Some Methods of Analysis in the Study of Microstructure

David Kinderlehrer
Department of Mathematics
Carnegie Mellon University
Pittsburgh, PA 15213-3890

Research Report No. 92-NA-037

October 1992

Some **methods of analysis in the study of microstructure**

David Kinderlehrer

Center for Nonlinear Analysis and Department of Mathematics
Carnegie Mellon University
Pittsburgh, PA 15213-3890

1. **Introduction** Fine scale morphology or microstructure is implicated in the macroscopic behavior of many materials, but the manifestations of this are often unclear[1]*[2]. We are in need of improved methods for studying this frequently encountered situation. In this report we describe in an expository fashion the initial developments of one such technique which has been applied in several instances especially related to certain alloys or other crystalline materials. Good examples where defect structures consisting of fine scale morphology are relatively simple are certain phase transformations of displacive or structural type and the mechanical behavior of shape memory alloys. Martensitic materials, in particular, exhibit fine twinned microstructures, often appearing as layers or layers within layers[3]. Although we often refer to microstructure, we are confronted with a primarily continuum phenomenon for which some authors use the term mesoscale. In these considerations, one issue is paramount: the presence of spatially oscillatory behavior and the means of understanding it constitutes the bridge from the fine scale to the large scale.

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

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

deformation alone need not be sufficient to characterize many of the properties of the limit configuration.

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

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

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

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

$$f^k\colon \Omega \to \mathbf{R}^N,\ k = 1,2,\ldots, \tag{2.1}$$

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

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

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

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

Another one is

$$f^k(x) = \begin{cases} -1 & \frac{j-1}{k} < x < \frac{j-\frac{1}{2}}{k} \\ 1 & \frac{j-\frac{1}{2}}{k} \le x \le \frac{j}{k} \end{cases} \qquad 1 \le j \le k, \; 0 \le x \le 1. \tag{2.3}$$

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

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

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

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

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

The association

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

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

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

which has the property

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

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

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

Examples

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

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

while for (2.3),

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

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

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

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

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

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

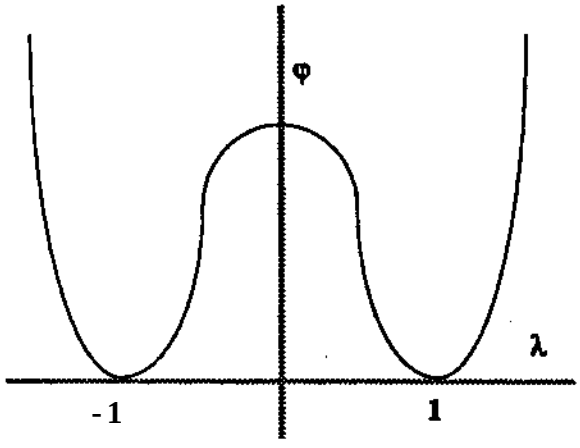


Figure 1 A typical double well potential in one variable.

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

$$v = \tfrac{1}{2}(\delta_{-1} + \delta_{+1}). \qquad (2.12)$$

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

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

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

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

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

studying this with a theory of magnetoelastic interactions based on the micromagnetics of W. F. Brown, Jr. [6,7,8] and the symmetry considerations introduced by Ericksen [16-24]. For a complete discussion, we refer to James and Kinderlehrer [32]. It has some similarities with Toupin's theory of the elastic dielectric [54]. We then apply it to the equilibrium microstructure of $TbDyFe_2$. The primary mechanism of magnetostriction appears to be an exhange of stability of mechanical variants under the influence of a change in the magnetic field, but we do not discuss this in detail here.

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

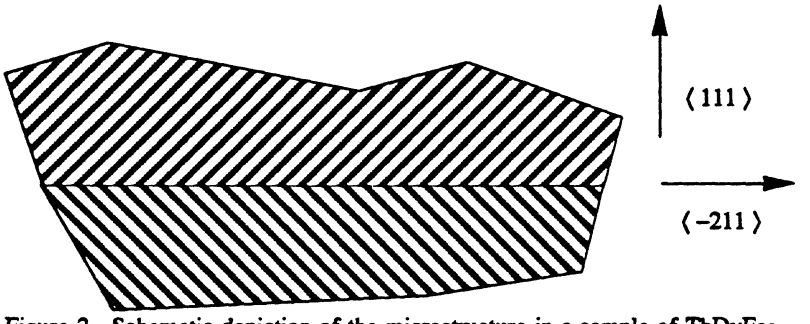


Figure 2. Schematic depiction of the microstructure in a sample of $TbDyFe_2$ illustrating the herringbone structure of two sets of laminar fine structures. Crystallographic directions are with reference to the high temperature nonmagnetic phase.

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

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

subject to the condition of frame indifference

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

and material symmetry

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

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

Requiring W to depend on the deformation gradient $F = \nabla y$ and magnetization m but not on $\nabla^2 y$ and ∇m indicates that any energy associated with mechanical twin walls and Bloch walls is neglected. In this formulation, there may be infinitely fine twins or infinitely fine magnetic

domains, as we have suggested earlier. Since on a macroscopic level, the materials of interest display highly mobile domain configurations, any wall energies need be very small. The analytical benefit is that in the limit of infinite fineness we are able to determine rather accurately the arrangement and location of variants within the material, although not their dimensions.

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

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

and the field energy density is given by

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

The saturation constraint leads to

$$\left|\frac{M}{\rho}\right| = f(\theta) \qquad \text{in the body,} \tag{3.5}$$

where ρ is the density.

