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TWINNING IN NONLINEARLY ELASTIC MONATOMIC CRYSTALS

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Abstract—Two-phase mixtures are admitted to the energy criterion of stability. This generality allows phase transitions to be interpreted as global instabilities, and so enables the prediction of the onset of these transitions. Stability is assessed in various loading environments, corresponding broadly to the well known hard and soft devices. The work is illustrated mainly by reference to deformation twinning.

1. INTRODUCTION

The natural occurrence of twinned crystals of quartz, phenomena such as the martensitic transformation of steel, and a recent paper of Ericksen[1] concerning the stability of nonlinearly elastic bars all suggest that it may be profitable to allow more than one phase in an equilibrium theory of the mechanics of crystals. That some such effects may be modelled by an elastic constitutive law is suggested by the remarkable fact that as a perfect crystal of calcite may be twinned by the pressure of a single knife edge into the appropriate lattice plane so may the twinned crystal be "untwinned" by the application of pressure to the same material plane.

A homogeneously deformed crystal is said to be composed of one phase. With each phase is associated an unique matrix of deformation gradients. Thus a two-phase mixture may be represented by two matrices of deformation gradients provided that these matrices are commensurate, in the sense that each transforms the (undeformed) common boundary of the phases in the same way. Displacements are required to be continuous, for we are unable to allow for the fracture of the material. So, piecewise constant strains are admitted to the energy criterion of stability. This generality allows phase transitions to be interpreted as global instabilities, and enables the prediction of the onset of these transitions. Briefly, the total energy per unit reference volume is required to be a strong minimum in any globally stable equilibrium configuration, this configuration being generally a mixture of various phases.

Loosely, a homogeneous (one-phase) configuration ceases to be strictly stable when the constitutive law ceases to be uniquely invertible. This is an inherently nonlinear effect. We assess the stability in loading environments which are such as to reduce the problem to a set of one-dimensional problems, each analogous to that one set and solved in [1].

The article begins with a review of the ideas of crystal symmetry, for symmetry is a key feature of instabilities such as twinning. Following Ericksen[2] and Parry[3], the symmetry transformations of the crystal are not required to be rotations. It is apparent that a given stress may then correspond to more than one strain, and that some kind of instability is likely.

Next, the stability criterion is precisely stated and the loading environments are prescribed. We do not suppose that it is possible to perform experiments where these loading conditions are exactly obtained, but we are content to observe that phase transitions of some description occur in each class of device. Two classes of global instability are defined, one arising from the crystal symmetry, the other not.

Finally, the twinning mode of instability is analysed. In this mode, one phase is the mirror image of the other in the common boundary, the mode is at least neutrally stable in some configurations of high symmetry. Generally, there is a profusion of possible twinning modes in any given state; it is an open problem to determine the operative modes in this situation. The selection criterion should presumably combine some energetic factor with the purely geometric criterion used in the crystallographic literature.

2. CRYSTAL SYMMETRY

Assume that the crystal possesses a strain energy function, w_k say, relative to some reference configuration k and relative to the referential axes of the matrix of deformation gradients, A say. The relation $w_k(A)$ is supposed objective, so that

$$w_k(A) = w_k(RA), \tag{2.1}$$

where R is any proper or improper orthogonal transformation.

All information about the symmetry of the crystal is contained in the isotropy group $\mathscr{G}^k$ relative to k. The elements G^k of $\mathscr{G}^k$ are unimodular (density-preserving) transformations of the reference configuration which leave the strain energy invariant. Thus

$$w_k(A) = w_k(AG^k). \tag{2.2}$$

Under a change of reference configuration, $k \to \bar{k}$ say, $\mathscr{G}^k$ maps into a conjugate group $\mathscr{G}^{\bar{k}}$ according to Noll's rule

$$G^{\bar{k}} = PG^kP^{-1} \tag{2.3}$$

where P maps k into $\bar{k}$. From (2.3), the components of one type of mixed tensor, representing the symmetry elements, are invariant with respect to change of reference configuration. Accordingly, it is sufficient to consider the symmetry of just one monatomic lattice. For the sake of simplicity, we consider only two dimensional problems and choose to investigate the simple square lattice.

Let w denote the strain energy relative to the simple square lattice as reference. Following Ericksen[2], w is assumed to depend only on the sites of the atoms in the lattice, and not on the identity of the occupants of the individual sites. Thus rearrangements of the lattice, which map these sites onto themselves, constitute symmetry transformations. Denote the group of these rearrangements by Γ. Then,

$$\Gamma = \{\gamma_{ij};\ \gamma_{ij} \text{ are integers, } \det(\gamma_{ij}) = \pm 1\}.$$

Γ is generated by three elements, viz.

$$F = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad G = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad H = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \tag{2.4}$$

so that any element of Γ is some product of the powers and inverses of F, G and H. F represents rotation through a right angle, G reflection in a coordinate plane and H simple shear parallel to one axis through one unit of lattice spacing.

