Finite Deformation by Mechanical Twinning

RICHARD D. JAMES

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1. The phenomenon of twinning

The application of force to solid bodies often gives rise to pairs of homogeneously deformed regions, each pair separated by a common plane. Sometimes adjoining *homogeneous bands* of this kind are called *twins*, sometimes not. As is common in the interpretation of experiment, the phenomenon observed, in this case twinning, does not always lead to an exact, well-defined concept in mathematical theory. Quartz, for example, occurs in four kinds of twinned configurations [1]; two of these are of the kind described above and two are *interpenetrating twins*. The two individuals of an interpenetrating twin are not simply separated by a plane, but rather by an irregular surface or a collection of planes joined along edges.

I shall be concerned throughout this paper only with so-called *mechanical twins* – those produced by the application of stress. *Annealing* or *growth twins* are formed during the growth of a crystal. The theory of growth twinning must necessarily account for the processes of nucleation and diffusion, and therefore must be rather different from the theory of mechanical twinning.

Crystals suffer large deformation by gliding and twinning [2]. During gliding, adjacent planes of atoms slide past one another aided by the movement of dislocations. On the contrary, it is generally agreed that mechanical twins are produced by continuous deformation.

The most elementary view of the twinning operation begins with a simple monatomic lattice filling all of space divided by a plane of atoms called the *plane of composition*. The atoms in one half-space remain fixed while those in the other half-space undergo a simple shear parallel to the twin plane, the amount of shear determined by the condition that the lattice in one half-space be a reflection, or a 180° rotation, of the lattice in the other, but that the two lattices not be related by a rigid translation. This elementary concept of a twin has been extended to a wide class of crystal lattices by EVANS [3], who has studied the pure geometry of twinned crystals. EVANS' definition excludes the curious Dauphiné twin of quartz, studied by THOMAS & WOOSTER [4] and more recently by McLELLAN [5]. The Dauphiné twin of quartz is an interpenetrating twin in which the two individuals are separated by irregular surfaces. The elementary view of twinning fails in another way for the Dauphiné twin; the two individuals are not related by a simple shear. In fact, the overall deformation needed to deform one individual into its twin is of the order of molecular distances. On the molecular scale the twinning transformation is accomplished by rotation of the tetrahedron of oxygen atoms which surrounds each silicon atom through an angle of 38°; this amount of rotation of the tetrahedra is just enough to cause one individual of the twin to be identical to a 180° rotation of the other individual. From the descriptions of BRAGG & CLARINGBULL and of THOMAS & WOOSTER the transformation can be easily understood. The Dauphiné twin of quartz illustrates the fact that whereas the macroscopic deformation is continuous across the surface of composition, other fields, in particular those which reflect the internal rearrangement of atoms relative to the skeletal lattice, may well be discontinuous. It is clear that a constitutive theory for quartz must take account of these additional fields in some way.[1]

Material scientists [*e.g.* 6] call the deformation of the skeletal lattice, or 'superlattice', a *lattice-distortive displacement*, and the deformation relative to the skeletal lattice a *shuffle displacement*. PARRY [7] terms these *configurational transitions* and *structural transitions*, respectively.

I have mentioned the Dauphiné twin of quartz simply because it illustrates plainly the diversity of the concept of twinning. My interest in the phenomenon of twinning arose rather from its importance to the explanation of the shape-memory effect. The shape-memory alloys, the most important being the nearly equiatomic alloy of nickel and titanium called nitinol, have the curious property of returning to their original shape after having been apparently permanently deformed at room temperature and then heated. Although the precise mechanism for the shape memory effect is still being debated, it is generally agreed [8] that twins are present in the subcritical martensitic phase; when the material is deformed, new twins are created and planes of composition of existing twins propagate normal to themselves so as to be compatible with the gross change of shape. Upon heating, the planes of composition move back to their original positions

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[1] The phenomenon of the co-existence and growth of Dauphiné twins under applied stress is termed *piezocrescence* by THOMAS & WOOSTER. They advance a linearized theory for the phenomenon based upon the energy criterion for stability. The theory is apparently due to RIVLIN.

causing a return to the original shape. It is appealing to view the phenomenon as a problem of the exchange of stability between twinned and untwinned configurations.

WANG [9] offers a detailed explanation of how the twins may occur in the crystal lattice of nitinol. Some twins he shows involve co-operative shear; atoms move parallel to the plane of composition, all in the same direction, by an amount which increases as their distance from the plane of composition, simple shear being a special case. Others, apparently not so important for the shape memory effect, involve unco-operative shear reminiscent of the Dauphiné twinning of quartz; adjacent planes of atoms shear parallel to the plane of composition by small amounts in opposite directions, so as to cause no overall deformation. Still others constitute trilling, the separation of three regions by three half planes which share a common edge so that each pair of adjacent regions is a twin.

Even more complicated arrangements of twins are commonly seen in deformation-induced martensite[2].

A theory for the kinematics of martensitic transformations has been proposed by BOWLES & MACKENZIE [11]. It is generally agreed[3] that martensitic transformations are lattice-distortive, unlike Dauphiné twinning.

Aside from the recent work of PARRY [12] and the forthcoming work by ERICKSEN [13] and PITTERI [14], I have uncovered only two theories of mechanical twinning which treat something more than kinematics. The first is a theory based upon linear elasticity given by VLADIMIRSKII [15]. Not surprizingly, the linear theory is totally inadequate as shown by HALL [16, p. 109]; according to it the traction required to form a twin in cadmium disagrees with the experimental value by a factor of about 5000. Nevertheless, some of VLADIMIRSKII'S conclusions can be supported by the theory I present. The generalization of VLADIMIRSKII'S theory by LIFSHITS [17] partly removes the assumption of a linearly elastic constitutive relation. The second is the theory of THOMAS & WOOSTER for Dauphiné twinning. Their theory turns out to be consistent with my definition of a twin in the context of TOUPIN'S theory of the elastic dielectric, after the proper linearization.

I propose to study the kinematics, equilibrium and stability of mechanical twins, and collections of mechanical twins, in the framework of continuum mechanics. A precise definition of a twin is laid down which generalizes, and in some cases corrects, the definitions used informally in the literature. I find it more efficient to eschew the details of molecular theory, and to frame the definition around a constitutive theory general enough to include the successful phenomenological theories of crystalline materials of which I am aware. To promote confidence in the definition, I study its implications for two special theories, finite elasticity and the theory of the elastic dielectric. The definition of a twin leads directly to the kinematical problem posed in § 2. I find that collections of twins cannot be put together in an arbitrary way. It is found by a systematic procedure that the simplest arrangement of deformations which is kinematically possible has the kinematic properties of a mechanical twin; the next simplest has the

[2] *Cf.* [6, 10].
[3] *Loc. cit.*

kinematic properties of a mechanical trilling. The simplest arrangement which does not have an axis we term a *tetrad.* I study a tetrad in detail because of its possible importance to the formation of martensite.

For the remainder of the paper I specialize the definition of a twin to piecewise homogeneous deformations in finite elasticity. The equilibrium equations in that case reduce to algebraic equations about which much can be said. In § 4b, I study the stability of twinned deformations under dead loading, and compare and contrast ordinary piecewise homogeneous deformations with those piecewise homogeneous deformations which are also twins. The existence and qualitative properties of a stable twin depend significantly upon the class of competitors allowed in the definition of stability. The status of a theorem of PARRY [12], which states that the traction on a twin boundary must vanish, is investigated.

The work clarifies the theories of VLADIMIRSKII and THOMAS & WOOSTER.

2. The definition of a twin

To formulate a continuum definition for mechanical twinning, I must adopt constitutive relations to describe the material. Let $\mathscr{R}$ be the reference shape of a body $\mathscr{B}$. A **deformation** of $\mathscr{R}$ is an invertible function

$$\chi : \mathscr{R} \to \chi(\mathscr{R}) \tag{2.1}$$

which maps the reference shape $\mathscr{R}$ onto the present shape $\chi(\mathscr{R})$. I shall assume that the reference shape $\mathscr{R}$ is fixed throughout this paper. The deformation describes the overall distortion of $\mathscr{B}$, that is, the distortion of the skeletal lattice or superlattice which determines the observed change of shape of $\mathscr{B}$. If χ is differentiable at $X \in \mathscr{R}$, we call

$$F = \nabla\chi(X) \tag{2.2}$$

the **deformation gradient** at X. I shall assume throughout this work, in addition to the invertibility of χ, that $\det F > 0$ is always met by the deformation gradient.

The response of some crystalline bodies is thought to be influenced by more than simply the deformation gradient. With the overall deformation fixed, there may occur movement of atoms relative to the skeletal lattice which affect the behavior of the material, *e.g.* the structural transitions or shuffles mentioned in § 1. Dauphiné twinning is one example. To describe the effects of these shuffles, it is traditional to use a set of **polarization vectors**,

$$p_1, \ldots, p_n, \tag{2.3}$$

each one viewed as a field dependent upon $X \in \mathscr{R}$.

I shall assume that the material is governed by a stored energy function of the form

$$\psi(F, p_1, \ldots, p_n). \tag{2.4}$$

I assume $\psi(\cdot, \cdot, \ldots, \cdot)$ is defined on a domain $\mathscr{D}$. For the definition of a twin we need not lay down any assumptions of smoothness for ψ, but for the interpretation of the theory we have in mind that the reference shape is untwinned.

The function ψ will be an invariant function under the groups $\mathscr{o}^+$ and $\mathscr{g}$ which embody the concepts of Galilean invariance and material symmetry. Since the action of elements of these groups upon ψ is different for different theories, I shall represent them abstractly. Let $\mathfrak{T}$ represent a Galilean transformation

$$(\bar{F}, \bar{p}_1, \ldots, \bar{p}_n) = \mathfrak{T}(F, p_1, \ldots, p_n), \quad \mathfrak{T} \in \mathscr{o}^+, \tag{2.5}$$

$\mathscr{o}^+$ being the proper orthogonal group. Assume $1 \in \mathscr{o}^+$ is the identity transformation. Let $\mathfrak{F}$ denote a transformation belonging to the **symmetry group** of $\mathscr{B}$ relative to the reference shape $\mathscr{R}$:

$$(\hat{F}, \hat{p}_1, \ldots, \hat{p}_n) = \mathfrak{F}(F, p_1, \ldots, p_n), \quad \mathfrak{F} \in \mathscr{g}. \tag{2.6}$$

We assume that[4]

$$\mathfrak{T}\mathfrak{F} = \mathfrak{F}\mathfrak{T}, \quad \forall \mathfrak{T} \in \mathscr{o}^+, \quad \forall \mathfrak{F} \in \mathscr{g}. \tag{2.7}$$

If ψ is independent of the vectors $p_1, \ldots, p_n$, the material is elastic; if thermoelastic, $n = 1$, and p is one dimensional and represents the entropy or temperature. The description (2.4) covers TOUPIN'S theory of the elastic dielectric [18] and ERICKSEN'S theory of diatomic crystals [19] with $n = 1$ and p interpreted as a polarization vector.

Since $\mathscr{g}$ and $\mathscr{o}^+$ are invariance groups for ψ we have, for each $\mathfrak{T} \in \mathscr{o}^+$ and each $\mathfrak{F} \in \mathscr{g}$,

$$(F, p_1, \ldots, p_n) \in \mathscr{D} \Leftrightarrow \mathfrak{T}\mathfrak{F}(F, p_1, \ldots, p_n) \in \mathscr{D}, \tag{2.8}$$

and

$$\psi(F, p_1, \ldots, p_n) = \psi(\mathfrak{T}\mathfrak{F}(F, p_1, \ldots, p_n)). \tag{2.9}$$

The elementary view of twinning begins with a lattice filling all of space divided by a plane of composition. On one side of this plane the lattice remains fixed, while on the other side the lattice undergoes a simple shear parallel to the plane of composition. As I have mentioned in § 1, this view is too simple to serve as the basis of a general definition of mechanical twinning. First, the two individuals need not be separated by a plane, but only by a *surface of composition*. The elementary view, however, does suggest that the surface be smooth, at least that the surface have a unique tangent plane at each point.[5] The two individuals need not be homogeneously deformed, as demanded by the elementary view. In continuum theory we simply focus upon the limiting values of the important functions χ $\nabla\chi$ and p_k as the surface of composition is approached from either side. All examples that I have encountered suggest that χ is continuous across the twin

[4] This assumption is consistent with all theories governed by stored energies of the form (2.4) of which I am aware.

[5] BASINSKI & CHRISTIAN [20] discuss a model for the tapering of twin boundaries in indium-thallium alloys which indicates that the twin boundary, viewed macroscopically, may not be smooth, but this example is isolated, and their explanation of the tapering may not be the only one possible. In fact, this tapering could be caused by inhomogeneous deformation, which seems not to have been considered.

boundary while F and p_k may have jump discontinuities. The limiting values $(F^+, p_1^+, \ldots, p_n^+)$ and $(F^-, p_1^-, \ldots, p_n^-)$ are not arbitrary. They must be consistent with the basic requirement that there is a reflection or a 180° rotation which, when applied to a small part of the body lying on one side and very near to the surface of composition, yields a part which is indistinguishable from a part of the body lying just on the other side of this surface. By 'very near to the surface of composition' we shall mean that the condition applies to the limiting values of F and $p_1, \ldots, p_n$ on each side. The word 'indistinguishable' shall be given its conventional meaning in continuum mechanics: the response of each part to any *subsequent* deformation shall be the same.

Materials scientists abundantly agree that, unlike a grain boundary, a surface of composition of a twin contains few, if any, molecules which are severely misplaced relative to the lattice on either side of the surface. It is said that a surface of composition of a twin is one of low energy. I shall take this to mean that a superficial free energy need not be assigned to this surface, that the constitutive description (2.4) suffices.

These remarks, when formalized, lead to the

Definition (*mechanical twin*). *Let the body* $\mathcal{B}$ *have a free energy function* $\psi(F, p_1, \ldots, p_n)$ *defined relative to a reference shape* $\mathcal{R}$. *Let a part* $\mathcal{P} \subset \mathcal{R}$ *undergo a deformation* $\chi(X), X \in \mathcal{P}$, *and be subject to a field of polarization* $p_1(X), \ldots, p_n(X)$, $X \in \mathcal{P}$. *The part* $\mathcal{P}$ *contains a twin if the following are true.*

(i) $\mathcal{P}$ *is diffeomorphic*[6] *to a sphere bisected by a plane passing through its center. Let the image of this plane under the diffeomorphism be the surface* $\mathcal{S} \subset \mathcal{P}$.