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

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

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

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

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

subject to the constraints,

$$\operatorname{div}_y\left(-\nabla_y U + \frac{1}{\det \nabla y}\, m\right) = 0 \quad \text{in } \mathbf{R}^3. \tag{3.7}$$

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

From (3.7), we may also write the energy in the form

$$E(y,m) = \int_\Omega fw(Vy,m,e)dx + \int_{y(\Omega)} f\frac{1}{\det \nabla y} m\text{-}V_yU\ dy\ . \qquad (3.8)$$

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

$$\mathrm{div}(-\nabla u\, C^{-1} \det F + mF\text{-}T) = 0 \quad \text{in } R^3, \qquad (3.9)$$

and the saturation condition is simply

$$Iml = 1 \quad \text{in Q.} \qquad (3.10)$$

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

$$E(yjn) = \int_\Omega fw(Vy,m,9)dx + \int_{R^3} fVu\ C^\wedge\text{-}Vu \det F\ dx, \qquad (3.11)$$

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

$$E(y,m) = \int_\Omega fw(Vy,m,9)dx + \int_{R^3} fVumF\text{-}Tdx. \qquad (3.12)$$

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

$$W(Ui,mi,9) \leq W(F,m,e) \quad \text{for Fe D, Iml = 1.} \qquad (3.13)$$

Generally, Ui and mi depend on temperature. The conditions (3.2) and (3.3) imply the existence of other minima by (2.9). Assume that *the full set cf minima is determined by the orbits* o/(Ui,mi) *under these actions.* Thus

$$\inf W = W(RUiH,miRT,e) < W(Fjn,9) \quad \text{for Re SO(3), } He \text{ P}$$
$$\text{and Fe M, Iml = 1, with } (F,m) \# (RUiH,miR^T). \qquad (3.14)$$

The potential wells are described as

$$(RU_1,m_1R^T), \quad R\ e\ SO(3),$$

$$(RU_2,m_2R^T), \quad R \in SO(3),$$

$$(RU_n,mnR^T), \quad R \in SO(3),$$

where

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

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

Our idea of a variational principle is to find a pair (yon) such that

$$E(yon) = inffEOMi): (TUO \text{ subject to } (3.9)\}.$$

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

$$infE = minWIftl. \tag{3.15}$$

4. The variational context

4.1 The variational context: energetics

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

$$infE(y,m) \ll minWIQI, \tag{4.1}$$

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

$$E(y^*,m^*) = minWIQI. \tag{4.2}$$

We are led in this manner to consider a sequence of deformation fields and magnetization fields (y^k,m^k) subject to (3.9) for which (dependence on 8 suppressed)

$$E(y^kjn^k) \text{ -+ } minWIQI. \tag{4.3}$$

and

$$Vy^k \text{ -» } V\bar{y} \quad \text{and} \quad m^k \text{ -> } \bar{m},$$

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

The only way for (4.3) to occur is if

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

Since

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

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

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

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

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

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

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

4.2 The variational context: kinematics

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

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

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

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

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

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

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

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

It is worthwhile pointing out that for the special case of an infinitely fine laminate supported on two deformation gradients Mi and M2, that is,

$$\int_{\Sigma} f v(A) dv_x(A,n) = (1-G)v(Mi) + 6y(M_2), \qquad (4.10)$$

for some 0, 0 < 0 < 1, the minors relations imply that

$$M2 - Mi = a \otimes n = \text{rank one}, \qquad (4.11)$$

and the { Mj} may represent the deformation gradients of twin related variants with normal n. A sequence of deformations which determines (4.10) with 0 = | is given by

$$Vyk(x) = Mi + \frac{1}{2}(1 + f^*(x-n))a \otimes n, \quad x \in Q, \qquad (4.12)$$

where f^t) is defined in (2.3).

