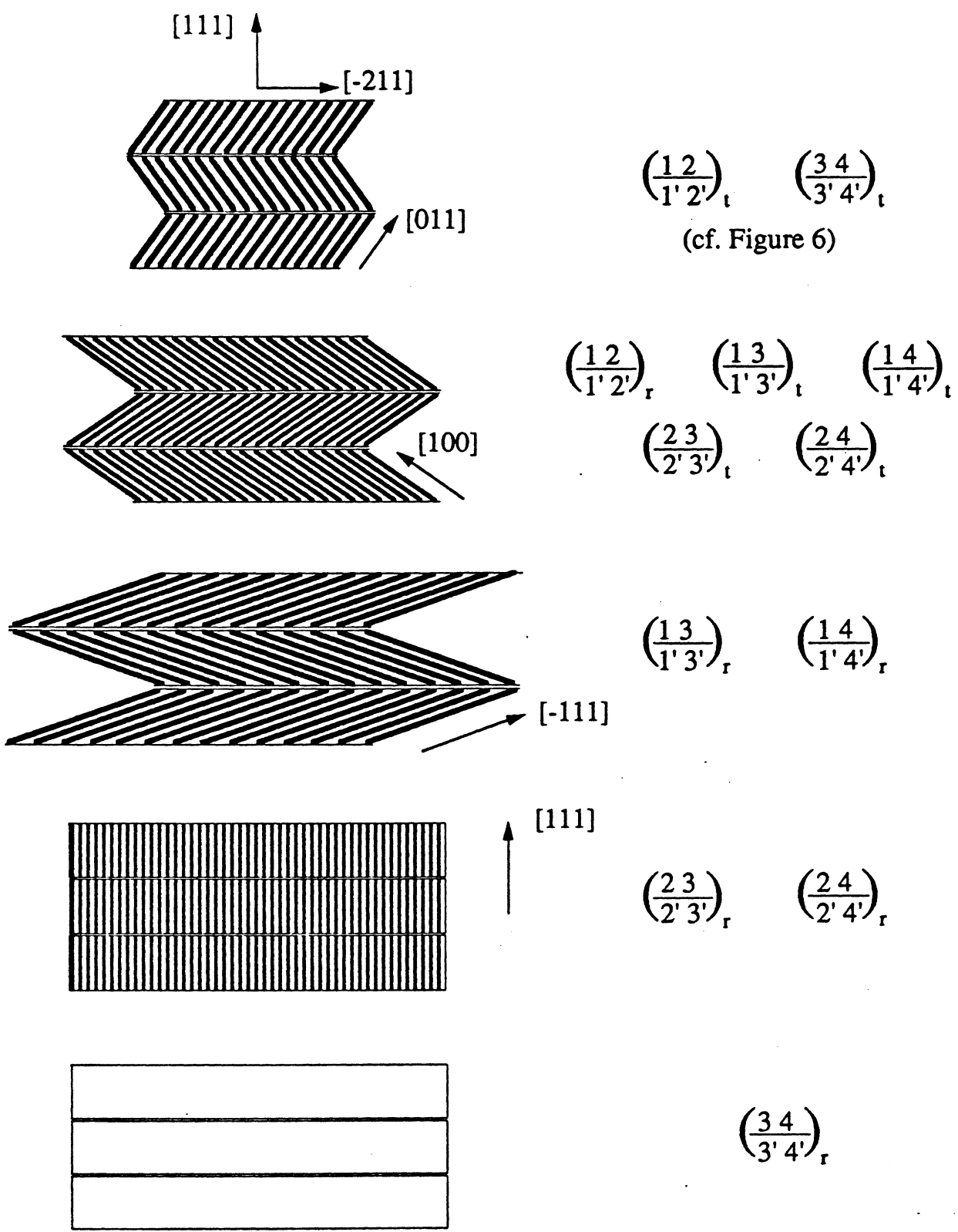
$$\left(\frac{3\,4}{3'\,4'}\right)_r$$

Figure 9. Appearance of the predicted minimizing sequences on the (0-11) plane.

same length is obtained by embedding the line segment in Ω_2, as can be seen by operating $(6.38)_3$ on **e**.

We are interested here in computing the maximum and minimum values of (6.76) as γ goes from 0 to 1 for a given pair of variants i and j, and then comparing among the different pairs of variants. The results of these calculations are presented in Table 2. We note that the length (6.75) is a positive-definite quadratic function of γ. Hence, the maximum value of this length is achieved at $\gamma = 0$ or 1. In all cases it turns out that the minimum is achieved also at $\gamma = 0$ or 1 except for variants 3 4, for which the minimum is achieved at $\gamma = \frac{1}{4}$. For the reciprocally twinned pair $(3\ 4)_r$ the length is independent of γ, so this pair is particularly useless for inducing magnetostriction.

The first remark is that for typical values of η_1 and η_2 for $Tb_xDy_{1-x}Fe_2$, a growth twinned crystal as analyzed above achieves nearly the maximum uniaxial magnetostriction that could be achieved (in a minimizing sequence) for a single crystal or for any other composite. With $\eta_2 > \eta_1$ the maximum strain experienced by a line segment is less than

$$\frac{\eta_2 - \eta_1}{\eta_1}. \tag{6.77}$$

This result can be formulated precisely and proved using the Young measure and minors relations (Ball and James [1992]) but is intuitively clear. The maximum strain given in Table 2 is

$$\frac{\triangle l}{l} = \frac{(\eta_1^2 + \frac{8}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}} - \eta_1}{\eta_1} \doteq \frac{8}{9}(\frac{\eta_2 - \eta_1}{\eta_1}) \tag{6.78}$$

Hence, there would hardly seem to be any advantage, from the viewpoint of large magnetostriction, to attempt to make single crystals of this alloy.