(ii) χ *is continuous on* $\mathcal{P}$. $F = \nabla \chi$ *and* $p_1, \ldots, p_n$ *have limiting values* $(F^+, p_1^+, \ldots, p_n^+)$ *and* $(F^-, p_1^-, \ldots, p_n^-)$ *as* $\mathcal{S}$ *is approached from either side.*

(iii) *There is a symmetry transformation* $\mathfrak{F} \in g$ *and a Galilean transformation* $\mathfrak{T} \in o^{+}$[7] *such that at each point of* $\mathcal{S}$,

$$(F^+, p_1^+, \ldots, p_n^+) = \mathfrak{T}\mathfrak{F}(F^-, p_1^-, \ldots, p_n^-). \tag{2.10}$$

(iv) $\mathfrak{T}^2 = 1$ *but* $\mathfrak{T} \neq 1$[8].

The surface $\mathcal{S}$ of this definition is called the **surface of composition.**

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[6] A diffeomorphism is an invertible continuously differentiable map with a continuously differentiable inverse. Thus, according to (i) there is a diffeomorphism $\mu : S \to \mathcal{P}$, S being a sphere bisected by a plane $\mathcal{P}_N$ passing through its center, such that $\mathcal{S} = \mu(\mathcal{P}_N)$.

[7] In special cases the free energy may be invariant under the full orthogonal group $\mathcal{O}$ if its domain is properly extended, even though the concept of Galilean invariance applies only to proper transformations. Finite elasticity theory is one example. In these special cases we may replace $\mathcal{O}^+$ by $\mathcal{O}$, but not in general.

[8] The definition may include certain specious twins like those discussed in Remark 5 in the special case of finite elasticity. I do not know how to exclude them in the general case. Dr. MARIO PITTERI has informed me that he has solved this problem for a broad class of crystal lattices from the point of view of molecular theory.

Remarks and Examples.

1. According to a theorem of MAXWELL, the condition (ii) of the definition implies the existence of an **amplitude** $\boldsymbol{a}$ such that at each point of $\mathscr{S}$,

$$\boldsymbol{F}^{+} = \boldsymbol{F}^{-} + \boldsymbol{a} \otimes \boldsymbol{N}, \tag{2.11}$$

$\boldsymbol{N}$ being the unit normal to $\mathscr{S}$. To be definite I shall always assume $\boldsymbol{N}$ points into $\mathscr{P}^{+}$.

This part of the definition shows plainly that the definition does not apply to growth twinning.

2. Let the connected part $\mathscr{P} = \mathscr{P}^{-} \cup \mathscr{P}^{+}$, $\mathscr{S} = \overline{\mathscr{P}^{-}} \cap \overline{\mathscr{P}^{+}}$, $\mathscr{S}$ being a smooth surface. Suppose $\nabla \chi = \boldsymbol{F}^{+}$ is constant on $\mathscr{P}^{+}$ and $\nabla \chi = \boldsymbol{F}^{-}$ is constant on $\mathscr{P}^{-}$. Then the deformation χ is **pairwise homogeneous**.

A short argument based upon (2.11) shows that *if χ is pairwise homogeneous, then $\mathscr{S}$ is a plane.* Part of the purpose of this work is to distinguish ordinary pairwise homogeneous deformations from the special ones which are mechanical twins.

Piecewise homogeneous deformations are defined analogously.

3. The condition (iv) is abstracted from many different observations of twins in nature, and must be included in the definition of a twin. On the other hand, many of the conclusions I shall draw would still be true if $\mathfrak{T}^2 \neq 1$ as long as $\mathfrak{T} \in \mathscr{o}^{+}$. I have found no examples of this kind in nature although my observations have been confined to crystalline minerals and metals. Apparently twins are observed in polyethylene, and perhaps it is in polymers that the more general possibility is realized.

4. The definition of a mechanical twin can be extended to the case of mechanical trilling. A trilling consists of a part $\mathscr{P} \subset \mathscr{R}$ diffeomorphic (see footnote 8) to a sphere trisected by three distinct half planes all of whose edges coincide with a line containing a diameter of the sphere, and a continuous deformation $\chi : \mathscr{P} \to \chi(\mathscr{P})$ such that each pair of adjoining regions is a twin. Thus for a trilling $\mathscr{P}$ is trisected into three regions $\mathscr{P}_1$, $\mathscr{P}_2$, $\mathscr{P}_3$ by three surfaces $\mathscr{S}_1$, $\mathscr{S}_2$, $\mathscr{S}_3$ which meet along a curve. This curve is called the *axis* of the **trilling**.

In § 3 I shall study the next least complex configurations, after twinning and trilling, which can arise from a continuous deformation.

5. (Finite elasticity.) If the body is elastic and homogeneous, the stored energy function is independent of $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n$:

$$\psi(\boldsymbol{F}, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_n) = W(\boldsymbol{F}), \quad \boldsymbol{F} \in \mathscr{D}. \tag{2.12}$$

The groups $\mathscr{g}$ and $\mathscr{o}^{+}$ are represented by groups of second order tensors $\mathscr{G}$ and second order proper orthogonal tensors $\mathscr{O}^{+}$, respectively, according to the rules

$$\begin{aligned} \mathfrak{T}(\boldsymbol{F}) &= \boldsymbol{Q}\boldsymbol{F}, \quad \boldsymbol{Q} \in \mathscr{O}^{+}, \\ \mathfrak{F}(\boldsymbol{F}) &= \boldsymbol{F}\boldsymbol{H}, \quad \boldsymbol{H} \in \mathscr{G}; \end{aligned} \tag{2.13}$$

thus the stored energy function and its domain satisfy

$$\begin{aligned} &F \in \mathscr{D} \Leftrightarrow QFH \in \mathscr{D}, \\ &W(F) = W(QFH) \quad \forall Q \in \mathcal{O}^+, \quad \forall H \in \mathscr{G}, \quad \forall F \in \mathscr{D}. \end{aligned} \tag{2.14}$$

I shall assume that $\mathscr{G}$ is contained in the group of second order unimodular tensors: $\mathscr{G} \subset \mathscr{U}$. If this assumption is not adopted, one can cause the volume of the deformed shape of $\mathscr{B}$ to become arbitrarily large or arbitrarily small, by the use of repeated symmetry transformations, while leaving the total stored energy of $\mathscr{B}$ unchanged. For crystalline bodies the group $\mathscr{G}$ generally neither contains, nor is contained within, the group $\mathcal{O}^+$ although $\mathscr{G}$ may contain some orthogonal tensors.

If a twin is contained in the elastic body $\mathscr{B}$, the limiting values F^+ and F^- of the deformation gradient must satisfy

$$\begin{gathered} F^+ = F^- + a \otimes N = QF^-H, \\ \text{for some } Q \in \mathcal{O}^+,\ Q \neq 1, \text{ and some } H \in \mathscr{G}, \end{gathered} \tag{2.15}$$

according to the definition of a twin. In finite elasticity theory certain specious twins may occur. Suppose F^+ and F^-, in addition to satisfying (2.15), also fulfill the condition $F^+ = F^-M$ for some $M \in \mathscr{G}$. Then the response of one side of the surface of composition to any deformation is the same as the response of the other side to the same deformation; in this sense no static experiment can detect the presence of the twin boundary. We shall call such twins *false twins*. A *true twin* in finite elasticity shall satisfy (2.15) as well as the condition

$$F^+ \neq F^-M \text{ for any } M \in \mathscr{G}. \tag{2.16}$$

If an elastic body $\mathscr{B}$ with symmetry group $\mathscr{G}$ relative to a fixed reference shape $\mathscr{R}$ supports a true twin, the requirement (2.16) shows that it does not generally follow that an elastic body $\mathscr{B}'$ with symmetry group $\mathscr{G}' \subset \mathscr{G}$ relative to the same reference shape supports a true twin. This statement can be easily visualized by the use of a molecular model; certain twins produced in a tetragonal lattice will disappear if the lattice parameters are changed slightly so as to make the lattice cubic.

The condition (2.15) and the assumption $\mathscr{G} \subset \mathscr{U}$ have an elementary consequence; since $H \in \mathscr{U}$ and $F^+ = QHF^-$, then $\det F^+ = \det F^-$. But, also from (2.16), we have

$$\begin{aligned} \det F^+ &= \det (F^- + a \otimes N) \\ &= (\det F^-)(\det (1 + (F^-)^{-1} a \otimes N)) \\ &= (\det F^-)(1 + (F^-)^{-1} a \cdot N). \end{aligned} \tag{2.17}$$

Therefore, since $\det F^- > 0$, we have

$$((F^-)^{-1} a) \cdot N = 0. \tag{2.18}$$

If the (—) side of the surface of composition of the twin is held fixed, $F^- = 1$; then $a \cdot N = 0$. If, in addition, the surface of composition is a plane and the amplitude is constant, then we recover a result commonly adopted without proof in textbooks on crystallography or metallurgy – the deformation on $\mathscr{P}^+$ is a simple shear (*cf.* [21]).

We conclude this subsection with some results we shall need later. The tensor

$$T \equiv W_F \tag{2.19}$$

is the Piola stress. If N is the unit normal of a surface $\mathscr{S}$ in the reference shape, TN is the force per unit area of $\mathscr{S}$ which acts on the deformed shape of $\mathscr{S}$.

6. (Elastic dielectric.) The definition of a twin is framed within a theory of finite deformation and polarization. One of the best known and most successful of these theories, and one which involves a nontrivial dependence upon the polarization, is TOUPIN's theory of the elastic dielectric [11, 14]. I shall not attempt to construct a complete theory for twinning in an elastic dielectric, mainly because I am not aware of any comprehensive theory for the material symmetry of an elastic dielectric.[9] Actually, I think that many dielectric bodies may be described well by TOUPIN's theory, but that the symmetry group will operate upon the local deformation and polarization in rather different ways for different classes of materials. For this reason I shall treat a simple example which has clearly defined symmetry operations.

THOMAS & WOOSTER [4] describe a phenomenon occurring in quartz crystals. Untwinned crystals of quartz are piezoelectric; if equal and opposite forces are applied normal to the parallel lateral faces of a quartz crystal, a potential difference is created between the faces. If the crystal contains a Dauphiné twin, the effect is eliminated and no such potential difference is found to occur[10]. I seek an elementary explanation of the phenomenon, so as to illustrate the definition of a twin in a theory where the dependence upon polarization is nontrivial.

Let us assume that quartz is described by a stored energy function of the form

$$\Sigma(F, \pi), \tag{2.20}$$

F being the deformation gradient and π being the polarization per unit mass. Let a slab

$$\mathscr{R} = \{X \mid 0 \leqq X \cdot N \leqq A\} \tag{2.21}$$

of density $\varrho_{\mathscr{R}}$ be deformed by a homogeneous deformation $\chi = \hat{F}X$, $\hat{F} =$ constant, and subject to a homogeneous field of polarization $\hat{\pi} =$ constant $\neq 0$. Assume the polarization vanishes outside the slab. The deformed shape of the slab is

$$\chi(\mathscr{R}) = \{x \mid 0 \leqq x \cdot \hat{n} \leqq \hat{a}\}, \tag{2.22}$$

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[9] TOUPIN discussed the matter in [18, § 13].

[10] It was this observation that urged THOMAS & WOOSTER to study the untwinning of quartz crystals which already contained Dauphiné twins. In their investigation they did not attempt to establish a theory for the piezoelectric effect in quartz, but rather they laid down an elementary theory for the untwinning of crystals by deformation. They found that inhomogeneous deformation, mainly torsion and flexure, could be applied to eliminate the Dauphiné twins.

in which

$$\hat{\boldsymbol{n}} = \frac{1}{|(\hat{\boldsymbol{F}}^{-1})^T \boldsymbol{N}|} (\hat{\boldsymbol{F}}^{-1})^T \boldsymbol{N} \quad \text{and} \quad \hat{a} = \frac{A}{|(\hat{\boldsymbol{F}}^{-1})^T \boldsymbol{N}|}. \tag{2.23}$$

Suppose the deformed shape of the slab is equilibrated by a Cauchy traction $\boldsymbol{t} = -\hat{p}\hat{\boldsymbol{n}}$ applied normal to the faces $\boldsymbol{x} \cdot \hat{\boldsymbol{n}} = \hat{a}$ and $\boldsymbol{x} \cdot \hat{\boldsymbol{n}} = 0$. Assume that neither *bulk charge* q nor *superficial charge* w are present on the slab. Let $\boldsymbol{\sigma}$ be the *Cauchy stress*, $\boldsymbol{E}$ be the *electric field*, ϕ be the *electrostatic potential*, $\boldsymbol{D}$ be the *electric displacement*, $\boldsymbol{P} = \varrho\boldsymbol{\pi}$ be the *polarization per unit volume*, $\varrho = \varrho_{\mathcal{R}} \det \boldsymbol{F}$ be the density, and $\varepsilon_0 =$ constant be the permittivity of free space. We have assumed that

$$\begin{aligned} &\boldsymbol{\sigma}\hat{\boldsymbol{n}} = -\hat{p}\hat{\boldsymbol{n}}; \\ &\boldsymbol{\pi} = 0 \quad \text{for} \quad \boldsymbol{x} \cdot \hat{\boldsymbol{n}} > \hat{a} \quad \text{and} \quad \boldsymbol{x} \cdot \hat{\boldsymbol{n}} < 0; \\ &\left.\begin{aligned} q &= 0 \\ w &= 0 \end{aligned}\right\} \quad \text{everywhere}. \end{aligned} \tag{2.24}$$

The polarization $\boldsymbol{\pi} = \hat{\boldsymbol{\pi}}$ inside the slab and $\boldsymbol{\pi} = \boldsymbol{0}$ outside the slab are subject to the equations of electrostatics:

$$\begin{aligned} \boldsymbol{E} &= -\operatorname{grad} \phi, & [\![\boldsymbol{E}]\!] &= E\boldsymbol{n}; \\ \operatorname{\boldsymbol{div}} \boldsymbol{D} &= q, & [\![\boldsymbol{D}]\!] \cdot \boldsymbol{n} &= w; \\ \boldsymbol{D} &= \varepsilon_0 \boldsymbol{E} + \boldsymbol{P}. \end{aligned} \tag{2.25}$$

The constants $\boldsymbol{F}$ and $\hat{\boldsymbol{\pi}}$ must also fulfill the equations of equilibrium for an elastic dielectric:

$$\begin{aligned} \boldsymbol{\sigma} &= \frac{\varrho}{\varrho_{\mathcal{R}}} \Sigma_{\boldsymbol{F}} \boldsymbol{F}^T - \boldsymbol{E} \otimes \boldsymbol{P} + \varepsilon_0 \left(\boldsymbol{E} \otimes \boldsymbol{E} - \frac{1}{2} |\boldsymbol{E}|^2 \boldsymbol{1} \right), \\ \operatorname{\boldsymbol{div}} \boldsymbol{\sigma} &= 0, \\ \Sigma_{\pi} &= \boldsymbol{E}. \end{aligned} \tag{2.26}$$

The bracket symbols $[\![\;]\!]$, as usual, denote the jump of the enclosed quantity across a singular surface with normal $\boldsymbol{n}$.