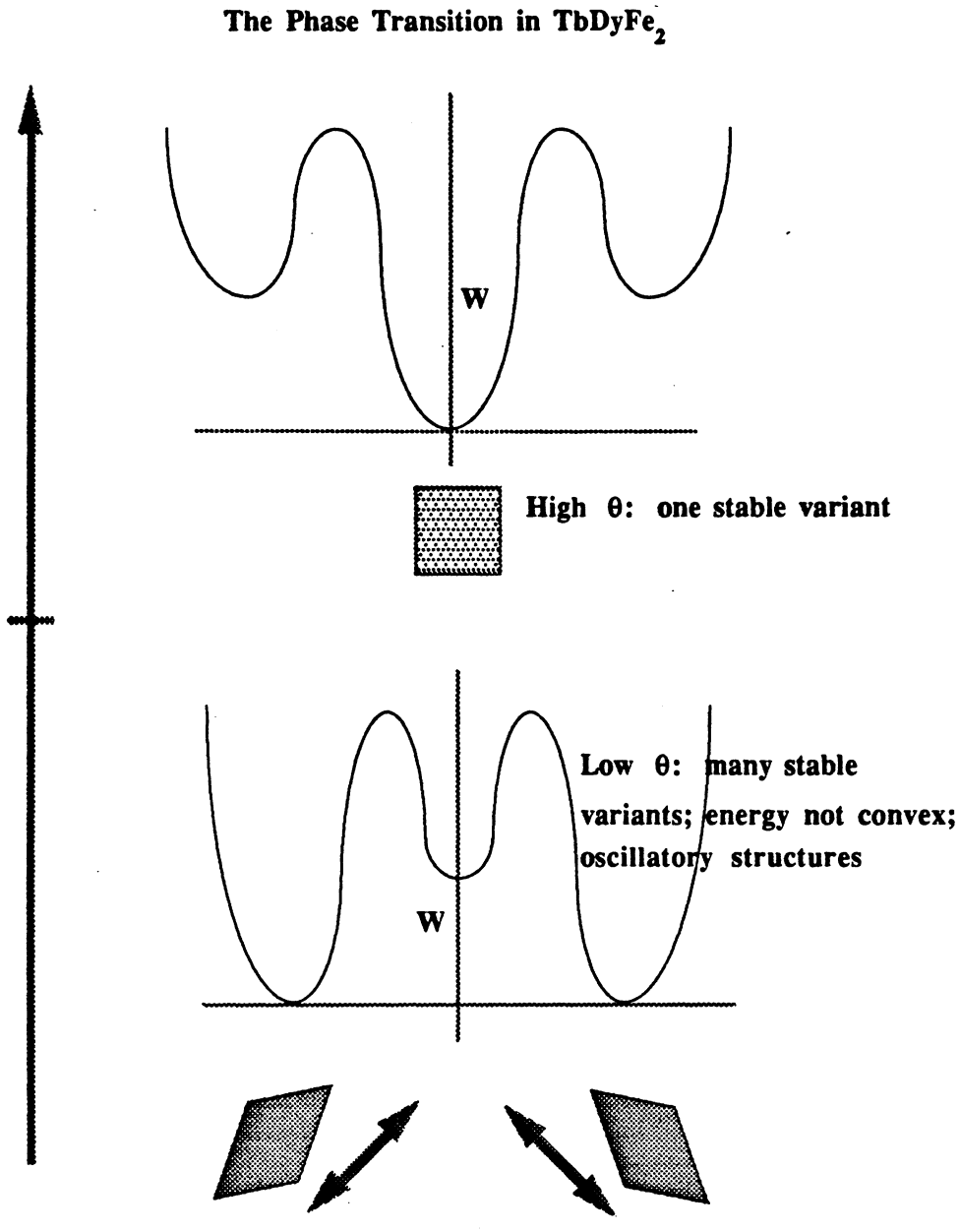


Figure 3 The phase transition in terfenol.

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

$$\bar{m}(x) = \int_{\Sigma} \mu \, d\nu_x(A,\mu) . \tag{4.13}$$

The new relation is that

$$\bar{m}(x)V\bar{y}(x)\text{-}T = \int_{\Sigma} A\text{-}T\,dv_x(A^{\wedge}), \tag{4.14}$$

with

$$\operatorname{div}(\pounds(V\bar{y})\text{-}T) = o \quad \text{in } R3. \tag{4.15}$$

4.3 Application

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

$$Ui = l + \pounds mi \circledR mi \quad \text{and} \quad mi = -^{\wedge}(1,1,1), \quad lei \text{ small}, \tag{4.1}$$

V3

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

$$Ui = 1 + e\,mi \circledR mi, \quad i = 23,4, \text{ with} \tag{4.2}$$
$$m_2 = \frac{1}{\sqrt{3}}(-l,l,D, \quad m_3 = \frac{1}{\sqrt{3}}p(l\text{-}U), \quad nu = \frac{1}{\sqrt{3}}p(U.\text{-}l).$$

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

To establish our result we wish to check that we may produce a minimizing sequence $(y^k jn^k)$ for the energy E(yon) with the potential well structure determined by (4.1) and (4.2) whose statistics, as determined by the "minors relations[1]" and their generalizations, (3.13) - (3.15), (3.20), and (3.21), deliver the observed crystallographic data, for example, of the lower laminate of Figure 1. We are able to do this using the wells determined by (Ui,mi) and (U_2,m_2).

Given any pair of transformation strains

$$Ui \ll 1 + e\pounds i \circledR \pounds i \quad \text{and} \quad U2 = 1 + e\pounds 2 \circledR \pounds 2>$$

$$I\,\pounds i\,I = 1, \ \pounds 1 \text{ and } \pounds 2 \text{ independent},$$

then the type I and type II twins (or twins and reciprocal twins) have normals

$$n^{+} = \pounds 1 + \%2 \text{ and } n^{-} = \xi_1 - \pounds 2.$$

There are rotations R*(e) and vectors tf^e) with

$$Ui = R\pm U_2(1 + a^{\pm}\otimes n^{\pm}) \qquad (4.3)$$

In this case with £i = mi, n+ = (100) and n~ = <011), in agreement with the observations of D. Lord [44,53].

A coherent laminate may be constructed from the deformation gradients Ui and R+U2 or from the deformation gradients Ui and R-U2, cf. also (3.16) - (3.19). We may construct a compatible sequence of magnetizations m^k with $m^k = \pm mi$ in the Ui regions and $m^k = \pm m2(R^+)^T$ in the R^+U2 regions with the property that the limit average $\bar{m} = 0$ so that

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

cf. Figure 2 below.