The double covariance expressed by (2.1) and (2.2) means that w may be defined arbitrarily only over subsets of the space of deformation gradients, see Parry[3]. Specifically, let

$$A'A = \begin{pmatrix} x & z \\ z & y \end{pmatrix}, \tag{2.5}$$

where A' denotes the transpose of A, then w may be defined arbitrarily, e.g., only over the "least domain", denoted $\mathscr{D}$, given by

$$y \geq x \geq 2z \geq 0. \tag{2.6}$$

Once defined in $\mathscr{D}$, w is generated throughout the space of the Cauchy Green tensor via (2.2), and then throughout the space of the deformation gradients via (2.1). Thus, e.g. in simple shear, where

$$A = \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix},$$

one finds from (2.6) that w may be defined arbitrarily only over

$$\mathscr{D} = \{\lambda:\ 0 \leq \lambda \leq \tfrac{1}{2}\}.$$

3. THE STABILITY CRITERION

The stability of piecewise homogeneous configurations of the body is assessed with respect to perturbations which are themselves piecewise homogenoeus. Any internal boundaries of such configurations must be planar. Consequently, two-phase perturbations admitted to the stability criterion must be such that (in plane strain) there exists a nonzero vector **x** such that

$$A_1\mathbf{x} = A_2\mathbf{x}, \tag{3.1}$$

where A_1 and A_2 are the matrices of deformation gradients in the two phases, the common boundary of the two phases being parallel to **x**. From (3.1), one phase must be related to the other via a shear parallel to **x** and a compression (or extension) perpendicular to **x**. We shall say that strains corresponding to deformation gradients related via (3.1) are commensurable.

Let $\mathscr{E}_k$ be the total energy per unit reference volume of the body in any configuration k with continuous displacements and piecewise constant gradients. The configuration k is then called stable, neutrally stable or unstable with respect to the perturbation to $\bar{k}$ according as $(\mathscr{E}_{\bar{k}} - \mathscr{E}_k)$ is positive, zero or negative. This is the energy criterion. Thus a configuration is judged at least neutrally stable to all disturbances if and only if the total energy per unit reference volume is a strong global minimum.

We catalogue various loading devices. Firstly, imagine a soft dead loading device where the nominal stress is constrained to be constant, N^0 say, throughout the body and throughout the virtual strain. Then the total energy per unit volume is

$$\mathscr{E}_k = \frac{1}{V}\int \{w(A) - tr\, N^\circ A\}\, \mathrm{d}V, \tag{3.2}$$

where the integration extends over the reference configuration of the body (of volume V).

Secondly, consider a related hard dead loading device where some linear combination of the overall deformation gradients per unit reference volume remains constant. Thus

$$tr \frac{1}{V} P \int A\, \mathrm{d}V = k \tag{3.3}$$

where P is a constant matrix, and k a constant scalar. As is customary, assume that the forces of constraint do no work in perturbations satisfying the constraints. Then

$$\mathscr{E}_k = \frac{1}{V}\int w(A)\, \mathrm{d}V. \tag{3.4}$$

Evidently, (3.3) may be satisfied by the application of the appropriate surface displacements.

Finally, imagine a generalized soft device wherein the body is *homogeneously* deformed so that a given conjugate stress (in the sense of Hill (4)) remains constant, T° say. Let the corresponding strain measure be denoted by E. Then

$$\mathscr{E}_k = \frac{1}{V}\int \{w(E) - trT^\circ E\}\, \mathrm{d}V. \tag{3.5}$$

Notice that the related generalized hard device, where

$$\frac{1}{V} tr P \int E\, \mathrm{d}V$$

is constrained to be constant, may not generally be controlled by surface displacements. Therefore we pursue it no further.

For either dead loading device, a necessary condition that the phase corresponding to A be globally stable is that

$$w(\bar{A}) - w(A) - trN^\circ(\bar{A} - A) > 0, \tag{3.6}$$

for all $\bar{A}$, where N° is the given nominal stress in the soft device, and where

$$N^\circ = \mu P, \tag{3.7}$$

where μ is an unknown Lagrange multiplier, in the hard device. Conversely, by integration, (3.6) is sufficient for strict stability with respect to all admissible perturbations. Notice that (3.6) fails if the perturbation is a superposed infinitesimal rigid rotation.