Under the assumptions laid down, the field equations and jump conditions become

$$\begin{aligned} &\boldsymbol{\sigma}(\hat{\boldsymbol{F}}, \hat{\boldsymbol{\pi}})\, \hat{\boldsymbol{n}} = -\hat{p}\hat{\boldsymbol{n}}, \\ &\Sigma_{\pi}(\hat{\boldsymbol{F}}, \hat{\boldsymbol{\pi}}) = \hat{\boldsymbol{E}}, \\ &\boldsymbol{E}_{\hat{a}} - \hat{\boldsymbol{E}} = \left(\frac{\hat{\varrho}}{\varepsilon_0} \hat{\boldsymbol{\pi}} \cdot \hat{\boldsymbol{n}} \right) \hat{\boldsymbol{n}}, \\ &\boldsymbol{E}_0 - \hat{\boldsymbol{E}} = \left(\frac{\hat{\varrho}}{\varepsilon_0} \hat{\boldsymbol{\pi}} \cdot \hat{\boldsymbol{n}} \right) \hat{\boldsymbol{n}}, \\ &\operatorname{\boldsymbol{div}} \operatorname{\boldsymbol{grad}} \phi = 0, \quad \boldsymbol{x} \cdot \hat{\boldsymbol{n}} > \hat{a}, \quad \boldsymbol{x} \cdot \hat{\boldsymbol{n}} < 0; \\ &\operatorname{\boldsymbol{grad}} \phi \cdot \hat{\boldsymbol{n}} = -\boldsymbol{E}_{\hat{a}} \cdot \hat{\boldsymbol{n}} \quad \text{at} \quad \boldsymbol{x} \cdot \hat{\boldsymbol{n}} = \hat{a} + 0, \\ &\operatorname{\boldsymbol{grad}} \phi \cdot \hat{\boldsymbol{n}} = -\boldsymbol{E}_0 \cdot \hat{\boldsymbol{n}} \quad \text{at} \quad \boldsymbol{x} \cdot \hat{\boldsymbol{n}} = 0^-. \end{aligned} \tag{2.27}$$

Here $\boldsymbol{E}_0$ and $\boldsymbol{E}_{\hat{a}}$, which both must be constant by $(2.27)_{3,4}$, are the limiting values of the electric field at $\boldsymbol{x} \cdot \hat{\boldsymbol{n}} = 0$ and $\boldsymbol{x} \cdot \hat{\boldsymbol{n}} = \hat{a}$ as the slab is approached from outside. So as to forbid the influence of an applied field, we assume that the continuous function ϕ tends to constants as $\boldsymbol{x} \cdot \hat{\boldsymbol{n}}$ tends to $+\infty$ and $-\infty$. Then ϕ is determined up to a constant by $(2.27)_{5,6,7}$.

We seek a solution $(\hat{\boldsymbol{F}}, \hat{\boldsymbol{\pi}})$ of (2.27) corresponding to an electric field $\hat{\boldsymbol{E}}$ inside the slab. If $\hat{\boldsymbol{F}}$, $\hat{\boldsymbol{\pi}}$ and $\hat{\boldsymbol{E}}$ are known, then the electric field outside the slab is determined by $(2.27)_{3-7}$. In fact, ϕ is given by

$$\phi = \begin{cases} c = \text{constant} & \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{n}} < 0, \\ -\hat{E}(\boldsymbol{x} \cdot \hat{\boldsymbol{n}}) + c & 0 < \boldsymbol{x} \cdot \hat{\boldsymbol{n}} < \hat{a}, \\ -\hat{E}\hat{a} + c & \boldsymbol{x} \cdot \hat{\boldsymbol{n}} > \hat{a}, \end{cases} \tag{2.28}$$

which shows that $\hat{\boldsymbol{E}} = \hat{E}\boldsymbol{n}$ inside the slab. Therefore, given $\hat{p}$ there is a solution $\hat{\boldsymbol{F}}$, $\hat{\boldsymbol{\pi}}$ of (2.27) corresponding to an electrostatic potential ϕ if and only if there is a constant $\hat{E}$ such that

$$\begin{aligned} \sigma(\hat{\boldsymbol{F}}, \hat{\boldsymbol{\pi}})\, \hat{\boldsymbol{n}} &= -\hat{p}\hat{\boldsymbol{n}}, \\ \Sigma_\pi(\hat{\boldsymbol{F}}, \hat{\boldsymbol{\pi}}) &= \hat{E}\hat{\boldsymbol{n}}, \\ \hat{E} + \frac{\hat{\varrho}}{\varepsilon_0}(\hat{\boldsymbol{\pi}} \cdot \hat{\boldsymbol{n}}) &= 0. \end{aligned} \tag{2.29}$$

We imagine that the slab has the properties of a section cut out of quartz crystal normal to the axis of the crystal, with $\boldsymbol{N}$ normal to one of the six lateral faces. Let $\boldsymbol{V}$ be a unit vector along the axis of the crystal and let $\{\boldsymbol{N}, \boldsymbol{W}, \boldsymbol{V}\}$ be a right-handed orthonormal basis (see Figure 1). We may contemplate that (2.29) is

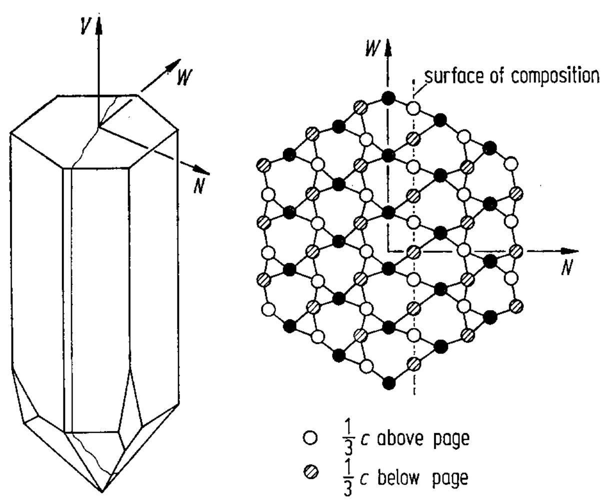

Fig. 1. Dauphiné twinning. A crystal of quartz with a Dauphiné twin (left); positions of the silicon atoms near a Dauphiné twin (right). $c = 5.40$ Å.

solved by a deformation gradient $\hat{F}$ which yields a pure stretch in the direction V and a polarization normal to V:

$$\hat{F}V = \hat{\lambda}V, \quad \hat{F}^T V = \hat{\lambda}V, \quad \hat{\pi} \cdot V = 0. \tag{2.30}$$

Relative to the basis $\{N, W, V\}$, $\hat{F}$ has the form

$$\begin{bmatrix} \hat{F}_{11} & \hat{F}_{12} & 0 \\ \hat{F}_{21} & \hat{F}_{22} & 0 \\ 0 & 0 & \hat{\lambda} \end{bmatrix}. \tag{2.31}$$

I assume[11] *there is at least one solution* $(\hat{F}, \hat{\pi})$ *of* (2.29), $\hat{F}, \hat{\pi}$ *restricted by* (2.30). Let $\hat{E} = \hat{E}n$ be the corresponding electric field.

Since there is a potential difference of $\hat{E}\hat{a}$ across the slab, the piezoelectric effect is exhibited.

Now I wish to consider the same kind of problem for a quartz crystal which contains a Dauphiné twin. To do so I must ascertain the symmetry transformation which determines the Dauphiné twin. The task is made easy due to a lucid description of the mechanism for the piezoelectric effect in quartz by VIGOUREUX & BOOTH [23] based on earlier work by GIBBS and BRAGG. These authors make it clear that the symmetry group of quartz includes the transformations

$$\mathfrak{Y}(F, \pi) = \left(FH_{\frac{n\pi}{3}}, \pi\right), \tag{2.32}$$

$H_{\frac{n\pi}{3}}$ being any rotation of $n\dfrac{\pi}{3}$, $n =$ integer, about the axis V. We have tacitly assumed here that Σ is defined relative to the usual undistorted reference shape of a quartz crystal. Of course, we have invariance under the Galilean group which acts upon (F, π) according to the rule

$$\mathfrak{T}(F, \pi) = QF, Q\pi), \quad Q \in \mathcal{O}^+. \tag{2.33}$$

The Dauphiné twin is a mechanical twin characterized by two properties. First, the deformation gradient is continuous across the surface of composition, and second, the two individuals may be brought into coincidence by a rotation of π about the axis of the crystal, which may itself become distorted by the deformation. Thus, using the notation for a general mechanical twin, we have the

Definition (*Dauphiné twin*). *Let $\Sigma(F, \pi)$ be the stored energy function for quartz deformed relative to an undistorted reference shape $\mathcal{R}$. Let V be a unit vector along the axis of the crystal in the reference shape. A part $\mathcal{P} = \mathcal{P}^+ \cup \mathcal{P}^- \subset \mathcal{R}$ deformed by χ, subject to a field of polarization π, contains a Dauphiné twin if it contains a*

---

[11] The assumption is plausible but would require a deep investigation of symmetry and stability to justify. Typically we shall have $\hat{F}$ near $\mathbf{1}$ and $\hat{\pi}$ near $\mathbf{0}$.

mechanical twin for which the limiting values $(F^{\pm}, \pi^{\pm})$ *satisfy*

$$F^{+} = QF^{-}H_{\frac{n\pi}{3}} = F^{-}, \quad \pi^{+} = Q\pi^{-}, \tag{2.34}$$

Q being a rotation of π about the axis $F^{+}V$, and $H_{\frac{n\pi}{3}}$ being a rotation of $\frac{n\pi}{3}$, $n =$ integer, about the axis V.[12]

Having the definition of a Dauphiné twin, we return to the problem of the piezoelectric effect in a twinned slab. We shall suppose that the slab contains no free charge and is subject to a hydrostatic pressure $\hat{p}$, as before (*cf.* (2.24)). However, now let the slab $\chi(\mathscr{R})$ contain a Dauphiné twin, with constants (F^{+}, π^{+}) on $\frac{1}{2}\hat{a} < x \cdot \hat{n} < \hat{a}$ and (F^{-}, π^{-}) on $0 < x \cdot \hat{n} < \frac{1}{2}\hat{a}$.

I claim that if we put $F^{+} = F^{-} = \hat{F}$, $\pi^{+} = \hat{\pi}$ and $\pi^{-} = -\hat{\pi}$, then we will satisfy not only the conditions for a Dauphiné twin, but also the equations of electromagnetism (2.25) and the equations of equilibrium for an elastic dielectric (2.26). Here $(\hat{F}, \hat{\pi})$ are the deformation gradient and polarization found for an untwinned crystal.

First we show that the conditions define a Dauphiné twin. If we put $Q = H_{\pi}$, we see that that from (2.30) $Q\hat{F}H_{\pi} = \hat{F}$. Also from (2.30) we have $Q\hat{F}V = Q\hat{\lambda}V = \hat{\lambda}H_{\pi}V = \hat{\lambda}V = \hat{F}V$. Thus Q has as axis $\hat{F}V$. Since $\hat{\pi} \cdot V = 0$, we have $Q\hat{\pi} = -\hat{\pi}$. Therefore, the conditions $F^{+} = F^{-} = \hat{F}$, $\pi^{+} = \hat{\pi}$, $\pi^{-} = -\hat{\pi}$ define a Dauphiné twin of the slab.

Second we show that the equations of electromagnetism and the equilibrium equations for an elastic dielectric are fulfilled. Note that now we must also satisfy the jump conditions across the surface of composition $x \cdot \hat{n} = \frac{1}{2}\hat{a}$. For $\frac{1}{2}\hat{a} < x \cdot \hat{n} < \hat{a}$, $F^{+} = \hat{F}$, $\pi^{+} + \hat{\pi}$ so that all of the equations are satisfied on this region with $E^{+} = \hat{E}n$. By (2.32) and (2.33) we have

$$\begin{aligned} H_{\pi}\Sigma_{\pi}(F^{-}, \pi^{-}) &= \Sigma_{\pi}(F^{+}, \pi^{+}), \\ H_{\pi}\Sigma_{F}(F^{-}, \pi^{-})\, F^{-T}H_{\pi} &= \Sigma_{F}(F^{+}, \pi^{+})\, F^{+T}. \end{aligned} \tag{2.35}$$

From (2.35) it is easy to show that all of the remaining equations and jump conditions are satisfied if we put $E^{-} = -\hat{E}\hat{n}$.

But now we see that the piezoeletric effect has been eliminated, for the potential for the twinned slab is

$$\phi = \begin{cases} c = \text{constant} & x \cdot \hat{n} < 0, \\ \hat{E}(x \cdot \hat{n}) + c & 0 < x \cdot \hat{n} < \frac{1}{2}\hat{a}, \\ -\hat{E}(x \cdot \hat{n}) + \hat{a}\hat{E} + c & \frac{1}{2}\hat{a} < x \cdot \hat{n} < \hat{a}. \end{cases} \tag{2.36}$$

This completes the example.

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[12] The theory of Rivlin for Dauphiné twinning, presented by Thomas & Wooster, can be obtained from the theory presented here by linearizing Σ about the values (F^{-}, π^{-}) and (F^{+}, π^{+}), and then by using a simple form of the energy criterion for stability.