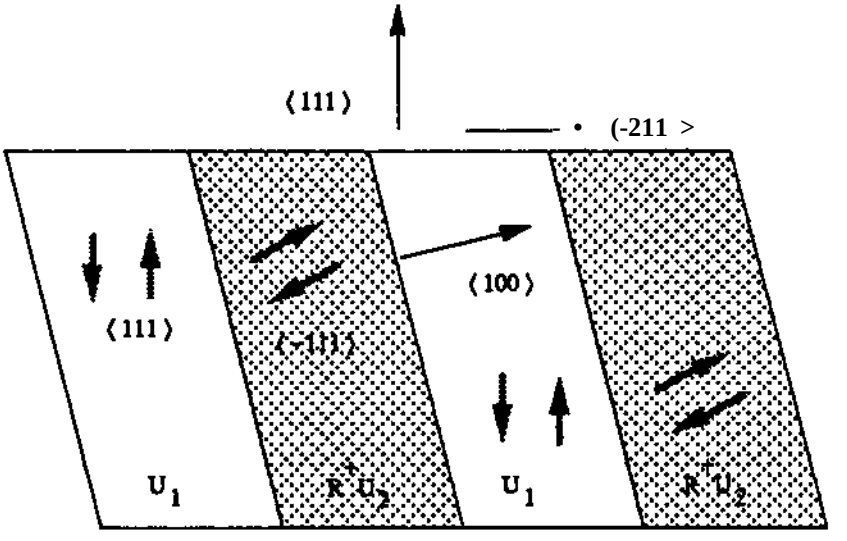


Figure 4. The equilibrium microstructure of a laminate with parameters predicted by the theory. The gray arrows represent directions of the magnetization within the mechanical layers. In the Ui layers they are ± mi where mi is a < 111 > direction and in the shaded layers they are $\pm m2(R^+)^T$ where 012 is a < -111) direction.

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

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

where $0 \le X \le 1$.

Our analysis suggests however that Figure 2 above is not the only solution and need not be the only one the laboratory photographs show either. A laminate may also be realized with

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

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

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

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

$$\begin{aligned} &-\operatorname{div} q(\nabla u) + \frac{\partial u}{\partial t} = 0 \quad \text{in } \Omega \times (0,\infty) \\ &u\,|_{\Omega\times(0)} = u_o \\ &u\,|_{\partial\Omega\times(0,\infty)} = 0 \end{aligned} \tag{5.1}$$

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

The functional

$$I(v) = \int_\Omega (\varphi(\nabla v) + \tfrac{1}{2h}(v - w)^2)\,dx, \quad h > 0, \tag{5.2}$$

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

$$\int_\Omega (\varphi(\nabla v) + \tfrac{1}{2h}(v - u^{h,k-1})^2)\,dx \;\to\; \min \tag{5.3}$$

where the competing $v \in H^1_o(\Omega)$, for example. The $\nu^{h,k}$ and $u^{h,k}$ satisfy

$$\int_\Omega (\bar{q}> + \frac{1}{2h}(v - iM^{-1})^2)\,dx = \min, \tag{5.4}$$

$$\bar{tfx}) = \int_{R^N} U(X)dv^h{}_x{}'^k(X) \quad .with$$

$$suppvhi \quad c \quad \{\lambda: \varphi(\lambda) = <f^{**}(k)\}. \tag{5.5}$$

where <p** denotes the convexifled <p, which is its relaxation in this situation. Moreover, it is possible to show that

$$-div\ \bar{q}h + J(u^{h,k} - u^{h,k-1}) = 0, \text{ where} \tag{5.6}$$

$$\bar{q}^h(x) = \int q^h(X)dv^h{}_x{}'^k a) \ .$$

We next assemble the v^{*1*} and $u^h{}'^k$, defining u^n to be the linear interpolant of the $(u^{h,k})$ and v^h the piecewise constant in time measure equal to v^ in $(k-1)h < t \leq kh$. We obtain in this fashion a family of approximants which are "maximally dissipative" because of (5.5) and converge to a Young measure solution of (5.1).

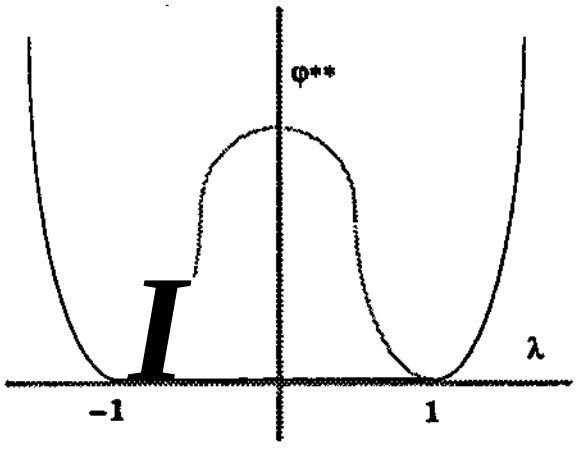
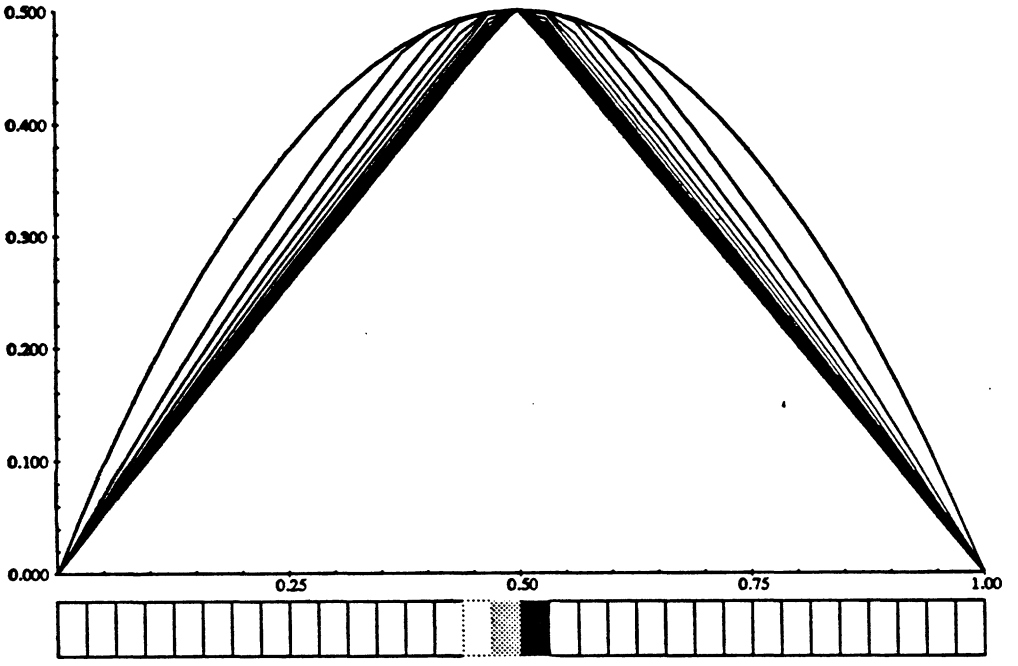


