MINIMIZING SEQUENCES AND THE MICROSTRUCTURE OF CRYSTALS

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SYNOPSIS

We present a model for predicting the detailed three dimensional microstructure of a crystal which undergoes a diffusionless phase transformation involving a change of symmetry. The model is not restricted to states of zero stress or to small strains and rotations. Any such model has the property that in many cases stable domain patterns necessarily involve fine mixtures of the phases. Mathematically, these patterns emerge as minimizing sequences which make the total free energy smaller and smaller but which do not in general converge to minimizers. We work out the details of this for martensite, relating the results to the crystallographic theory.

Our model does not place any *a priori* geometric restrictions on the shapes or arrangements of the regions in which the new phase forms; this is necessary to determine microstructures which occur in complex stress fields, or to explore the possibility of new and unusual microstructures which may occur for special values of the material parameters.

§1. INTRODUCTION

The general aim of this work is to develop mathematical models capable of predicting the detailed microstructure of a crystal which undergoes a diffusionless solid-solid phase transformation involving a change of symmetry. A principal motivation is the well known mathematical fact that 'non-elliptic' integrals of the calculus of variations do not in general attain a minimum, while the corresponding minimizing sequences develop finer and finer oscillations reminiscent of a finely twinned microstructure. A standard and elementary illustration (cf. L.C. Young [8]) is afforded by the problem of minimizing

$$I(u) = \int_0^1 [((u')^2 - 1)^2 + u^2]dx \qquad (1)$$

among real-valued functions $u(x)$ satisfying $u(0) = u(1) = 0$. In (1) u' denotes the derivative of u with respect to x. In this problem $I(u) \geqslant 0$ and the sequence $u^{(j)}$ shown in Figure 1 satisfies $I(u^{(j)}) \to 0$ as $j \to \infty$. But there is no u satisfying the end conditions and $I(u) = 0$, so that there is *no* minimizer of $I(u)$. (In multidimensional problems it is not necessary to have dependence of the energy on u as well as on u' to get this phenomenon.) This suggests that microstructure such as that

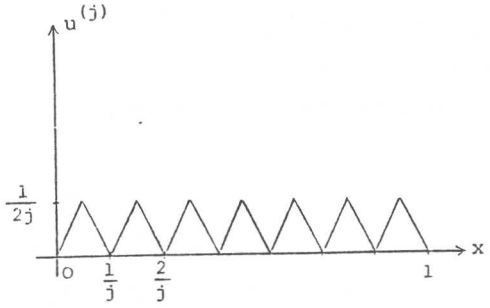

Figure 1

observed in a region containing a finely-twinned martensite/austenite interface (see Christian [2] and Figure 2) can be modelled by temporarily

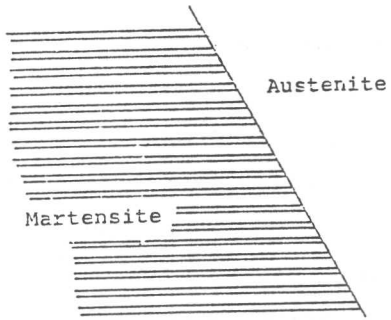

Figure 2

ignoring the phase-boundary energies and looking for minimizing sequences of a corresponding bulk elastic energy whose minimum is not in general attained.

§2. THE MODEL

In adopting an appropriate expression for the bulk elastic energy it is important to use nonlinear elasticity theory; indeed, for the rotations with respect to the austenite phase occurring in Figure 2 use of linear elasticity would predict grossly inaccurate stresses. Following Gibbs' [5] chapter on solids in contact with fluids we take for the bulk elastic energy the expression

$$I_\theta(\mathbf{y}) = \int_\Omega \Phi(\nabla \mathbf{y}(\mathbf{x}), \theta)\, d\mathbf{x}, \tag{2}$$

where $\mathbf{y}(\mathbf{x})$ denotes the deformed position of the particle occupying the position $\mathbf{x}$ in a reference configuration Ω, $\nabla \mathbf{y}(\mathbf{x})$ the gradient of $\mathbf{y}$ with respect to $\mathbf{x}$ and θ the temperature. The stored-energy function $\Phi = \Phi(\mathbf{F}, \theta)$ is assumed to be defined for 3×3 matrices $\mathbf{F}$ satisfying $\det \mathbf{F} > 0$, and satisfies for any crystal the frame-indifference condition

$$\Phi(\mathbf{RF}, \theta) = \Phi(\mathbf{F}, \theta) \quad \text{for all rotations } \mathbf{R}. \tag{3}$$

The Born analogy between molecular and continuum theory gives the condition

$$\Phi(\mathbf{F}\bar{\mathbf{R}}, \theta) = \Phi(\mathbf{F}, \theta) \text{ for all } \bar{\mathbf{R}} \in P^\nu, \tag{4}$$

where P^ν denotes a finite group of rotations of order ν. (Larger symmetry groups are considered by Ericksen [3]). In the case when the symmetry in the reference configuration is cubic, for example, $\nu = 24$ and P^ν is the group of rotations which map a cube into itself.