3. Kinematics of twinning, trilling, etc.

A point in a body $\mathscr{B}$ can belong to the intersection of several surfaces of composition. If a small neighborhood of the point is bisected by one such surface, the limiting values of the deformation gradient as the surface is approached from either side must fulfill the condition (2.11). If a point ξ lies on the axis of a trilling (*cf.* Remark 4 of § 2), the three limiting values of the deformation gradient $\boldsymbol{F}_1$, $\boldsymbol{F}_2$, $\boldsymbol{F}_3$ obtained by approaching ξ from each of the regions of continuity of $\nabla\chi$ must satisfy

$$\begin{aligned} \boldsymbol{F}_2 - \boldsymbol{F}_1 &= \boldsymbol{a}_1 \otimes \boldsymbol{N}_1, \\ \boldsymbol{F}_3 - \boldsymbol{F}_2 &= \boldsymbol{a}_2 \otimes \boldsymbol{N}_2, \\ \boldsymbol{F}_1 - \boldsymbol{F}_3 &= \boldsymbol{a}_3 \otimes \boldsymbol{N}_3; \end{aligned} \tag{3.1}$$

$$\det \boldsymbol{F}_1 > 0, \quad \det \boldsymbol{F}_2 > 0, \quad \det \boldsymbol{F}_3 > 0, \tag{3.2}$$

for some nonvanishing amplitudes $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$. The unit vectors $\boldsymbol{N}_1$, $\boldsymbol{N}_2$ and $\boldsymbol{N}_3$ are the limiting unit normal vectors to the surfaces $\mathscr{S}_1$, $\mathscr{S}_2$ and $\mathscr{S}_3$ at the point ξ (*cf.* 3 of § 2). Note that the normal vectors $\boldsymbol{N}_1$, $\boldsymbol{N}_2$, $\boldsymbol{N}_3$ must be coplanar; since $\mathscr{S}_1$, $\mathscr{S}_2$, $\mathscr{S}_3$ all contain the axis of the trilling, then the normal vectors $\boldsymbol{N}_1, \boldsymbol{N}_2, \boldsymbol{N}_3$ must all lie in a plane normal to this axis.

Conversely, if there are constants $\boldsymbol{F}_1$, $\boldsymbol{F}_2$, $\boldsymbol{F}_3$ and $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ which satisfy (3.1) and (3.2) for an assigned set of coplanar, non-collinear normal vectors $\boldsymbol{N}_1$, $\boldsymbol{N}_2$, $\boldsymbol{N}_3$, then there is a piecewise homogeneous deformation having the deformation gradients $\boldsymbol{F}_1$, $\boldsymbol{F}_2$, $\boldsymbol{F}_3$. That is, we simply erect three half planes having the normal vectors $\boldsymbol{N}_1$, $\boldsymbol{N}_2$, $\boldsymbol{N}_3$ whose edges coincide, and we assign *constant* deformation gradients $\boldsymbol{F}_1$, $\boldsymbol{F}_2$, $\boldsymbol{F}_3$ in the included regions. Of course, we cannot say that this deformation is a trilling since we have not assigned a stored energy function.

Collections of neighboring deformations more complicated than those which arise from twinning and trilling are commonly observed, especially in deformation-induced martensite [15]. Whether or not the adjacent individuals of these collections form twins, the limiting values of the deformation gradients must satisfy conditions analogous to (3.1), if the deformation which creates these collections is continuous.

I propose to study in this section the kinematic restrictions which arise when regions with different deformation gradients meet at a point. The analysis will lead to the definitions of the next least complicated arrangements, after those which arise from twinning and trilling, which are kinematically possible. I shall also give an algorithm whereby the kinematic restrictions on any system of adjacent individuals can be solved or judged unsolvable.

The analysis provides necessary conditions on collections of twins. It does not guarantee that for any particular material the relations of symmetry for twinning (*i.e.* equation (2.10)) are fulfilled. However, the analysis delivers *necessary and sufficient* conditions that a collection of regions separated by surfaces of discontinuity of the deformation gradient be kinematically possible. Of course, the deformation gradient need not suffer a discontinuity across a surface of composition as we have seen in the example of Dauphiné twinning (Remark 6 of § 2).

Surfaces of composition which are surfaces of discontinuity of F are associated with lattice-distortive deformations. The kinematics of collections of twins which are not lattice distortive, *i.e.* do not contain surfaces of discontinuity of the deformation gradient, is trivial.

The analysis of (3.1) and (3.2) is simple and serves as an example. We assume N_1, N_2, N_3 are assigned, coplanar unit vectors. Without loss of generality, let

$$N_3 = \alpha N_1 + \beta N_2. \tag{3.3}$$

If we eliminate F_1, F_2 and F_3 from (3.1), we obtain

$$a_1 \otimes N_1 + a_2 \otimes N_2 + a_3 \otimes N_3 = 0, \tag{3.4}$$

which, after use of (3.3), becomes

$$(a_1 + \alpha a_3) \otimes N_1 + (a_2 + \beta a_3) \otimes N_2 = 0. \tag{3.5}$$

If N_1 is not parallel to N_2, an elementary theorem of linear algebra implies that

$$\begin{aligned} a_1 + \alpha a_3 &= 0, \\ a_2 + \beta a_3 &= 0; \end{aligned} \tag{3.6}$$

(3.6) has non-vanishing solutions (a_1, a_2, a_3) if and only if both $\alpha \neq 0$ and $\beta \neq 0$. Note that if (a_1, a_2, a_3) solve (3.6), then so do $(\lambda a_1, \lambda a_2, \lambda a_3)$ for any $\lambda \neq 0$. The deformation gradients F_1, F_2 and F_3 are determined by (3.1); let F_3 be assigned such that $\det F_3 > 0$. Let $(\lambda a_1, \lambda a_2, \lambda a_3)$ obtained from (3.6) be inserted into the right hand sides of (3.1), so that (F_1, F_2) are determined by $(3.1)_{2,3}$. Then (3.5) implies that (3.1) is fulfilled by (F_1, F_2). If λ is sufficiently small, $\det F_1 > 0$ and $\det F_2 > 0$. Therefore, if N_1 is not parallel to N_2 and $\alpha \neq 0$, $\beta \neq 0$, then both (3.1) and (3.2) have a solution.

Of course, the definition of a trilling does not permit N_1, N_2 and N_3 to be all parallel, since the part $\mathscr{P} \subset \mathscr{R}$ which contains the trilling must be diffeomorphic to a sphere trisected by three *distinct* half planes. If we were to relax this requirement, and consider three regions separated by surfaces which meet along a curve, we would obtain the possibilities shown in Figure 2c.

In summary, we have the existence of solutions $a_1 \neq 0$, $a_2 \neq 0$, $a_3 \neq 0$, F_1, F_2, F_3 of (3.1) *for* N_1 *not parallel to* N_2 *if and only if there are constants* $\alpha \neq 0$ *and* $\beta \neq 0$ *such that*

$$N_3 = \alpha N_1 + \beta N_2. \tag{3.7}$$

See Figures 2a and 2b.

Before turning to the general problem, we consider cusps, like the ones shown in Figure 2c. My definition of a trilling has excluded them by the condition that the reference shape be diffeomorphic to a sphere trisected by three *distinct* half planes (*cf.* 3 of § 2). Cusps are dificult to analyze from a general standpoint so the definition of a partition I shall state presently will exclude them.

To formulate the general problem, let a finite number of points (*vertices*) be given on the surface of a sphere S. Suppose a connected set of *edges*, each one being an arc of a great circle of ∂S, join the points in pairs. That is, the end-points of each edge are distinct vertices and no vertices are contained in the interior of an edge. Assume that at least two edges meet at a vertex. The edges divide ∂S into a finite number of connected, open, non-empty *faces*. Assume that each edge separates two distinct faces. A set of e edges, v vertices and f faces formed by these rules[13] is termed a partition of ∂S. Since the EULER characteristic of ∂S is two, we have for any partition $f - e + v = 2$.

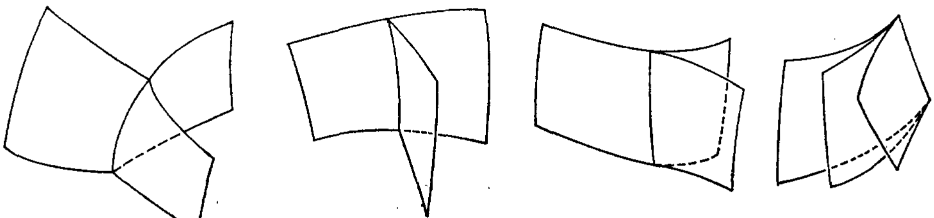
a b c

Fig. 2a–c. Kinematics of mechanical trilling. a Kinematically possible; b Not kinematically possible; c Kinematically possible configurations which are not trillings.

Let a straight line segment join each vertex of a partition to the center of S. Each edge and the two line segments joining its terminal vertices to the center determine a plane (since the edges are arcs of great circles). A total of e planes with unit normals $N_1, \ldots, N_e$ are formed in this way. The planes divide up the interior of the sphere into f open, connected, non-empty regions $R_1, \ldots, R_f$. The interior of the intersection of each region with ∂S is a face. Without confusion[14] I shall also call the collection of regions $R_1, \ldots, R_f$ a partition of S. A partition shall be labelled by a hollow letter, *e.g.* $\mathbb{P}$.

My basic assumption is that a part $\mathscr{P}$ of the reference shape $\mathscr{R}$ of the body $\mathscr{B}$ is diffeomorphic to a partitioned sphere S: there is an invertible, continuously differentiable map $\mu : S \to \mathscr{P}$, with a continuously differentiable inverse. The images of $\mathscr{R}_1, \ldots, \mathscr{R}_f$ under μ are certain regions $r_1, \ldots, r_f$, on each of which there is defined a continuous field of deformation gradient. I assume that there is a *continuous* deformation χ of $\mathscr{P}$ whose gradient coincides with each of the fields of deformation gradient on each of the regions $r_1, \ldots, r_f$.

Without loss of generality, we may assume that the reference shape $\mathscr{P}$ is S, *i.e.* that μ is the identity. We simply recognize that the assumption that $\mathscr{P}$ is deformed continuously by χ with continuous fields of deformation gradient in $r_1, \ldots, r_f$ is equivalent to the assumption that S is deformed continuously by $\chi \circ \mu$ with continuous fields of deformation gradient in $\mathscr{R}_1, \ldots, \mathscr{R}_f$.

Thus assume that $\mathscr{P} = S$, that $F_1, \ldots, F_f$ are fields of deformation gradient defined on $\mathscr{R}_1, \ldots, \mathscr{R}_f$, respectively, that $F_i = \nabla\chi$, $i = 1, \ldots, f$, for a continuous deformation χ of S, and that if $\hat{F}_i$ and $\hat{F}_j$, $i \neq j$, are the limiting values of the

[13] It is easy to show that these rules are self-consistent.

[14] There is no possibility of confusion since a partition of ∂S uniquely determines $R_1, \ldots, R_f$.

deformation gradient as the center of S is approached from adjacent regions $\mathscr{R}_i$, $\mathscr{R}_j$, then $\hat{F}_i - \hat{F}_j \neq 0$. Here, the word 'adjacent' means that the faces F_i, F associated with the regions $\mathscr{R}_i$, $\mathscr{R}_j$ share a common edge: $\partial F_i \cap \partial F_j \subset E_k$, for some edge E_k. According to MAXWELL's Theorem, there is an amplitude $\boldsymbol{a}_k$ such that

$$\hat{\boldsymbol{F}}_i - \hat{\boldsymbol{F}}_j = \boldsymbol{a}_k \otimes \boldsymbol{N}_k, \qquad |\boldsymbol{a}_k| \neq 0, \tag{3.8}$$

$\boldsymbol{N}_k$ being the normal vector of the plane through the edge E_k. There are e systems of equations like (3.8) that must be satisfied, one system for each edge.

One way to organize and study these equations is to define incidence matrices like those used in algebraic topology [24]. Let faces $F_1, \ldots, F_f$ and edges $E_1, \ldots, E_e$ belong to a partition $\mathbb{P}$ of the surface of a sphere S. The **incidence matrix** η_{ij} of $\mathbb{P}$ is defined by

$$\eta_{ij} = \begin{cases} 1 & \text{if} \quad E_i \subset \partial F_j, \\ 0 & \text{if} \quad E_i \subset \partial F_j. \end{cases} \tag{3.9}$$

The incidence matrix has e rows and f columns, as well as the properties summarized in

Lemma 1. *For the incidence matrix of any partition,*
(I) *each row contains exactly two ones*;
(II) *each column contains at least two ones.*

The proof of Lemma 1 follows easily from the definition of a partition and I shall omit it. Lemma 1 states that each edge separates exactly two faces, and the boundary of each face consists of at least two edges. Since at least two vertices must belong to a partition, we have, by EULER's relation, $e = f + v - 2 \geqq f$.

Let the **signed incidence matrix** $\bar{\eta}_{ij}$ be obtained from η_{ij} by changing the 1 which appears *second* in each row to -1. Let $\hat{\boldsymbol{F}}_1, \ldots, \hat{\boldsymbol{F}}_f$ be the limiting values of the deformation gradient as the center of S is approached from each of the regions $\mathscr{R}_1, \ldots, \mathscr{R}_f$. Then the equations (3.8) can be written

$$\sum_{j=1}^{f} \bar{\eta}_{ij} \hat{\boldsymbol{F}}_j = \boldsymbol{a}_i \otimes \boldsymbol{N}_i, \qquad i = 1, \ldots, e \quad (\text{no sum over } i). \tag{3.10}$$

We must also assure that

$$\det \hat{\boldsymbol{F}}_j > 0, \qquad j = 1, \ldots, f. \tag{3.11}$$

As before, we view the partition of ∂S as given. Therefore, in (3.10) $\boldsymbol{N}_1, \ldots, \boldsymbol{N}_e$ and $\bar{\eta}_{ij}$ are given; we seek a solution $\boldsymbol{a}_1 \neq 0, \ldots, \boldsymbol{a}_e \neq 0$; $\boldsymbol{F}_1, \ldots, \boldsymbol{F}_f$ of (3.10) and (3.11).

Conversely, if there is a solution, $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_e$; $\boldsymbol{F}_1, \ldots, \boldsymbol{F}_f$ of (3.10) and (3.11), then there is a continuous deformation of S with *constant* deformation gradients $\boldsymbol{F}_1, \ldots, \boldsymbol{F}_f$ defined on the regions $\mathscr{R}_1, \ldots, \mathscr{R}_f$.