Figure 5. The relaxation <p** of 9 plays an important role in the solution of the problem. Where <p is different from <p** is shown in dotted lines.

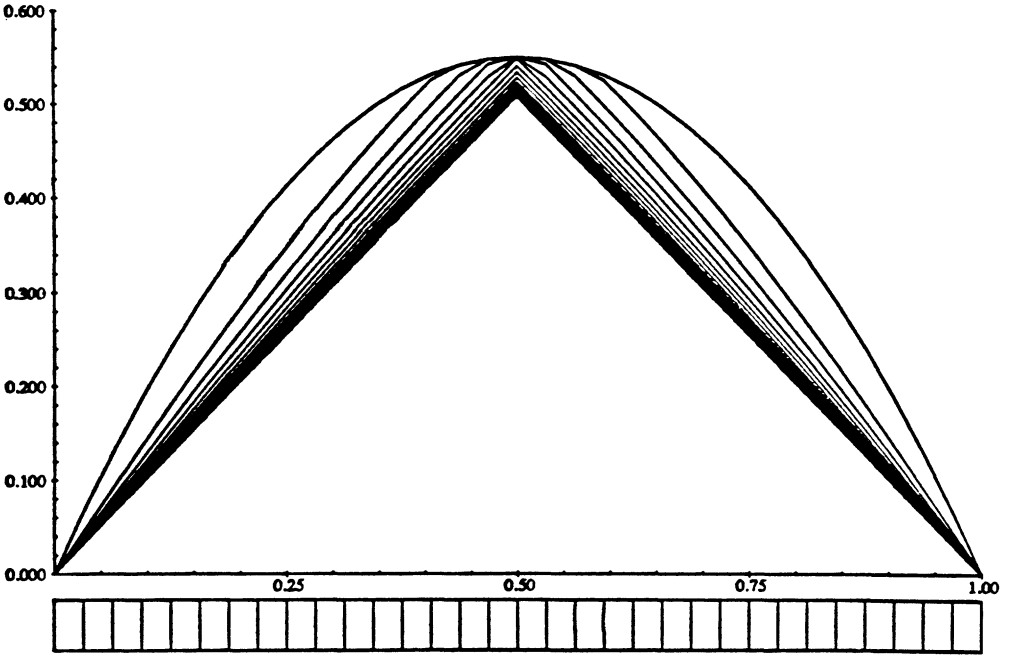
It turns out that the solution u^{*1*} of the basic variational principle is the unique solution of the relaxed problem for this principle which is strictly convex in v, but not in Vv. Some convex analysis thai tells us that u^h is unique and so is its limit u as h—»0. The Young measure need not be unique.

This is an opportunity to study the pure generation of oscillations in a new context The underlying solution is known. What statistics are possible for the sequences which generate this solution and can we compute them? How do they evolve in time? Using an algorithm specifically designed to compute Young measures by Nicolaides and Walkington, Walkington has computed several examples of this behavior, shown in Figure 6. Although in these pictures, the solution decreases monotonically to its limit

$$u(x,«0 = \begin{cases} j\ *\ \sim\ x & 0 < x \leq 0.5 \\ & 0.5 < x < 1 \end{cases}$$



$u(x,0) = 2x(1-x)$



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

Figure 6 Computation of the solution of (5.6) by a Young measure algorithm.

this is not the case for general initial values u(x,0), although the energy integral is a decreasing function of t We refer also to their article in these proceedings.

The author wishes to thank his colleagues and coworkers, especially R. James, R. Nicolaides, P. Pedregal, and Noel Walkington, for their assistance and advice in preparing this account

References

[I] Ball, J. M. and James, R. 1987 Fine phase mixtures as minimizers of energy, Arch. Rat Mech. Anal.,100,15-52

[2] Ball, J. M. and James, R. 1991 Proposed experimental tests of a theory of tine microstructure and the two well problem, Phil. Trans. Roy. Soc. Lond. (to appear)

[3] Barrett, C. and Massalski, T. B. 1980 *Structure of Metals*, 3rd rev. ed., Pergamon

[4] Battacharya, K. Self accomodation in martensite, Arch. Rat. Mech. Anal, (to appear)

[5] Battacharya, K. Wedge-like microstructure in martensite, (to appear)

[6] Brown, WJF. 1962 *Magnetostalic Principles in Ferromagnetism*, Vol. 1 of Selected Topics in Solid Slate Physics (ed. EJ>. Wohlfarth), North-Holland.