Let $\mathbf{U} = \sqrt{\mathbf{F}^T\mathbf{F}}$. Necessary and sufficient conditions for (3) and (4) to hold are then that

$$\Phi(\mathbf{F}, \theta) = \Phi(\mathbf{U}, \theta) = \Phi(\bar{\mathbf{R}}^T\mathbf{U}\bar{\mathbf{R}}, \theta) \text{ for all } \bar{\mathbf{R}} \in P^\nu. \tag{5}$$

To model a cubic-tetragonal transformation, for instance, we take for the reference configuration the undistorted cubic phase at the transformation temperature θ_0, and suppose that, as a function of the positive symmetric matrix $\mathbf{U}$, $\Phi(\mathbf{U}, \theta_0)$ has precisely the minimizers 1, corresponding to

austenite, and $\bar{R}^T U \bar{R}$, $\bar{R} \in P^\nu$, corresponding to the variants of martensite, where $U_0 = \mathrm{diag}(\eta_2, \eta_1, \eta_1)$ is the transformation strain. In fact there are only three such variants, namely U_0, $\mathrm{diag}(\eta_1, \eta_2, \eta_1)$ and $\mathrm{diag}(\eta_1, \eta_1, \eta_2)$. As θ passes through θ_0 these minimizers change so that the austenite has lower energy for $\theta > \theta_0$ and the martensite has lower energy for $\theta < \theta_0$.

§3. MAIN RESULTS

From now on we consider an unloaded crystal at temperature θ_0. An *interface* with normal n corresponds to deformation gradients F^+, F^- which have corresponding strains U^+, U^- that are minimizers of $\Phi(U, \theta_0)$ and are such that $F^+ - F^- = a \otimes n$ for some a. An analysis shows that there are no austenite/austenite or austenite/martensite interfaces, while (cf Ericksen [4], Gurtin [6]) the martensite/ martensite interfaces correspond to compound twins. A partial analysis of the minimizing sequences $y^{(j)}$ of $I_{\theta_0}(y)$ is given in Ball & James [1] together with a discussion of related mathematical issues. Such a minimizing sequence possesses a subsequence converging in an appropriate sense (that of *weak convergence*) to a configuration y that is typically *not* a minimizer of I_{θ_0}, just as for the example (1). The theory is related to the crystallographic theory of martensite by means of the following result, a more precise description of which is given in [1]. *Let* Ω *consist of two disjoint connected regions* Ω_M *and* Ω_A *separated by an interface* S *of arbitrary geometry. Then a minimizing sequence* $y^{(j)}$ *of* I_{θ_0} *exists with the properties that in* Ω_M $\nabla y^{(j)}$ *takes more and more closely the two values* F^+, F^- *corresponding to a given twin, while in* Ω_A $\nabla y^{(j)}$ *tends to* 1, *if and only if (i)* S *is part of a plane* $\{x \cdot m = \mathrm{const}\}$, $|m| = 1$, *and (ii)* $\lambda F^+ + (1-\lambda)F^- = 1 + b \otimes m$ *for some* $0 < \lambda < 1$ *and* b. The possible solutions for the normal m of the habit plane, the relative proportion λ of the twins, and the amplitude b are precisely those given by the crystallographic theory [7]. (Necessary and sufficient conditions for the existence of solutions are also presented in [1] for the case when the transformation strain U_0 is a general positive symmetric matrix.) The theory presented here has, however, the advantages that (a) it delivers both the twins and the habit plane simultaneously on the basis of an explicit energy calculation, (b) that it assumes less geometry, and (c) that it should be capable of predicting other microstructures even when part of the boundary of the crystal is acted on by loads which may vary from place to place or when the crystal is subjected to a temperature gradient. Note that for the case of an unloaded crystal at the transformation temperature θ_0 the minimum energy is in fact attained, e.g. by $y(x) = x$ (pure austenite), or by $y(x) = F^{\pm}x$ (pure martensite). However, in the presence of small temperature or concentration gradients, or of other inhomogeneities, we expect that the bulk energy would not in general attain a minimum, leading to minimizing sequences with finer and finer twinning as above. An example of this type is given in [1, section 7a].

Other topics discussed in [1] are the effect of surface energy on limiting fineness, fine wrinkling at the boundary of a body, and fractal triangular domain patterns similar to those observed for Dauphine twins in quartz. We believe that many such finely oscillating phase mixtures are associated with minimization problems which have minimizing sequences which do not converge to minimizers.

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