According to the Fredholm alternative, the system (3.10) has a solution $\boldsymbol{a}_1 \neq 0, \ldots, \boldsymbol{a}_e \neq 0$; $\boldsymbol{F}_1, \ldots, \boldsymbol{F}_f$ if and only if a certain homogeneous system of linear equations involving only $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_e$ is satisfied. Let the rank of $\bar{\eta}_{ij}$ be r.

The signed incidence matrix $\bar{\eta}_{ij}$ can be put in upper triangular form by elementary row operations; in fact because of the special form of η_{ij} one need only use three elementary transformations, namely, exchange of rows, multiplication of a row by -1, and addition of rows, to triangularize $\bar{\eta}_{ij}$. Let $\bar{\eta}^*_{ij}$ be upper triangular form of $\bar{\eta}_{ij}$. The last $(e-r)$ rows of $\bar{\eta}^*_{ij}$ will be composed of zeros. If now the same operations which were used to transform $\bar{\eta}_{ij}$ to $\bar{\eta}^*_{ij}$ are applied to the right hand side of (3.10), we see that the last $(e-r)$ rows of the transformed system (3.10) become

$$\begin{gathered} \pm \boldsymbol{a}_{m_{(r+1)}} \otimes \boldsymbol{N}_{m_{(r+1)}} \pm \cdots \pm \boldsymbol{a}_{p_{(r+1)}} \otimes \boldsymbol{N}_{p_{(r+1)}} = 0 \\ \vdots \qquad\qquad\qquad\qquad \vdots \\ \pm \boldsymbol{a}_{m_e} \otimes \boldsymbol{N}_{m_e} \pm \quad \cdots \quad \pm \boldsymbol{a}_{p_e} \otimes \boldsymbol{N}_{p_e} = 0. \end{gathered} \tag{3.12}$$

The indices $m_{(r+1)} \dots p_e$ are determined by the signed incidence matrix. Equation (3.10) has a solution $\boldsymbol{a}_1 \neq 0, \dots, \boldsymbol{a}_e \neq 0$, $\boldsymbol{F}_1, \dots, \boldsymbol{F}_f$ if and only if (3.12) has a solution $\boldsymbol{a}_1 \neq 0, \dots, \boldsymbol{a}_e \neq 0$. The first r rows of the transformed system determine $\boldsymbol{F}_1, \dots, \boldsymbol{F}_f$, some of which can be chosen arbitrarily. The system (3.12) is homogeneous; therefore if $\boldsymbol{a}_1, \dots, \boldsymbol{a}_e$ is a solution, then so is any constant multiple of $\boldsymbol{a}_1, \dots, \boldsymbol{a}_e$. By making this constant multiple sufficiently small, and choosing all of the free values of the deformation gradient to have a positive determinant, we can also satisfy (3.11).

The algorithm is easy to carry out by hand, even for complicated partitions, since the rows of $\bar{\eta}_{ij}$ continue to have one 1 and one -1 and $(f-2)$ zeros, or else all zeros, after each row operation.

Given a certain number of edges, faces and vertices consistent with EULER'S relation, there are an infinite number of possible partitions. If (3.12) is not too complicated, all of these can be analyzed without great difficulty because only the unit normal vectors enter (3.12). I have carried this out in the following way; I fix the number e of edges and consider $f = 2, \dots, e$. For each e and f, I calculate the number v of vertices and consider all possible partitions of ∂S having e edge, f faces and v vertices. I analyze the equations (3.12) to see if any of those partitions are kinematically possible. The results of this calculation are summarized in Table 1.

In the column labeled *morphology* I have given names to the simplest partitions which are kinematically possible. The phrase 'same as' means that the only kinematically possible partition is governed by the same equations as the earlier partition indicated. Note that the simplest partitions belong to a twin and a trilling, which suggests, perhaps, that we are on the right track. As I have emphasized earlier in this section, the words 'twin' and 'trilling' only indicate that the kinematic conditions for twinning or trilling have been met.

It must not be thought that greater complexity of the partition implies greater likelihood of being able to solve (3.12). Given an arbitrary partition, however complicated, it is always possible to add two more edges and one more face such that the equations (3.12) have no non-trivial solutions.

Motivated by these results we shall define a fourling, fiveling and, in general-an n-ling in the following way.

Table 1. Kinematics of the partitions with a small number of edges. See text for details.

e	f	v	morphology
2	2	2	**twin**
3	2	3	same as (2, 2, 2)
3	3	2	**trilling**
4	2	4	same as (2, 2, 2)
4	3	3	same as (3, 3, 2)
4	4	2	**fourling**
5	2	5	same as (2, 2, 2)
5	3	4	same as (3, 3, 2)
5	4	3	same as (4, 4, 2)
5	5	2	**fiveling**
6	2	6	same as (2, 2, 2)
6	3	5	same as (3, 3, 2)
6	4	4	**tetrad**, or same as (4, 4, 2)
.	.	.	.
.	.	.	.
.	.	.	.

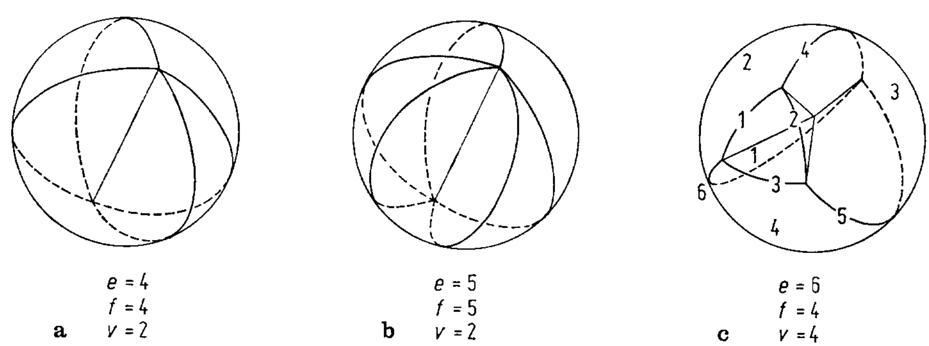

Fig. 3a–c. Kinematically possible partitions. See Table 1 and text.

Definition. *A mechanical n-ling* (n = *integer* $\geqq 4$) *is a part* $\mathscr{P} \subset \mathscr{R}$ *deformed by a continuous map* χ, *subject to a field of polarization* $\mathbf{p}_1, \ldots, \mathbf{p}_n$, *such that*

(I) $\mathscr{P}$ *is diffeomorphic to a partitioned sphere with* $e = n$, $f = n$, $v = 2$. *Let* $\mathscr{R}_1, \ldots, \mathscr{R}_n$ *be the regions of the partition.*

(II) *Each pair of adjoining regions* $\mathscr{R}_i$ *and* $\mathscr{R}_j$ *forms a mechanical twin.*

The terms fourling, fiveling, *etc.* are used in crystallography to denote collections of twins [26]. Most examples of multiple twinning occur as growth twins, although a mechanical fourling is found at the intersection of two twin bands [26, p. 65; see also 10, p. 360].

The first kinematically possible partition to appear in Table 1 which has more than two vertices corresponds to $e = 6$, $f = 4$, $v = 4$. I have called it a *tetrad*; it is pictured in Figure 2c. Because of its possible importance to the martensitic transformations, I shall analyze it explicitly.

By a process of exhaustion, one can show that if a partition with $e = 6$, $f = 4$, $v = 4$ is kinematically possible, it must be true that either

α. two, and only two, vertices are not connected by an edge, or

β. every vertex is connected to every other vertex by exactly one edge.

The former satisfies the same kinematic equations (*i.e.* (3.12)) as a partition with $e = 4$, $f = 4$, $v = 2$; an example is pictured in Figure 2a. *Any kinematically possible partition with* $e = 6$, $f = 4$, $v = 4$ *satisfying* β *is, by definition, a* **tetrad.** Based on the numbering of vertices, edges and faces shown in Figure 2c, the signed incidence matrix for a tetrad is

$$\|\bar{\eta}_{ij}\| = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 \end{bmatrix} \tag{3.13}$$

which has rank 3. The triangulation of (3.10) is

$$\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{F}_1 \\ \boldsymbol{F}_2 \\ \boldsymbol{F}_3 \\ \boldsymbol{F}_4 \end{bmatrix} = \begin{bmatrix} \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 \\ \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 - \boldsymbol{a}_1 \otimes \boldsymbol{N}_1 \\ \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 - \boldsymbol{a}_2 \otimes \boldsymbol{N}_2 \\ \boldsymbol{a}_4 \otimes \boldsymbol{N}_4 + \boldsymbol{a}_1 \otimes \boldsymbol{N}_1 - \boldsymbol{a}_2 \otimes \boldsymbol{N}_2 \\ \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 - \boldsymbol{a}_2 \otimes \boldsymbol{N}_2 - \boldsymbol{a}_5 \otimes \boldsymbol{N}_5 \\ -\boldsymbol{a}_6 \otimes \boldsymbol{N}_6 - \boldsymbol{a}_1 \otimes \boldsymbol{N}_1 + \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 \end{bmatrix}. \tag{3.14}$$

Thus the equations analogous to (3.12) are

$$\begin{aligned} \boldsymbol{a}_4 \otimes \boldsymbol{N}_4 + \boldsymbol{a}_1 \otimes \boldsymbol{N}_1 - \boldsymbol{a}_2 \otimes \boldsymbol{N}_2 &= 0, \\ \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 - \boldsymbol{a}_2 \otimes \boldsymbol{N}_2 - \boldsymbol{a}_5 \otimes \boldsymbol{N}_5 &= 0, \\ -\boldsymbol{a}_6 \otimes \boldsymbol{N}_6 - \boldsymbol{a}_1 \otimes \boldsymbol{N}_1 + \boldsymbol{a}_3 \otimes \boldsymbol{N}_3 &= 0. \end{aligned} \tag{3.15}$$

The normal vectors $\boldsymbol{N}_1, \ldots, \boldsymbol{N}_6$ here are not arbitrary since they must belong to a tetrad. From the definition of a tetrad three edges must meet at each vertex, so the normals corresponding to those edges must lie in one plane. If we number the normals as in Figure 2c, we must have scalars α_1, α_2, β_2, β_3, γ_1, γ_3, δ_4, δ_5 such that

$$\begin{aligned} \boldsymbol{N}_4 &= \alpha_1 \boldsymbol{N}_1 + \alpha_2 \boldsymbol{N}_2, \\ \boldsymbol{N}_5 &= \beta_2 \boldsymbol{N}_2 + \beta_3 \boldsymbol{N}_3, \\ \boldsymbol{N}_6 &= \gamma_1 \boldsymbol{N}_1 + \gamma_3 \boldsymbol{N}_3, \\ \boldsymbol{N}_6 &= \delta_4 \boldsymbol{N}_4 + \delta_5 \boldsymbol{N}_5. \end{aligned} \tag{3.16}$$

Also, we must have that N_1, N_2, N_3 are linearly independent. If we eliminate N_6 between the third and fourth of (3.16), and then eliminate N_4 and N_5 using the first two of (3.16), we obtain

$$\begin{aligned} N_6 = \gamma_1 N_1 + \gamma_3 N_3 &= \delta_4 N_4 + \delta_5 N_5 \\ &= \alpha_1\, \delta_4 N_1 + (\alpha_2\, \delta_4 + \beta_2\, \delta_5)\, N_2 + \beta_3\, \delta_5 N_3, \end{aligned} \tag{3.17}$$

whence

$$\gamma_1 = \alpha_1\, \delta_4, \qquad \gamma_3 = \beta_3\, \delta_5, \qquad \alpha_2\, \delta_4 = -\beta_2\, \delta_5. \tag{3.18}$$

The equations (3.18) imply that

$$\alpha_2 \gamma_1 \beta_3 + \beta_2 \gamma_3 \alpha_1 = 0. \tag{3.19}$$

We return now to (3.15). As always, we view the normals as assigned, consistent with (3.16). After substitution of (3.16), (3.15) becomes

$$\begin{aligned} (a_1 + \alpha_1 a_4) \otimes N_1 + (-a_2 + \alpha_2 a_4) \otimes N_2 &= 0, \\ (-a_2 - \beta_2 a_5) \otimes N_2 + \quad (a_3 - \beta_3 a_5) \otimes N_3 &= 0, \\ (-a_1 - \gamma_1 a_6) \otimes N_1 + \quad (a_3 - \gamma_3 a_6) \otimes N_3 &= 0. \end{aligned} \tag{3.20}$$

Since N_1, N_2, and N_3 are linearly independent, we must have

$$\begin{aligned} a_1 + \alpha_1 a_4 &= 0, & -a_2 + \alpha_2 a_4 &= 0, \\ -a_2 - \beta_2 a_5 &= 0, & a_3 - \beta_3 a_5 &= 0, \\ -a_1 + \gamma_1 a_6 &= 0, & a_3 - \gamma_3 a_6 &= 0. \end{aligned} \tag{3.21}$$

A necessary condition that (3.21) have a solution $a_1 \neq 0, \dots, a_6 \neq 0$ is that $\alpha_1 \neq 0, \dots, \gamma_3 \neq 0$. Suppose $\alpha_1 \neq 0, \dots, \gamma_3 \neq 0$. Then (3.21) implies that

$$a_1 \parallel a_2 \parallel a_3 \parallel a_4 \parallel a_5 \parallel a_6. \tag{3.22}$$

For some fixed a, $|a| = 1$, let

$$a_i = \eta_i a, \qquad \eta_i \neq 0, \qquad i = 1, \dots, 6. \tag{3.23}$$

Then (3.20) is equivalent to the system

$$\begin{aligned} \eta_1 + \alpha_1 \eta_4 &= 0, & -\eta_2 + \alpha_2 \eta_4 &= 0, \\ -\eta_2 - \beta_2 \eta_5 &= 0, & \eta_3 - \beta_3 \eta_5 &= 0, \\ -\eta_1 - \gamma_1 \eta_6 &= 0, & \eta_3 - \gamma_3 \eta_6 &= 0, \end{aligned} \tag{3.24}$$

which is to be solved for non-vanishing $\eta_1, \dots, \eta_6$, the other parameters $\alpha_1, \dots, \gamma_3$ being assigned non-zero constants which fulfill (3.18). The determinant of the system (3.24) is $\alpha_2 \gamma_1 \beta_3 + \beta_2 \gamma_3 \alpha_1$, which vanishes by (3.19). Thus there is a solution $(\eta_1, \dots, \eta_6)$ of (3.24), not all of $\eta_1, \dots, \eta_6$ being zero. However, it must follow from (3.24) that there is a solution with none of the $\eta_1, \dots, \eta_6$ equal to zero, for if one of $\eta_1, \dots, \eta_6$ vanishes, then by (3.24) all of $\eta_1, \dots, \eta_6$ must vanish. Hence by reversing the argument we deduce that for a normalized amplitude

$\boldsymbol{a}$, $|\boldsymbol{a}| = 1$, (3.15) has a solution,

$$\boldsymbol{a}_i = \eta_i \boldsymbol{a}, \quad i = 1, \ldots, 6. \tag{3.25}$$

We have found the perhaps unexpected result that *the amplitudes of all edges of a tetrad are parallel.*

In summary we have found

Properties of a tetrad:

1. $e = 6$, $f = 4$, $v = 4$.
2. Each vertex is connected to every other vertex by an edge.
3. Each pair of edges meeting at a vertex have non-parallel normal vectors.
4. The amplitudes of all edges are parallel $\boldsymbol{a}_i = \eta_i \boldsymbol{a}$, $|\boldsymbol{a}| = 1$, the non-zero η_i, $i = 1, \ldots, 6$ being determined up to a constant multiple by (3.24).