[7] Brown, W.F. 1963 *Micromagnetics*, John Wiley and Sons, New York.

[8] Brown, W.F. 1966 *Magnetoelastic Interactions*, Vol. 9 of Springer Tracts in Natural Philosophy (ed. C. Truesdell), Springer-Verlag.

[9] Chipot, M. and Kinderlehrer, D. 1988 Equilibrium configurations of crystals, Arch. Rat Mech. Anal. 103, 237-277

[10] Chipot, M. Numerical analysis of oscillations in nonconvex problems,(to appear)

II1] Clark, A. E. 1980 Magnetostrictive rare earth - Fe2 compounds, *Ferromagnetic Materials, Vol 1* (Wohlfarth, E. P. ed) North Holland, 532 - 589

[12] Collins, C. and Luskin, M 1989 The computation of the austenitic-martensitic phase transition, Lecture Notes in Physics 344 (ed. M. Rascle, D. Serre and M. Slemrod), Springer-Verlag, 34-50.

[13] Collins, C. and Luskin, M. Numerical modeling of the microstructure of crystals with symmetry-related variants, *Proc. ARO US-Japan Workshop on SmartlIntelligent Materials and Systems*, Technomic

[14] Collins, C. and Luskin, M. Optimal order error estimates for the finite element approximation of the solution of a nonconvex variational problem, to appear

[15] Collins, C, Kinderlehrer, D., and Luskin, M. 1991 Numerical approximation of the solution of a variational problem with a double well potential, SIAM J. Numer. Anal., 28, 321-333

[16] Ericksen, J. L. 1979 On the symmetry of deformable crystals, Arch. Rat Mech. Anal. 72,1-13

[17] Ericksen, J. L. 1980 Some phase transitions in crystals, Arch. Rat Mech. Anal. 73, 99-124

[18] Ericksen, J. L. 1981 Changes in symmetry in elastic crystals, IUTAM Symp. Finite Elasticity (Carlson, D£. and Shield R.T., eds.) M. Nijhoff, 167-177

[19] Ericksen, J. L. 1982 Crystal lattices and sublattices, Rend. Sem. Mat Padova, 68,1-9

[20] Ericksen, J. L. 1984 The Cauchy and Born hypotheses for crystals, *Phase Transformations and Material Instabilities in Solids*, (Gurtin, M., ed) Academic Press, 61-78

[21] Ericksen, J. L. 1986 Constitutive theory for some constrained elastic crystals, Int J. Solids Structures, 22,951 - 964

[22] Ericksen, J. L. 1987 Twinning of crystals I, *Metastability and Incompletely Posed Problems*, IMA Vol. Math. Appl. 3,(Antman, S., Ericksen, JX., Kinderlehrer, D_M MttUer, L,eds) Springer, 77-96

[23] Ericksen, J. L. 1988 Some constrained elastic crystals, *Material Instabilities in Continuum Mechanics*, (Ball, J. ed.) Oxford, 119 -136

[24] Ericksen, J. L. 1989 Weak martensitic transformations in Bravais lattices, Arch. Rat Mech. Anal, 107, 23 - 36

[25] Firooze, N. and Kohn, R. 1991 Geometric parameters and the relaxation of multiwell energies, IMA preprint Series 765

[26] Fonseca, L 1988 The lower quasiconvex envelope of the stored energy function for an elastic crystal, J. Math, pures et appl, 67,175-195

[27] James, R. D. 1988 Microstructure and weak convergence, *Proc, Symp. Material Instabilities in Continuum Mechanics*, Heriot-Watt, (Ball, J. M., ed.), Oxford, 175-196

[28] James, R. D. 1989 Relation between microscopic and macroscopic properties of crystals undergoing phase transformation, in *Proc. 7th Army Conf. on Applied Mathematics and Computing* (ed. F. Dressel).

[29] James, R. D. and Kinderlehrer, D. 1989 Theory of diffusionless phase transitions, *PDE's and continuum models of phase transitions*, Lecture Notes in Physics, 344,(Rascle, M., Serre, D., and Slemrod, M., eds.) Springer, 51-84

[30] James, R. D. and Kinderlehrer, D. 1990 An example of frustration in a ferromagnetic material, Nematics: Mathematical and Physical Aspects, (Coron, J.-M., Ghidaglia, J.-M., and Hélein, F., eds), Kluwer NATO ASI series, 201-222

[31] James, R. D. and Kinderlehrer, D. 1990 Frustration in ferromagnetic materials, Cont. Mech. Therm. 2, 215-239

[32] James, R. D. and Kinderlehrer, D. A theory of magnetostriction with application to $TbDyFe_2$ (to appear)

[33] James, R.D. and Müller, S. to appear

[34] Khachaturyan, A. G. 1983 *Theory of structural phase transformations*, Wiley

[35] Kinderlehrer, D. 1988 Remarks about the equilibrium configurations of crystals, *Proc. Symp. Material instabilities in continuum mechanics*, Heriot-Watt (Ball, J. M. ed.) Oxford, 217-242

[36] Kinderlehrer, D. and Pedregal, P. 1991 Characterizations of Young measures generated by gradients, Arch. Rat. Mech. Anal., 115, 329-365