More interesting is another observation which goes beyond the scope of the present theory. The present theory treats all minimizing sequences on equal footing, but obviously there will be a difference between microstructures formed from the pairs $(2\ 3)_t$, $(3\ 4)_t$ and

variants	length	length with $\eta_1 = 0.9992$, $\eta_2 = 1.0016$
1 2	min η_1	0.9992
	max $(\eta_1^2 + \frac{8}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	1.00133
1 3	min η_1	0.9992
	max $(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	0.99973
1 4	min η_1	0.9992
	max $(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	0.99973
2 3	min $(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	0.9997
	max $(\eta_1^2 + \frac{8}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	1.00133
3 4	min $(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2) - \frac{(\eta_1^2 - \eta_2^2)^2}{3(2\eta_2^2 + \eta_1^2)})^{\frac{1}{2}}$	0.99947
	max $(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	0.99973
$(3\ 4)_r$	min=max=$(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	0.99973
2 4	min $(\eta_1^2 + \frac{2}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	0.99973
	max $(\eta_1^2 + \frac{8}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}}$	1.00133

Table 2. The minimum and maximum macroscopic lengths of a line oriented along $[-211]$ which in the reference configuration had unit length. Except for the variant-pair (3 4), the lengths are independent of whether twins or reciprocal twins are used in the computation. See text.

$(2\ 4)_t$ and the other pairs. That is, $(2\ 3)_t$, $(3\ 4)_t$ and $(2\ 4)_t$ need not exhibit refinement at the growth twin boundary, in contrast to the variant pairs $1\ 2$, $1\ 3$ and $1\ 4$. The total energy we have given omits any contribution of interfacial energy, either on discontinuities of $\nabla \mathbf{y}^{(k)}$ or of $\mathbf{m}^{(k)}$. With the variant pairs $1\ 2$, $1\ 3$ and $1\ 4$, the surface area of discontinuities of $\nabla \mathbf{y}^{(k)}$ goes to ∞ as $k \to \infty$. Ultimately, this will be energetically unfavorable and the final value of k may be determined by a compromise between the energy calculated in this paper and surface energy. We note that there are alternative explanations for limited fineness based on dynamic inaccessibility (see Ball, Holmes, James, Pego and Swart [1990]). In any case our expectation is that the sequences with variants $(2\ 3)_t$, $(3\ 4)_t$ and $(2\ 4)_t$ are likely to be preferred, based on considerations of small energies. However, these variants do *not* give the largest magnetostrictive strain along $[-211]$, as can be seen from Table 2. More specifically, the variant pairs $(2\ 3)_t$ and $(2\ 4)_t$ have the same maximum length, but the minimum length of a line segment using $(2\ 3)_t$ or $(2\ 4)_t$ is greater than the minimum length for variants $1\ 2$. Thus, speculating a little, we could suggest the following mechanism. With small compressive stress on a $[-211]$ rod we could imagine that the observed magnetostriction due to an applied field is caused by the variation of γ between 0 and 1 for the exactly compatible variant pair $(2\ 3)_t$, $(2\ 4)_t$ or perhaps $(3\ 4)_t$. This might be associated with λ-jumping of Clark, Teter and McMasters [1988]; see also Clark [1992]. The maximum strain available using either variants $(2\ 3)_t$ or $(2\ 4)_t$ is

$$\frac{\Delta l}{l} \;=\; \frac{(\eta_1^2 + \tfrac{8}{9}(\eta_2^2 - \eta_1^2))^{\frac{1}{2}} - (\eta_1^2 + \tfrac{2}{9}(\eta_1^2 - \eta_1^2))^{\frac{1}{2}}}{(\eta_1^2 + \tfrac{2}{9}(\eta_1^2 - \eta_1^2))^{\frac{1}{2}}} \;\doteq\; \frac{2}{3}\left(\frac{\eta_2 - \eta_1}{\eta_1}\right). \qquad (6.79)$$

With a larger compressive stress, we could imagine that the material switches to variants $1\ 2$, because the minimum length of a line segment achieves the smaller value $\eta_1 < (\eta_1^2 + \tfrac{2}{9}(\eta_1^2 - \eta_1^2))^{\frac{1}{2}}$. Then, the strain available would be the value given by (6.71). The ratio of the values (6.72) and (6.71), which is 3/4, would then represent the ratio of observed magnetostrictive strains with small and moderate compressive stress. This agrees pretty closely with what we are able to read off the graphs.

How would we recognize the change from the variant pair $(2\ 3)_t, (2\ 4)_t$ or $(3\ 4)_t$ to 1 2? First, we might recognize an abrupt increase of the fineness on application of a compressive stress. Second, if we were observing a (0-11) plane, we could turn to Table 1 and check the traces of the twin plane on the plane of observation. From Table 1, we expect the [100] or [011] trace at small or zero stress, but 1 2 can have either a [011] or a [100] trace. We also note that if we are only interested in biasing the material toward the smallest strain, we could also use the pairs 1 3 or 1 4, which can give [−111] traces. One general fact that emerges from Table 1 is that coarse microstructures have [100] or [011] traces, while all other traces are expected to exhibit fine mixtures.

We were encouraged to make these speculative remarks based on the apparent good agreement with Lords' picture, Figure 6. An analysis of minimizing sequences is needed under applied fields and stresses. With recent results of DeSimone [1992] and computational advances by Luskin and Ma [1990] it appears that such predictions will be feasible, at least in the large specimen limit discussed here.

Acknowledgement

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