According to our argument the first three of these properties can serve to define a tetrad. The fourth follows from (3.23), (3.24) and the accompanying argument. The η_i, $i = 1, \ldots, 6$, are determined up to a constant multiple because the coefficient matrix of (3.24) has rank 5.

Before closing this section, I wish to draw attention to a special tetrad. It has been said [6] that martensitic transformations are always accompanied by "a structural change having a dominant deviatoric component." In the context of the present discussion, the phrase quoted may be interpreted as saying that the equations $\boldsymbol{a} \cdot \boldsymbol{N}_{i=0}$, $i = 1, \ldots, e$, are approximately satisfied. In fact, a special tetrad has this property. If we take the vertices in the foreground of Figure 3c and move them around to the far side of the sphere, we get the structure shown in Figure 4. If we choose the normalized amplitude $\boldsymbol{a}$ of this tetrad to be parallel to a line segment which joins the central vertex to the center of S the equations $\boldsymbol{a} \cdot \boldsymbol{N}_i = 0$, $i = 1, \ldots, 6$, are approximately satisfied, the approximation getting closer as the three outer vertices approach the central one.

Several plane slices through this tetrad are also shown in Figure 4. They look remarkably similar to the 'needles' commonly seen in deformation-induced martensite. The book by HALL [26, Fig. 85] shows a particularly nice specimen, but they are common to many kinds of martensite [6, p. 164; 10, p. 348, 354; 26; p. 110]. One also commonly sees plates and 'butterflies' [6, p. 53] in martensite and these are all consistent with the results presented here.

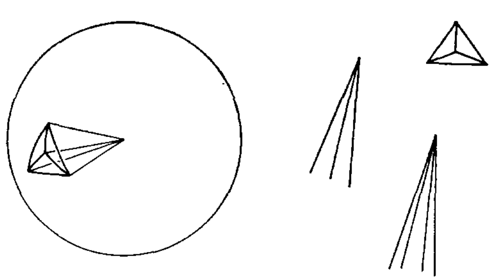

Fig. 4. A special tetrad, with plane slices.

4. Static theory of piecewise homogeneous deformations in finite elasticity

From now on I shall confine attention to the special case of finite elasticity. The definition of a twin, specialized to finite elasticity, and of a piecewise homogeneous deformation were given in Remarks 2 and 4 of § 2.

a. Equilibria

Let an elastic body $\mathscr{B}$ have a stored energy function $W(\boldsymbol{F})$ defined on a domain $\mathscr{D}$ relative to a reference shape $\mathscr{R}$. Suppose $\mathscr{R}$ is a sphere S[15] partitioned into regions $\mathscr{R}_1, \ldots, \mathscr{R}_f$. Let η_{ij}, $i = 1, \ldots, e, j = 1, \ldots, f$, be the incidence matrix for the partition. On each of the regions $\mathscr{R}_i$, $i = 1, \ldots, f$, let a constant deformation gradient $\boldsymbol{F}_i$ be assigned, consistent with the kinematic restrictions (3.10) and (3.11). The equilibrium equations for an elastic body free of body forces are

$$\int_{\partial \mathscr{P}} \boldsymbol{T}(\boldsymbol{F}) \boldsymbol{N} \, dA = 0, \quad \forall \mathscr{P} \subset \mathscr{R} \text{ with sufficiently regular boundaries.} \tag{4.1}$$

Here $\boldsymbol{T}$ is the Piola stress defined by (2.19). Under the conditions we have laid down on the deformation, the equilibrium equations (4.1) are equivalent to the conditions

$$\boldsymbol{Div}\, \boldsymbol{T}(\boldsymbol{F}) = 0 \quad \text{on} \quad \mathscr{R}_1, \ldots, \mathscr{R}_f, \tag{4.2}$$

and

$$(\boldsymbol{T}(\boldsymbol{F}_i) - \boldsymbol{T}(\boldsymbol{F}_j))\, \boldsymbol{N}_k = 0 \text{ whenever } \eta_{ki} = 1 \text{ and } \eta_{kj} = 1, \; k = 1, \ldots, e. \tag{4.3}$$

Of course, the equations (4.2) are already satisfied since $\boldsymbol{F}$ has been assumed constant on each of the regions $\mathscr{R}_1, \ldots, \mathscr{R}_f$. Thus, the study of equilibria of piecewise homogeneous deformations in finite elasticity is reduced to a study of the jump conditions (4.3)[16].

In this subsection I propose to study in general the equilibrium equations (4.3) for piecewise homogeneous deformations. I shall not impose particular boundary conditions, although I will give a characterization of equilibria which should help if one should wish to solve a particular boundary value problem. As mentioned in § 1, I shall illuminate the difference between ordinary piecewise homogeneous deformations and those special piecewise homogeneous deformations which are also twins.

By their silence on the matter, books (*e.g.* [2]) that discuss twinning suggest that a twin is, by definition, equilibrated. This is not true according to the definition I have given, even if the deformation is pairwise homogeneous. A non-trivial problem, which I shall discuss later in this Section, must be solved to assure the equilibrium of a twin.

---

[15] More generally, we could assume that $\mathscr{R}$ be diffeomorphic to S. See § 3 for the definition of a partition and the incidence matrix.

[16] Parry [9, (4.1) bis] takes the equilibrium equations to be $[\![\boldsymbol{T}]\!] = 0$. His conditions are therefore sufficient but not necessary for equilibrium. These jump conditions have also been given by Vladimirskii [15].

I shall begin with a pairwise homogeneous deformation; two regions $\mathscr{R}^+$ and $\mathscr{R}^-$ are separated by a plane P_N with normal N. I seek constant deformation gradients $F^- = F$ on $\mathscr{R}^-$ and $F^+ = F + a \otimes N$ on $\mathscr{R}^+$ such that

$$t(a, N, F) = (T(F + a \otimes N) - T(F))\, N = 0. \tag{4.4}$$

KNOWLES & STERNBERG [27] have shown that (4.4) can be recast in the form

$$t(a, N, F) = \int_0^1 [W_{FF}(F + \lambda a \otimes N) \cdot (a \otimes N)]\, N\, d\lambda. \tag{4.5}$$

They note that the necessary conditions $a \cdot t(a, N, F) = 0$, which follows immediately from (4.5), implies that there is a value $0 < \lambda^* < 1$ such that

$$[W_{FF}(F + \lambda^* a \otimes N) \cdot (a \otimes N)] \cdot (a \otimes N) \leqq 0. \tag{4.6}$$

In rectangular Cartesian components, (4.6) is

$$\frac{\partial^2 W(F + \lambda^* a \otimes N)}{\partial F^i_\alpha\, \partial F^j_\beta}\, a_i a_j N^\alpha N^\beta \leqq 0. \tag{4.7}$$

That is[17], *a necessary condition that the deformation*

$$\chi = \begin{cases} FX, & X \in \mathscr{R}^- \\ FX + a(N \cdot X), & X \in \mathscr{R}^+ \end{cases} \tag{4.8}$$

be equilibrated is that the condition of strong ellipticity, i.e.

$$[W_{FF}(G) \cdot (b \otimes M)] \cdot (b \otimes M) > 0 \quad \forall b, M,$$

fails for some $G \in \{A \mid A = F + \lambda a \otimes N$ *for some* $\lambda \in (0, 1)\}$.

Thus ellipticity fails somewhere in the domain of the stored energy function. To be definite I shall assume that the stored energy function has the qualitative features shown in Figure 5: There is an open set $\mathscr{S} \subset \mathscr{D}$ such that the condition of *ellipticity* fails in $\mathscr{S}$, and the condition of *strong ellipticity* holds in $\mathscr{D} - \overline{\mathscr{S}}$. For the rest of this paper all stored energy functions shall have this property.

In § 5 I shall study the stability of piecewise homogeneous deformations. The least restrictive kind of stability I shall consider, the kind which most clearly embodies the concept of 'infinitesmal stability', is that of a weak relative minimizer. A necessary condition that a point $X \in \mathscr{R}$ of differentiability of χ is a weak relative minimizer of the total energy (*cf.* § 4 for details) is that $\nabla\chi(X)$ be a point of ellipticity of the function W. For the stored energy functions considered here, every piecewise homogeneous weak relative minimum of the total energy must satisfy

$$F_i \in \mathscr{D} - \mathscr{S}, \quad i = 1, \ldots, f. \tag{4.9}$$

In my search for piecewise homogeneous equilibria, I will allow only deformation gradients which meet (4.9).

[17] KNOWLES & STERNBERG [27, § 3].

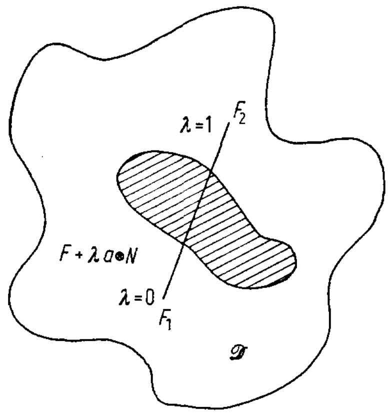

Fig. 5. The domain of the stored energy function. The condition of *strong ellipticity* (5.8) is met outside, and the condition of *ellipticity* fails inside the hatched region.

To study piecewise homogeneous equilibria I find it convenient to define the following **excess function**:

$$\mathscr{E}(\boldsymbol{b}, \boldsymbol{M}, \boldsymbol{G}) = W(\boldsymbol{G} + \boldsymbol{b} \otimes \boldsymbol{M}) - W(\boldsymbol{G}) - \boldsymbol{b} \cdot W_{\boldsymbol{F}}(\boldsymbol{G})\, \boldsymbol{M}. \tag{4.10}$$

$\mathscr{E}$ is defined on the set

$$\{(\boldsymbol{b}, \boldsymbol{M}, \boldsymbol{G}) \mid \boldsymbol{G} \in \mathscr{D} \quad \text{and} \quad \boldsymbol{G} + \boldsymbol{b} \otimes \boldsymbol{M} \in \mathscr{D}\}. \tag{4.11}$$

If we take the gradient of $\mathscr{E}$ with respect to $\boldsymbol{b}$ we get

$$\mathscr{E}_{\boldsymbol{b}} = (\boldsymbol{T}(\boldsymbol{G} + \boldsymbol{b} \otimes \boldsymbol{M}) - \boldsymbol{T}(\boldsymbol{G}))\, \boldsymbol{M}, \tag{4.12}$$

whence

Lemma 2. *The pairwise homogeneous deformation* (4.8) *is equilibrated if and only if*

$$\mathscr{E}_{\boldsymbol{b}}(\boldsymbol{a}, \boldsymbol{N}, \boldsymbol{F}) = 0. \tag{4.13}$$

If we take the second gradient of $\mathscr{E}$ with respect to $\boldsymbol{b}$, we get

$$\boldsymbol{l} \cdot \mathscr{E}_{\boldsymbol{b}\boldsymbol{b}} \boldsymbol{l} = [W_{\boldsymbol{F}\boldsymbol{F}}(\boldsymbol{G} + \boldsymbol{b} \otimes \boldsymbol{M}) \cdot (\boldsymbol{l} \otimes \boldsymbol{M})] \cdot (\boldsymbol{l} \otimes \boldsymbol{M}), \tag{4.14}$$

so we have

Lemma 3. $\mathscr{E}_{\boldsymbol{b}\boldsymbol{b}}$ *is positive-definite if and only if*

$$\boldsymbol{G} + \boldsymbol{b} \otimes \boldsymbol{M} \in \mathscr{D} - \overline{\mathscr{S}}. \tag{4.15}$$

Of special interest, especially for mechanical twinning, is the effect of the invariance groups (*cf.* (2.14)–(2.16)) upon the function $\mathscr{E}$ and the domain $\mathscr{S}$.

Lemma 4. *Let the stored energy $W(\boldsymbol{G})$ have a symmetry group $\mathscr{G}$ and let $\mathscr{O}^+$ denote the group of proper orthogonal tensors. Then, for each $\boldsymbol{Q} \in \mathscr{O}^+$ and $\boldsymbol{H} \in \mathscr{G}$,*

$$\boldsymbol{G} \in \mathscr{S} \Leftrightarrow \boldsymbol{Q}\boldsymbol{G}\boldsymbol{H} \in \mathscr{S}. \tag{4.16}$$

The function $\mathscr{E}(\boldsymbol{b}, \boldsymbol{M}, \boldsymbol{G})$ *meets the restrictions*

$$\mathscr{E}(\boldsymbol{Qb}, \boldsymbol{H}^T\boldsymbol{M}, \boldsymbol{QGH}) = \mathscr{E}(\boldsymbol{b}, \boldsymbol{M}, \boldsymbol{G}) \tag{4.17}$$

for all $\boldsymbol{Q} \in \mathscr{O}^+$, *all* $\boldsymbol{H} \in \mathscr{G}$, *and all* $(\boldsymbol{b}, \boldsymbol{M}, \boldsymbol{G})$ *in the domain of* $\mathscr{E}$.