[37] Kinderlehrer, D. and Pedregal, P. 1991 Charactérisation des mesures de Young associées à un gradient, C.R.A.S. Paris, 313, 765-770

[38] Kinderlehrer, D. and Pedregal, P. 1992 Gradient Young measures generated by sequences in Sobolev spaces (to appear)

[39] Kinderlehrer, D. and Pedregal, P. 1992 Remarks about the analysis of gradient Young measures, Pitman Res Notes Math 269 (Miranda, M., ed), 125-150

[40] Kinderlehrer, D. and Pedregal, P. 1992 Weak convergence of integrands and the Young measure representation, SIAM J. Math Anal.,23,1 - 19

[41] Kinderlehrer, D. and Pedregal, P. Remarks about Young measures supported on two wells, (to appear)

[42] Kohn, R. V. 1991 The relaxation of a double-well energy, Cont. Mech. Therm., 3, 193-236

[43] Kohn, R.V. 1989 The relationship between linear and nonlinear variational models of coherent phase transitions, in *Proc. 7th Army Conf. on Applied Mathematics and Computing* (ed. F. Dressel).

[44] Lord, D. 1990 Magnetic domain observations in $TbDyFe_2$, IMA lecture

[45] Luskin, M. and Ma, L. 1990 Analysis of the finite element approximation of microstructure in micromagnetics, UMSI report 90/164

[46] Ma, L. to appear

[47] Matos, J. The absence of fine microstructure in α–β quartz, (to appear)

[48] Nicolaides, R. and Walkington, N. these proceedings

[49] Roitburd, A. L. 1978 Martensitic transformation as a typical phase transformation, *Solid State Phys* 33, Academic Press, 317-390

[50] Tartar, L. 1979 Compensated compactness and applications to partial differential equations, *Nonlinear analysis and mechanics: Heriot Watt Symposium, Vol I V*(Knops, R., ed.) Pitman Res. Notes in Math. 39, 136-212

[51] Tartar, L. 1983 The compensated compactness method applied to systems of conservation laws, *Systems of nonlinear partial differential equations* (Ball, J. M., ed) Riedel

[52] Tartar, L. 1990 H-measures, a new approach for studying homogenisation, oscillations and concentration effects in partial differential equations, Proc. R. Soc. Edin., 115, 193-230

[53] Teter, J.P., Mahoney, K., Al-Jiboory, M., Lord, D., and McMasters, O. D., 1991 Domain observation and magnetostriction in TbDyFe twinned single crystals, J. Appl. Phys, 69, 5768-5770

[54] Toupin, R. 1956 The elastic dielectric, J. Rat. Mech. Anal., 5, 849 - 915

[55] Young, L. C. 1969 *Lectures on calculus of variations and optimal control theory*, W.B. Saunders

Center for Nonlinear Analysis
Report Series

Nonlinear Analysis Series

No.

91-NA-001 [ ] Lions, P.L., **Jacobians and Hardy spaces**, June 1991

91-NA-002 [ ] Giga, Y. and Soto, M.-H., **Generalized interface evolution with the Neumann boundary condition**, July 1991

91-NA-003 [ ] Soner, H.M. and Souganidis, P.E., **Uniqueness and singularities of cylindrically symmetric surfaces moving by mean curvature**, July 1991

91-NA-004 [ ] Coleman, B.D., Marcus, M. and Mizel, V.J., **On the Thermodynamics of periodic phases**, August 1991

91-NA-005 [ ] Gurtin, M.E. and Podio-Guidugli, P., **On the formulation of mechanical balance laws for structured continua**, August 1991

91-NA-006 [ ] Gurtin, M.E. and Voorhees, P., **Two-phase continuum mechanics with mass transport and stress**, August 1991

91-NA-007 [ ] Fried, E., **Non-monotonic transformation kinetics and the morphological stability of phase boundaries in thermoelastic materials**, September 1991

91-NA-008 [ ] Gurtin, M.E., **Evolving phase boundaries in deformable continua**, September 1991

91-NA-009 [ ] Di Carlo, A., Gurtin, M.E., and Podio-Guidugli, P., **A regularized equation for anisotropic motion-by-curvature**, September 1991

91-NA-010 [ ] Kinderlehrer, D. and Ou, B., **Second variation of liquid crystal energy at x/|x|**, August 1991

91-NA-011 [ ] Baughman, L.A. and Walkington, N., **Co-volume methods for degenerate parabolic problems**, August 1991

91-NA-012 [ ] James, R.D. and Kinderlehrer, D., **Frustration and microstructure: An example in magnetostriction**, November 1991

91-NA-013 [ ] Angenent, S.B. and Gurtin, M.E., **Anisotropic motion of a phase interface**, November 1991

92-NA-001 [ ] Nicolaides, R.A. and Walkington, NJ_M **Computation of microstructure utilizing Young measure representations,** January **1992**

92-NA-002 [ ] Tartar, **L., On mathematical tools for studying partial differential equations of continuum physics: H-measures and Young measures,** January 1992

92-NA-003 [1 Bronsard, **L.** and Hilhorst, **D_M On the slow dynamics for the Cahn-Hilliard equation in one space dimension,** February 1992

92-NA-004 [] Gurtin, **M.E., Thermodynamics and the supercritical Stefan equations with nucleations,** March 1992

92-NA-005 [] Antonic, N., **Memory effects in homogenisation linear second order equation,** February 1992