The theory, it turns out, will determine only the *concentrations* of phases so that, at best, one expects only neutral stability, for different configurations may correspond to the same concentrations of the same phases. Therefore, in what follows, we seek equilibrium states which are *at least neutrally stable*, this being best possible.

Suppose that the linear path form A to $\bar{A}$ is in the domain of w. Let

$$A(s) = A + s[\bar{A} - A], \qquad s \in [0, 1]. \tag{3.8}$$

Then (3.6) may be rewritten as

$$Q = \int_0^1 F(s)\,\mathrm{d}s - F(0) > 0, \tag{3.9}$$

where

$$F(s) = tr\left\{\frac{\partial w}{\partial A(s)}(\bar{A} - A)\right\} \tag{3.10}$$

is the directional derivative of w along the specified linear path.

4. THE FORM OF THE STRAIN ENERGY FUNCTION

We shall specify a particular form of strain energy function. This implies that we cannot lay down the class of disturbances for which (3.6) is valid, but can only assess the stability of a particular configuration of the material. One cannot expect (3.6) to be valid for all disturbances. An "observable" configuration will be stable to infinitesimal perturbations and also, generally, to some larger set of finite perturbations, this larger set being determined once the strain energy function is prescribed.

In assessing the stability of phase mixtures, we shall allow only configurations such that there is no discontinuity of traction across any internal boundary. The condition may be satisfied by admitting only phases, A and $\bar{A}$, corresponding to the same nominal stress, N say. Thus

$$N(A) = N(\bar{A}) = N^\circ. \tag{4.1}$$

Suppose, following Ericksen[1], that F is not monotonic, but assumes the form shown below.

The functional Q measures the difference of the two areas shaded in Fig. 1.

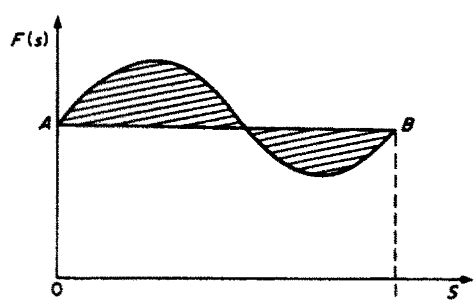

Fig. 1.

Imagine that the material may be held at a point (in the space of A) which is at least neutrally stable in either dead loading device. Consider, first of all, the soft dead loading device and, suppose that the constitutive law $N(A)$ is uniquely invertible at the value N°. Then there is only one solution to the problem of equilibrium. Suppose, now, that the $N(A)$ relation is such that there are two, and only two, phases A and $\bar{A}$ such that

$$N(A) = N(\bar{A}) = N^\circ, \tag{4.1 bis}$$

and such that the material is at least neutrally stable to some set of perturbations (including all infinitesimal perturbations) at both points, A and $\bar{A}$. Then either the point A or the point $\bar{A}$ is at least neutrally stable with respect to the other considered as a perturbation, depending on the sign of Q. Also, either A or $\bar{A}$ is at least neutrally stable with respect to all perturbations on the linear path which includes A and $\bar{A}$ (provided that F is not monotonic only in the interval $[0, 1]$), see Ericksen[1], and so, by continuity, at least neutrally stable with respect to some set of finite perturbations not necessarily on that path. With the assumption that Q varies smoothly as the material is constrained to move along some deformation path, it follows that the material should "snap", discontinuously, into another configuration, or phase, as Q changes sign, provided that there is sufficient energy to effect the perturbation. As remarked by Ericksen, when there is not sufficient energy some form of hysteresis is exhibited. For isotropic solids, Ogden[5] has shown that there are at least four distinct branches of the inversion $A(N)$. Some such transition as that indicated above is then to be expected, but we postpone a detailed consideration to a later work. Similar remarks apply to the generalized soft loading device.

Secondly, the hard dead loading device is such that N is constrained to be parallel to P, see (3.7). The one dimensional theory of Ericksen is readily generalized. Thus μ is chosen to minimise the total energy per unit reference volume, and it is found that in the range

$$trPA \leq k \leq trP\bar{A}, \tag{4.2}$$

where A and $\bar{A}$ are such that $Q = 0$, a phase mixture exists and is at least neutrally stable with respect to all perturbations on the specified linear path. The phase mixture will then also be at least neutrally stable with respect to some set of finite perturbations not necessarily on that path. The concentrations of the phases are determined from (3.3). There is an at least neutrally stable homogeneous configuration of the material outside the range given by (4.2).