The proof of (4.16) follows easily by differentiating twice the relation $W(\boldsymbol{QGH}) = W(\boldsymbol{G})$ with respect to $\boldsymbol{G}$, and then by contracting with the tensor $(\boldsymbol{b} \otimes \boldsymbol{M})$ twice. Equation (4.17) follows directly from the definition (4.10) of $\mathscr{E}$ and the invariance of W.

Lemma 4 implies that *if the limiting value of the deformation gradient on one side of a twin boundary lies in the domain of strong ellipticity of* W, *then so does the limiting value of the deformation gradient on the other side.*

If we take the gradient of (4.17) with respect to $\boldsymbol{b}$, and then use Lemma 2 we see that if $\boldsymbol{F}_0$ and $\boldsymbol{F}_0 + \boldsymbol{a}_0 \otimes \boldsymbol{N}_0$ are the deformation gradients of an equilibrated pairwise homogeneous deformation, then so are

$$\boldsymbol{QF}_0\boldsymbol{H} \quad \text{and} \quad \boldsymbol{QF}_0\boldsymbol{H} + \boldsymbol{Qa}_0 \otimes \boldsymbol{H}^T\boldsymbol{N} \tag{4.18}$$

for each $\boldsymbol{Q} \in \mathscr{O}^+$ and each $\boldsymbol{H} \in \mathscr{G}$. But more than that, if $\boldsymbol{F}_0$ and $\boldsymbol{F}_0 + \boldsymbol{a}_0 \otimes \boldsymbol{N}_0$ are the deformation gradients of an equilibrated homogeneous *twin*, then the pair of deformation gradients (4.18) also determine an equilibrated homogeneous twin. This is proved in

Lemma 5. *Let the homogeneous twin*

$$\hat{\boldsymbol{\chi}} = \begin{cases} \hat{\boldsymbol{F}}\boldsymbol{X}, & \boldsymbol{X} \in \hat{\mathscr{R}}^-, \\ \hat{\boldsymbol{F}}\boldsymbol{X} + \hat{\boldsymbol{a}}(\hat{\boldsymbol{N}} \cdot \boldsymbol{X}), & \boldsymbol{X} \in \hat{\mathscr{R}}^+, \end{cases} \tag{4.19}$$

$$\hat{\boldsymbol{F}} + \hat{\boldsymbol{a}} \otimes \hat{\boldsymbol{N}} = \hat{\boldsymbol{Q}}\hat{\boldsymbol{F}}\hat{\boldsymbol{H}},$$

be equilibrated:

$$\mathscr{E}_b(\hat{\boldsymbol{a}}, \hat{\boldsymbol{N}}, \hat{\boldsymbol{F}}) = 0. \tag{4.20}$$

Then, for any $\boldsymbol{Q} \in \mathscr{O}^+$ *and any* $\boldsymbol{H} \in \mathscr{G}$, *the deformation*,

$$\boldsymbol{\chi} = \begin{cases} \boldsymbol{Q}\hat{\boldsymbol{F}}\boldsymbol{H}\boldsymbol{X}, & \boldsymbol{X} \in \mathscr{R}^-, \\ \boldsymbol{Q}\hat{\boldsymbol{F}}\boldsymbol{H}\boldsymbol{X} + \boldsymbol{Q}\hat{\boldsymbol{a}}(\boldsymbol{H}^T\hat{\boldsymbol{N}} \cdot \boldsymbol{X}), & \boldsymbol{X} \in \mathscr{R}^+, \end{cases} \tag{4.21}$$

is an equilibrated homogeneous twin.

The statement made just before (4.18) shows that $\boldsymbol{\chi}$ is equilibrated. To prove that $\boldsymbol{\chi}$ is a twin, we must show that the conditions of invariance $(2.16)_2$ are fulfilled. But by (4.19)

$$\boldsymbol{Q}\hat{\boldsymbol{F}}\boldsymbol{H} + \boldsymbol{Q}\hat{\boldsymbol{a}} \otimes \boldsymbol{H}^T\hat{\boldsymbol{N}} = \boldsymbol{Q}(\hat{\boldsymbol{F}} + \hat{\boldsymbol{a}} \otimes \hat{\boldsymbol{N}})\boldsymbol{H} = \boldsymbol{Q}\hat{\boldsymbol{Q}}\hat{\boldsymbol{F}}\hat{\boldsymbol{H}}\boldsymbol{H}. \tag{4.22}$$

Let $\boldsymbol{R} = \boldsymbol{Q}\hat{\boldsymbol{Q}}\boldsymbol{Q}^T$, and $\boldsymbol{P} = \boldsymbol{H}^{-1}\hat{\boldsymbol{H}}\boldsymbol{H}$. Since $\mathscr{O}^+$ and $\mathscr{G}$ are groups $\boldsymbol{R} \in \mathscr{O}^+$ and $\boldsymbol{P} \in \mathscr{G}$. With these definitions (4.22) becomes

$$\boldsymbol{Q}\hat{\boldsymbol{F}}\boldsymbol{H} + \boldsymbol{Q}\hat{\boldsymbol{a}} \otimes \boldsymbol{H}^T\hat{\boldsymbol{N}} = \boldsymbol{R}(\boldsymbol{Q}\hat{\boldsymbol{F}}\boldsymbol{H})\,\boldsymbol{P}, \tag{4.23}$$

which shows that $\boldsymbol{\chi}$ is a twin. This completes the proof of Lemma 5.

The most interesting choices of Q and H in (4.21) are $\hat{Q}$ and $\hat{H}$, respectively. Then if we put $\hat{\mathscr{R}}^+ = \mathscr{R}^-$, we can combine the deformations $\hat{\chi}$ and χ to produce a collection of homogeneous equilibrated twins. That is, if $\hat{F}$ and $\hat{F} + \hat{a} \otimes \hat{N} = \hat{Q}\hat{F}\hat{H}$ form an equilibrated homogeneous twin having a twin plane with normal $\hat{N}$, then $\hat{Q}\hat{F}\hat{H}$ can form an equilibrated homogeneous twin with $\hat{Q}\hat{F}\hat{H} + \hat{Q}\hat{a} \otimes \hat{H}^T\hat{N}$ across a twin plane with normal $\hat{H}^T\hat{N}$. Complicated collections of equilibrated twins can be built up in this way, based upon the partitions analyzed in § 3. It is not my purpose to elaborate on this observation but only to provide some of the groundwork for the solution of such problems.

To form these collections of twins, one starts with a single pairwise homogeneous equilibrated twin. The existence of a single pairwise homogeneous equilibrated deformation actually implies the existence of many more than are indicated by (4.18). These are summarized in

Theorem 1. *Suppose the pairwise homogeneous deformation*

$$\chi_0 = \begin{cases} F_0X, & X \in \mathscr{R}^- \\ F_0X + a_0(N_0 \cdot X), & X \in \mathscr{R}^+ \end{cases} \tag{4.24}$$

is equilibrated,

$$\mathscr{E}_b(a_0, N_0, F_0) = 0 \tag{4.25}$$

and satisfies

$$F_0 \in \mathscr{D} - \bar{\mathscr{S}}, \quad F_0 + a_0 \otimes N_0 \in \mathscr{D} - \bar{\mathscr{S}}. \tag{4.26}$$

Then there is a unique, continuously differentiable function

$$a = \alpha(N, F), \quad \alpha(N_0, F_0) = a_0, \tag{4.27}$$

defined on a neighborhood $\mathscr{N}_0$ of (N_0, F_0) such that $\alpha(N, F)$ is the amplitude of an equilibrated pairwise homogeneous deformation:

$$\mathscr{E}_b(\alpha(N, F), N, F) = 0 \quad \forall (N, F) \in \mathscr{N}_0. \tag{4.28}$$

The domain of definition of $\alpha(N, F)$ may be extended to the set

$$\mathscr{N} \equiv \{(N, F) \mid (H^TN, QFH) \in \mathscr{N}_0 \text{ for some } Q \in \mathscr{O}^+ \text{ and some } H \in \mathscr{G}\}. \tag{4.29}$$

The function $\alpha(N, F)$ enjoys the invariance

$$\begin{aligned} Q\alpha(N, F) &= \alpha(H^TN, QFH), \\ &\forall Q \in \mathscr{O}^+ \\ &\forall H \in \mathscr{G} \\ &\forall (N, F) \in \mathscr{N}. \end{aligned} \tag{4.30}$$

Proof. The existence of $\alpha(N, F)$ follows from the implicit function theorem. Since

$$\mathscr{E}_b(a, N, F) = 0 \tag{4.31}$$

is satisfied at $(\boldsymbol{a}_0, \boldsymbol{N}_0, \boldsymbol{F}_0)$ and

$$\mathscr{E}_{bb}(\boldsymbol{a}_0, \boldsymbol{N}_0, \boldsymbol{F}_0) \tag{4.32}$$

is positive definite (Lemma 3 and (4.26)), there is a unique continuously differentiable function $\boldsymbol{a} = \boldsymbol{\alpha}(\boldsymbol{N}, \boldsymbol{F})$ defined on a neighborhood $\mathscr{N}_0$ of $(\boldsymbol{N}_0, \boldsymbol{F}_0)$ which satisfies (4.28). The extension of $\mathscr{N}_0$ to $\mathscr{N}$ is accomplished by the use of (4.17). Let $(\boldsymbol{N}, \boldsymbol{F}) \in \mathscr{N}_0$ and define

$$\boldsymbol{\alpha}(\boldsymbol{H}^T\boldsymbol{N}, \boldsymbol{QFH}) = \boldsymbol{Q}\boldsymbol{\alpha}(\boldsymbol{N}, \boldsymbol{F}),$$

to obtain the extension of $\boldsymbol{\alpha}$ to $\mathscr{N}$. It can easily be shown that the extended function $\boldsymbol{\alpha}(\cdot, \cdot)$ is uniquely defined, single valued, and continuously differentiable on $\mathscr{N}$. The invariance (4.30) then follows by (4.33). This completes the proof of Theorem 1.

b. Stability

We shall suppose an elastic body $\mathscr{B}$ deformed relative to a fixed reference shape $\mathscr{R}$ is governed by a stored energy function $W(\boldsymbol{F})$. This energy function shall have the properties summarized in Figure 5 and described in § 4a.

Let us be given the pairwise homogeneous deformation

$$\tilde{\boldsymbol{\chi}}(X) = \begin{cases} \boldsymbol{F}^-\boldsymbol{X}, & \boldsymbol{X} \in \mathscr{R}^-, \\ \boldsymbol{F}^+\boldsymbol{X} = \boldsymbol{F}^-\boldsymbol{X} + \boldsymbol{a}(\boldsymbol{N}\cdot\boldsymbol{X}), & \boldsymbol{X} \in \mathscr{R}^+; \end{cases} \tag{4.33}$$

$$\mathscr{R} = \mathscr{R}^+ \cup \mathscr{R}^-, \qquad \mathscr{P}_N = \overline{\mathscr{R}}^+ \cap \overline{\mathscr{R}}^-;$$

$$\boldsymbol{F}^+ \in \mathscr{D}, \qquad \boldsymbol{F}^- \in \mathscr{D}.$$

On $\partial\mathscr{R}$ there will occur Piola tractions $\boldsymbol{t}^+ = \boldsymbol{T}^+\boldsymbol{M}$ and $\boldsymbol{t}^- = \boldsymbol{T}^-\boldsymbol{M}$ produced by the Piola stress $\boldsymbol{T}^+ \equiv \boldsymbol{T}(\boldsymbol{F}^+)$ in $\mathscr{R}^+$ and $\boldsymbol{T}^- \equiv \boldsymbol{T}(\boldsymbol{F}^-)$ in $\mathscr{R}^-$.

To be definite I shall assume that the body $\mathscr{B}$ is loaded by dead loads corresponding to the surface tractions $\boldsymbol{t}^+$ on $\partial\mathscr{R}^+ - \mathscr{P}_N$ and $\boldsymbol{t}^-$ on $\partial\mathscr{R}^- - \mathscr{P}_N$. The reader is probably aware of the degeneracy, with respect to rigid rotations, implied by the dead load stability criterion; for compressive loads one might also wish to impose a zero-moment condition [28], or possibly additional kinematic boundary conditions, in order to obtain useful solutions. Here I shall avoid such additional restrictions and concentrate on the simplest kinds of problems.

I shall only treat pairwise homogeneous deformations and homogeneous twins although it is easy to see how the results can be generalized to include piecewise homogeneous deformations and homogeneous trillings, *etc.*

The total energy of $\mathscr{B}$, dead loaded by Piola surface tractions $\boldsymbol{t}^+$ on $\partial\mathscr{R}^+ - \mathscr{P}_N$ and $\boldsymbol{t}^-$ on $\partial\mathscr{R}^- - \mathscr{P}_N$, is defined by

$$E[\boldsymbol{\chi}] \equiv \int_{\mathscr{R}} W(\nabla\boldsymbol{\chi})\, dV - \int_{\partial\mathscr{R}^+ - \mathscr{P}_N} \boldsymbol{t}^+ \cdot \boldsymbol{\chi}\, dA - \int_{\partial\mathscr{R}^- - \mathscr{P}_N} \boldsymbol{t}^- \cdot \boldsymbol{\chi}\, dA. \tag{4.34}$$

The domain of $E[\cdot]$ consists of all deformations $\boldsymbol{\chi}$ such that $\nabla\boldsymbol{\chi}$ is well defined[18]

[18] *E.g.* $\boldsymbol{\chi}$ is continuous and weakly differentiable [29, p. 142]. Note that the definition (4.34) includes loading by a hydrostatic pressure if $\boldsymbol{t}^+ = \boldsymbol{t}^- = 0$ and if W is interpreted as the enthalpy.

almost everywhere and $\nabla\chi \in \mathscr{D}$ almost everywhere. I seek necessary and sufficient conditions that $\tilde{\chi}$ given by (4.33) is a minimizer of $E[\cdot]$ in a sense I shall presently make definite.

The study of problems of change of phase in elastic bar theory [30, 31] indicates that solid bars are likely to occur in 'metastable' as well as 'stable 'configurations. The terms stable and metastable refer to the size of the class of functions which compete for the minimum of $E[\cdot]$. These studies suggest that one should use caution when comparing the results of experiment with deformations which minimize $E[\cdot]$ with respect to all possible deformations. On the other hand, necessary conditions satisfied by weak relative minima of $E[\cdot]$ (defined below) seem to be consistent with all kinds of static experiments. This is not to say that absolute minimizers of $E[\cdot]$ are unimportant, just that caution should be used in their interpretation.