92-NA-006 [ ] Gurtin, M.E. and Voorhees, **P.W., The continuum mechanics of coherent two-phase elastic solids with mass transport,** March 1992

92-NA-007 [ ] Kinderlehrer, D. and Pedregal, **P., Remarks about gradient Young measures generated by sequences in Sobolev spaces,** March 1992

92-NA-008 [ ] **Workshop on Shear Bands,** March 23-25,1992 (Abstracts), March 1992

92-NA-009 [] Armstrong, R. W., **Microstructural/Dislocation Mechanics** Aspects **of Shear** Banding **in Polycrystals,** March 1992

92-NA-010 [] Soner, H. M. and Souganidis, **P.** E., **Singularities and Uniqueness of Cylindrically Symmetric Surfaces Moving by Mean Curvature,** April 1992

92-NA-011 [ ] Owen, David R., Schaeffer, Jack, andWang, Kerning, **A Gronwall Inequality for Weakly Lipschitzian Mappings,** April 1992

92-NA-012 [] Alama, Stanley and Li, **Yan Yan, On "Multibump" Bound States for Certain Semilinear Elliptic Equations,** April 1992

92-NA-013 [] Olmstead, W. E., Nemat-Nasser, S., and Li, **L., Shear Bands as Discontinuities,** April 1992

92-NA-014 [ ] Antonic, R, **H-Measures Applied to Symmetric Systems,** April 1992

92-NA-015 [] Barroso, Ana Cristina and Fonseca, Irene, **Anisotropic Singular Perturbations - The Vectorial Case,** April 1992

92-NA-016 [] Pedregal, Pablo, **Jensen's Inequality in the Calculus of Variations,** May 1992

92-NA-017 [] Fonseca, Irene and Muller, Stefan, **Relaxation of Quasiconvex Functional in BV(Q,SRP) for Integrands f(x,u,Vu),** May 1992

92-NA-018 [ ] Alama, Stanley and Tarantello, Gabriella, **On Semilinear Elliptic Equations with Indefinite Nonlinearities**, May 1992

92-NA-019 [ ] Owen, David R., **Deformations and Stresses With and Without Microslip**, June 1992

92-NA-020 [ ] Barles, G., Soner, H. M., Souganidis, P. E., **Front Propagation and Phase Field Theory**, June 1992

92-NA-021 [ ] Bruno, Oscar P. and Reitich, Fernando, **Approximation of Analytic Functions: A Method of Enhanced Convergence**, July 1992

92-NA-022 [ ] Bronsard, Lia and Reitich, Fernando, **On Three-Phase Boundary Motion and the Singular Limit of a Vector-Valued Ginzburg-Landau Equation**, July 1992

92-NA-023 [ ] Cannarsa, Piermarco, Gozzi, Fausto and Soner, H.M., **A Dynamic Programming Approach to Nonlinear Boundary Control Problems of Parabolic Type**, July 1992

92-NA-024 [ ] Fried, Eliot and Gurtin, Morton, **Continuum Phase Transitions With An Order Parameter; Accretion and Heat Conductor**, August 1992

92-NA-025 [ ] Swart, Pieter J. and Homes, Philip J., **Energy Minimization and the Formation of Microstructure in Dynamic Anti-Plane Shear**, August 1992

92-NA-026 [ ] Ambrosio, I., Cannarsa, P. and Soner, H.M., **On the Propagation of Singularities of Semi-Convex Functions**, August 1992

92-NA-027 [ ] Nicolaides, R.A. and Walkington, Noel J., **Strong Convergence of Numerical Solutions to Degenerate Varational Problems**, August 1992

92-NA-028 [ ] Tarantello, Gabriella, **Multiplicity Results for an Inhomogenous Neumann Problem with Critical Exponent**, August 1992

92-NA-029 [ ] Noll, Walter, **The Geometry of Contact, Separation, and Reformation of Continous Bodies**, August 1992

92-NA-030 [ ] Brandon, Deborah and Rogers, Robert C., **Nonlocal Superconductivity**, July 1992

92-NA-031 [ ] Yang, Yisong, **An Equivalence Theorem for String Solutions of the Einstein-Matter-Gauge Equations**, September 1992

92-NA-032 [ ] Spruck, Joel and Yang,Yisong, **Cosmic String Solutions of the Einstein-Matter-Gauge Equations**, September 1992

92-NA-033 [ ] **Workshop on Computational Methods in Materials Science (Abstracts)**, September 16-18, 1992.

92-NA-034 [ ] Leo, Perry H. and Herng-Jeng Jou, **Shape evolution of an initially circular precipitate growing by diffusion in an applied stress field**, October 1992

92-NA-035 [ ] Gangbo, Wilfrid, **On the weak lower semicontinuity of energies with polyconvex integrands**, October 1992

92-NA-036 [ ] Katsoulakis, Markos, Kossioris, Georgios T. and Retich, Fernando, **Generalized motion by mean curvature with Neumann conditions and the Allen-Cahn model for phase transitions**, October 1992

92-NA-037 [ ] Kinderlehrer, David, **Some methods of analysis in the study of microstructure**, November 1992

Stochastic Analysis Series

91-SA-001 [ ] Soner, H.M., **Singular perturbations in manufacturing**, November 1991

91-SA-002 [ ] Bridge, D.S. and Shreve, S.E., **Multi-dimensional finite-fuel singular stochastic control**, November 1991

92-SA-001 [ ] Shreve, S. E. and Soner, H. M., **Optimal Investment and Consumption with Transaction Costs**, September 1992