It is tacit that the strain energy function is such that the branches of the inversion $A(N)$ (along the path $N = \mu P$) are commensurable, in the sense that the points A and $\bar{A}$ such that

$$N(A) = N(\bar{A}) = \mu P, \tag{4.3}$$

are commensurable. This may be regarded as a rather weak constitutive requirement, or perhaps as a selection criterion.

The instabilities may be categorized. Suppose that A and $\bar{A}$ are such that $Q = 0$. Then if A and $\bar{A}$ correspond to rearrangements of the lattice, so that

$$\bar{A} = RAG, \tag{4.4}$$

where $RR' = I$ and $G \in \Gamma$, we shall say that the instability is induced by symmetry. For example, in assessing the stability of a stress-free state, (4.1) reduces to

$$w(A) - w(\bar{A}) > 0. \tag{4.5}$$

This inequality is violated by any rearrangement of the lattice. A combination of phases is to be expected in any continuing deformation of the crystal. Generally, when (4.9) does not hold, the instability depends on the details of w in $\mathcal{D}$.

5. TWINNING

Twinning is a symmetry induced instability.

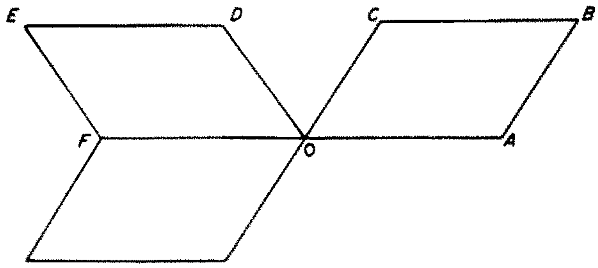

Fig. 2.

Let *OABC* be a cell which generates the deformed lattice. Then the twinned lattice is generated by *ODEF*, which is the mirror image, in the invariant line *FOA*, of a cell congruent to *OABC*. A simple shear parallel to *FOA* carries the sites of the original lattice points into the sites of the twin. The strain energies of the crystal and its twin are identical, for the twin is just the "left-handed" version of the crystal, as may be verified by Noll's rule.

Refer the deformation gradient to axes parallel and perpendicular to the invariant line. Then the crystal is neutrally stable to the twinning mode in dead loading provided that

$$tr N^{\circ}(A - \bar{A}) = 0, \tag{5.1}$$

where

$$A = \begin{pmatrix} 1 & \mu \\ 0 & \nu \end{pmatrix}, \quad \bar{A} = \begin{pmatrix} 1 & -\mu \\ 0 & \nu \end{pmatrix} \text{ say.}$$

Notice that

$$\bar{A} = RAG \tag{5.2}$$

where

$$R = G = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{5.3}$$

Let n^0_{ij} be the components of N°, then (5.1) reads

$$n^0_{21} = 0. \tag{5.4}$$

This relation ensures that the energy of the loading device is the same in both phases. We have also to ensure that the equilibrium equations are satisfied throughout the material. Therefore we require that

$$N(A) = N(\bar{A}) = N^{\circ}, \tag{4.1 bis}$$

or, in terms of the Cauchy stress, denoted $\Sigma(A)$,

$$A^{-1} \sum(A) = \bar{A}^{-1} \sum(\bar{A}) \tag{5.5}$$

Note that, from (5.5),

$$\sum(A)(A^{-1\prime}\nu) = \sum(\bar{A})(\bar{A}^{-1\prime}\nu) \tag{5.6}$$

where ν is an arbitrary vector. Choosing ν to be the normal to the phase boundary in the undeformed configuration, eqn (5.6) expresses the continuity of traction across that boundary.

The Cauchy stresses in the two phases are related via

$$\sum(\bar{A}) = R\sum(A)R', \tag{5.7}$$

by objectivity. Substituting in eqn (5.5), one finds

$$A^{-1}\sum(A) = RA^{-1}\sum(A)R', \tag{5.8}$$

and it follows that

$$\sigma_{12} = \sigma_{22} = 0, \tag{5.9}$$

where the components of $\Sigma(A)$ are denoted σ_{ij}. Equations (5.9) are sufficient that (5.4) hold. From (5.9), *twinning may occur if and only if the traction on the invariant line is zero.*

These calculations will be found most useful in a phenomenological theory of crystal behaviour. One envisages the construction of a hypothetical strain energy function, possibly using Ref. [3], and then, at any given strain, the calculation of the domain of stability (that is, the calculation of those $\bar{A}$ such that eqn (3.6) holds). If this domain is large enough, then the theory will allow phase transitions, and twinning, in particular. Notice that, in twinning, $\bar{A} - A$ may be arbitrarily small, so that this assumption is not too restrictive. Phase transitions are readily observed in practice, so that their prediction provides a convenient test of the suitability of a strain energy function.

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