We shall say that $\tilde{\chi}$ is a **weak relative minimizer** of $E[\cdot]$ if there is a $\delta > 0$ such that each χ in the domain of $E[\cdot]$ which meets the condition[19]

$$\|\nabla\chi - \nabla\tilde{\chi}\| < \delta \quad \text{a.e.}, \tag{4.35}$$

also satisfies

$$E[\tilde{\chi}] \leqq E[\chi]. \tag{4.36}$$

$\tilde{\chi}$ will be termed a **strong relative minimizer** of $E[\cdot]$ if for some $\varepsilon > 0$ and every χ in the domain of $E[\cdot]$ which satisfies

$$|\chi - \tilde{\chi}| < \varepsilon, \tag{4.37}$$

we have

$$E[\tilde{\chi}] \leqq E[\chi]. \tag{4.38}$$

Finally, $\tilde{\chi}$ is a **minimizer** of $E[\cdot]$ if for every χ in the domain of $E[\cdot]$,

$$E[\tilde{\chi}] \leqq E[\chi]. \tag{4.39}$$

We begin with a study of pairwise homogeneous weak relative minima. If $\tilde{\chi}$ given by (4.33) is a weak relative minimizer of $E[\cdot]$, then

(I) $\tilde{\chi}$ is equilibrated (*cf.* 4.3),

$$(\boldsymbol{T}(\boldsymbol{F}^+) - \boldsymbol{T}(\boldsymbol{F}^-))\,\boldsymbol{N} = 0, \text{ and} \tag{4.40}$$

(II) $\boldsymbol{F}^+$ and $\boldsymbol{F}^-$ are points of ellipticity of the function W.[20] (4.41)

Both of these conditions have been used in the study of equilibria § 3a. They are both true for a broad class of loading devices. By the use of (4.40) and the divergence theorem, we can write the total energy in the form

$$E[\chi] = \int_{\mathscr{R}^+} (W(\nabla\chi) - \boldsymbol{T}^+ \cdot \nabla\chi)\, dV + \int_{\mathscr{R}^-} (W(\nabla\chi) - \boldsymbol{T} \cdot \nabla\chi)\, dV. \tag{4.42}$$

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[19] By definition, $\|\boldsymbol{F}\| = (\boldsymbol{F} \cdot \boldsymbol{F})^{\frac{1}{2}} = tr\, \boldsymbol{F}\boldsymbol{F}^T$.

[20] See *e.g.* Coral [32]. Coral's proof is adapted to finite elasticity in the forthcoming book by Truesdell [33].

Let the competitor χ be given by

$$\chi(X) = \begin{cases} GX, & X \in \mathscr{R}^-, \\ GX + b(M \cdot X), & X \in \mathscr{R}^+; \end{cases} \tag{4.43}$$

$$G, b, M \text{ constant},$$

in which

$$\|G - F^-\| < \delta \tag{4.44}$$

and

$$\|G + b \otimes M - F^+\| < \delta. \tag{4.45}$$

Then, if δ is sufficiently small, χ is a competitor for the weak relative minimum. If we substitute χ into (4.42) and use (4.36), we find that for all constant G, b, M consistent with (4.44) and (4.45),

$$\begin{aligned} &\{W(G + b \otimes M) - W(F^+) - (G + b \otimes M - F^+) \cdot T^+\} V^+ \\ &\quad + \{W(G) - W(F^-) - (G - F^-) \cdot T^-\} V^- \geqq 0. \end{aligned} \tag{4.46}$$

Here V^+ and V^- are the volumes of the reference shapes $\mathscr{R}^+$ and $\mathscr{R}^-$, respectively. So far, I have been unable to show, and perhaps it is not true, that each bracketed term in (4.46) must necessarily be non-negative.

Suppose for a moment that each bracketed term of (4.46) by itself is non-negative for the specified set of G, b, M. Then, in particular,

$$W(G) - W(F^-) - (G - F^-) \cdot T^- \geqq 0 \quad \forall G \text{ such that } \|G - F^-\| < \delta. \tag{4.47}$$

By putting $K = G + b \otimes M$, we also have

$$W(K) - W(F^+) - (K - F^+) \cdot T^+ \geqq 0 \quad \forall K \text{ such that } \|K - F^+\| < \delta. \tag{4.48}$$

Let χ be any deformation in the domain of $E[\cdot]$ which meets the condition (4.35). Put $K = K(X) \equiv \nabla\chi(X)$, $X \in \mathscr{R}^+$, and $G = G(X) \equiv \nabla\chi(X)$, $X \in \mathscr{R}^-$. Then (4.47) and (4.48) hold at each X. If we then integrate (4.47) over $\mathscr{R}^-$ and (4.48) over $\mathscr{R}^+$ and add the two expressions, we recover (4.42). Summarizing these arguments, we have

Theorem 2. *Necessary conditions that the pairwise homogeneous deformation* $\tilde{\chi}$ *be a weak relative minimizer of* $E[\cdot]$ *are* (4.40) *and* (4.41), *as well as the inequality* (4.46).

Sufficient conditions that the pairwise homogeneous deformation $\tilde{\chi}$ *be a weak relative minimizer of* $E[\cdot]$ *are that* $\tilde{\chi}$ *be equilibrated* (cf. (4.40)) *and that the local inequalities* (4.47) *and* (4.48) *be satisfied.*

We now turn to a study of the strong relative minima of $E[\cdot]$. Already one theorem is known.[21] If $\tilde{\chi}$ is a strong relative minimum of $E[\cdot]$, then the condition

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[21] *Loc. cit.* CORAL and TRUESDELL.

of *rank-one convexity* holds at $\tilde{\chi}$, *viz*,

$$\begin{gathered} W(\boldsymbol{F}^{\pm} + \boldsymbol{b} \otimes \boldsymbol{M}) - W(\boldsymbol{F}^{\pm}) - \boldsymbol{b} \cdot \boldsymbol{T}^{\pm}\boldsymbol{M} \geqq 0 \\ \forall \boldsymbol{b}, \boldsymbol{M}, \text{ such that } \boldsymbol{F}^{\pm} + \boldsymbol{b} \otimes \boldsymbol{M} \in \mathscr{D}. \end{gathered} \tag{4.49}$$

If in (4.49) we choose $\boldsymbol{b} = \boldsymbol{a}$, $\boldsymbol{M} = \boldsymbol{N}$ and $(-)$, we get

$$W(\boldsymbol{F}^{+}) - W(\boldsymbol{F}^{-}) - \boldsymbol{a} \cdot \boldsymbol{T}^{-}\boldsymbol{N} = 0; \tag{4.50}$$

if we choose $\boldsymbol{b} = -\boldsymbol{a}$, $\boldsymbol{M} = \boldsymbol{N}$ and $(+)$, we get

$$W(\boldsymbol{F}^{-}) - W(\boldsymbol{F}^{+}) + \boldsymbol{a} \cdot \boldsymbol{T}^{+}\boldsymbol{N} \geqq 0. \tag{4.51}$$

Assuming the necessary condition $\boldsymbol{T}^{+}\boldsymbol{N} = \boldsymbol{T}^{-}\boldsymbol{N}$ to hold, (4.50) and (4.51) imply that

$$W(\boldsymbol{F}^{+}) - W(\boldsymbol{F}^{-}) - \boldsymbol{a} \cdot \boldsymbol{T}^{\pm}\boldsymbol{N} = 0. \tag{4.52}$$

If $\tilde{\chi}$ is also a mechanical twin, then $\boldsymbol{F}^{+} = \boldsymbol{Q}\boldsymbol{F}^{-}\boldsymbol{H}$ so $W(\boldsymbol{F}^{+}) = W(\boldsymbol{F}^{-})$; therefore (4.52) implies that $\boldsymbol{a} \cdot \boldsymbol{T}^{\pm}\boldsymbol{N} = 0$.

Theorem 3. *If* $\tilde{\chi}$ *given by* (4.33) *is a strong relative minimum of* $E[\cdot]$, *then*

$$W(\boldsymbol{F}^{+}) - W(\boldsymbol{F}^{-}) - \boldsymbol{a} \cdot \boldsymbol{T}^{\pm}\boldsymbol{N} = 0. \tag{4.53}$$

If, in addition, $\tilde{\chi}$ *is a mechanical twin, then the traction on the twin plane is perpendicular to the amplitude of the twin*:

$$\boldsymbol{a} \cdot \boldsymbol{T}^{\pm}\boldsymbol{N} = 0.\text{[22]} \tag{4.54}$$

We now assume $\tilde{\chi}$ is a minimizer of $E[\cdot]$. The necessary condition (4.46) still holds for minima, but for the large class of $(\boldsymbol{G}, \boldsymbol{b}, \boldsymbol{M})$ given by

$$\boldsymbol{G} \in \mathscr{D}, \qquad \boldsymbol{G} + \boldsymbol{b} \otimes \boldsymbol{M} \in \mathscr{D}. \tag{4.55}$$

Also, (4.53) is satisfied since every minimizer is a strong relative minimizer. Therefore, if in (4.46) we eliminate $W(\boldsymbol{F}^{+})$ by use of (4.53), if we replace $\boldsymbol{F}^{+}$ by $\boldsymbol{F}^{-} + \boldsymbol{a} \otimes \boldsymbol{N}$, and we put $\boldsymbol{b} = 0$, we obtain

$$\begin{gathered} \{W(\boldsymbol{G}) - W(\boldsymbol{F}^{-}) - (\boldsymbol{G} - \boldsymbol{F}^{-}) \cdot \boldsymbol{T}^{+}\}\, V^{+} \\ + \{W(\boldsymbol{G}) - W(\boldsymbol{F}^{-}) - (\boldsymbol{G} - \boldsymbol{F}^{-}) \cdot \boldsymbol{T}^{-}\}\, V^{-} \geqq 0 \qquad \forall \boldsymbol{G} \in \mathscr{D}. \end{gathered} \tag{4.56}$$

Equivalently, we have

$$W(\boldsymbol{G}) - W(\boldsymbol{F}^{-}) - (\boldsymbol{G} - \boldsymbol{F}^{-}) \frac{V^{+}\boldsymbol{T}^{+} + V^{-}\boldsymbol{T}^{-}}{V^{+} + V^{-}} \geqq 0 \qquad \forall \boldsymbol{G} \in \mathscr{D}. \tag{4.57}$$

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[22] Several of the results deduced in this section are true for a wide variety of deformations and loading devices. In particular, (4.54), (4.53) and (4.41) are true for a broad class of loading devices, and without the restriction to pairwise homogeneous deformations, as long as $\boldsymbol{F}^{+}$, $\boldsymbol{F}^{-}$, $\boldsymbol{T}^{+}$ and $\boldsymbol{T}^{-}$ are assumed to be limiting values as the surface of discontinuity is approached from either side.

Put $G = F^- + \mu K$, μ being a sufficiently small scalar and K being a momentarily fixed second order tensor. Then the left hand side of (4.57) becomes a non-negative function of μ which vanishes at $\mu = 0$. Thus the derivative of the left hand side of (4.57) must vanish at $\mu = 0$:

$$W_F(F^-) \cdot K - \left(\frac{V^+T^+ - V^-T^-}{V^+ + V^-}\right) \cdot K = 0. \tag{4.58}$$

Therefore

$$T^- = \frac{V^+T^+ + V^-T^-}{V^+ + V^-}, \tag{4.59}$$

that is,

$$T^- = T^+ \equiv T; \tag{4.60}$$

for pairwise homogeneous minima $\tilde{\chi}$ of $E[\cdot]$, the Piola stresses in $\mathscr{R}^+$ and $\mathscr{R}^-$ are the same.

Now (4.57) becomes

$$W(G) - W(F^-) - (G - F^-) \cdot T \geqq 0 \quad \forall G \in \mathscr{D}. \tag{4.61}$$

Since we may simply interchange the roles of (+) and (−) the inequality (4.61) also holds with F^- replaced by F^+. But (4.60), (4.61), and its counterpart for (+), are sufficient for $\tilde{\chi}$ to be a minimizer of $E[\cdot]$. To see this we simply repeat the argument given just before Theorem 2 with G and K only restricted by the conditions $G \in \mathscr{D}$ and $K \in \mathscr{D}$.

Still letting the minimizer $\tilde{\chi}$ be equilibrated by a constant Piola stress T, we note that the Cauchy stress σ defined by $\sigma \equiv (\det F)^{-1} T F^T$, is symmetric:

$$TF^T \text{ is symmetric for } F = F^+ \text{ or } F^-. \tag{4.62}$$

Therefore

$$T(F^-)^T \text{ is symmetric}$$

and

$$T(F^- + a \otimes N)^T \text{ is symmetric.} \tag{4.63}$$

If we eliminate $T(F^-)^T$ from $(4.63)_2$ by the use of $(4.63)_1$, we get

$$TN \otimes a = a \otimes TN; \tag{4.64}$$

that is, TN is parallel to a; *if $\tilde{\chi}$ is a pairwise homogeneous minimum of $E[\cdot]$, then the traction on $\mathscr{P}_N$ is parallel to the amplitude a.*

According to (4.54) the statement just made cannot be true for a twin unless the traction on $\mathscr{P}_N$ vanishes, a result obtained in a special case by PARRY [9]. I summarize these properties of pairwise homogeneous minima in

Theorem 4. *The pairwise homogeneous deformation $\tilde{\chi}$ of* (4.33) *is a minimizer of* $E[\cdot]$ *if and only if*

$$\begin{gathered} T^+ = T^-, \\ W(G) - W(F^-) - (G - F^-)\, T^- \geqq 0 \quad \forall G \in \mathscr{D}, \\ W(K) - W(F^+) - (K - F^+)\, T^+ \geqq 0 \quad \forall K \in \mathscr{D}. \end{gathered} \tag{4.65}$$

If $\tilde{\chi}$ is also a twin, the traction on $\mathscr{P}_N$ vanishes:

$$T^{+}N = 0. \tag{4.66}$$

These strong conditions suggest that it is unlikely that many of the deformations observed in experiment correspond to minimizers of $E[\cdot]$ under dead loading. The condition (4.54), however, is true for a large class of loading devices, and deserves further study.

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Division of Engineering
Brown University
Providence, Rhode Island

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