STABLE EQUILIBRIUM CONFIGURATIONS OF ELASTIC CRYSTALS

BY

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IMA Preprint Series # 177
September 1985

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STABLE EQUILIBRIUM CONFIGURATIONS OF ELASTIC CRYSTALS

J.L. Ericksen

For J.B. Serrin on his 60th birthday

I. Introduction

Nonlinear thermoelasticity theory for crystals is generating some knotty questions in the calculus of variations and in the theory of related partial differential equations. This stems from invariance assumptions which are suggested by molecular theory, and seem to be needed to analyze some commonly observed phenomena, such as twinning. What might be regarded as the simplest problem is to characterize the most stable configurations of unloaded crystals. Even this is difficult, because these are not at all unique, but form infinite sets. A number of these do seem to match configurations observed in real crystals. After elaborating this a bit, I will present methods for constructing solutions which are special, but resemble configurations which are observed.

2. Crystal Elasticity

Kinematical descriptions of crystal configurations and their symmetries are discussed in detail by Pitteri [1,2]. Some of the simpler kinds are adequately described by a set of three linearly independent vectors e_a ($a = 1,2,3$), called lattice vectors. Then, two such sets e_a and $\overline{e}_a$ describe the same configuration provided

$$\overline{e}_a = m_a^b e_b, \quad (2.1)$$

where the m_a^b are integers such that

$$\det m = \pm 1, \quad m \stackrel{\text{def}}{=} \|m_a^b\|. \quad (2.2)$$

Under the obvious rule for composing these linear transformations, they form a group G ,

$$m \in G, \quad (2.3)$$

which is infinite, discrete and not compact. Essentially, molecular theories of elasticity are schemes for calculating ϕ , the Helmholtz free energy per unit mass, as a function of lattice vectors and temperature T ,

$$\phi = \phi(e_a, T). \quad (2.4)$$

In some situations, for example for the quartz problems discussed by James [3], one finds that additional variables are needed, for an adequate description. Other difficulties are encountered in dealing with long range interactions. However, (2.4) seems to apply to a variety of crystals. When it does, one should get a single value of ϕ for a single configuration, so ϕ should be invariant under G ,

$$\phi(m_a^b e_b, T) = \phi(e_a, T), \quad m \in G. \quad (2.5)$$

The notion that rotating a configuration should not alter this energy gives rise to the additional invariance that, for any rotation R ,

$$R^{-1} = R^T, \quad \det R = 1, \quad (2.6)$$

$$\phi(R e_a, T) = \phi(e_a, T). \quad (2.7)$$

To get to elasticity or thermoelasticity theory, the usual practice is to introduce the Born hypothesis, which is discussed in detail by Ericksen [4].

Briefly, one picks some reference configuration, including a definite choice of (constant) reference lattice vectors E_a . Then, the assumption is that a macroscopic deformation $x = \chi(X)$, with gradient

$$F = \nabla \chi, \quad \det F > 0, \quad (2.8)$$

takes E_a to e_a , a possible set of lattice vectors in the deformed configuration, given by the formula

$$e_a = F E_a. \quad (2.9)$$

Thus

$$\phi(e_a, T) = \phi(F E_a, T) = \tilde{\phi}(F, T), \quad (2.10)$$

the E_a being regarded as fixed. To describe the invariance of $\tilde{\phi}$, we define, for each $m \in G$, a linear transformation $H(m)$ by the rule

$$H(m)E_a = m_a^b E_b, \quad (2.11)$$

such H satisfying

$$\det H = \pm 1, \quad (2.12)$$

and generating a group $\bar{G}$ conjugate to G . Then, by easy calculation,

$$\tilde{\phi}(RFH, T) = \tilde{\phi}(F, T), \quad H \in \bar{G}. \quad (2.13)$$

Commonly, such invariances are obscured by approximations made in calculating thermodynamic potentials from molecular theory. However, examples of molecular theories consistent with the above description can be found, for example in the works of Eftis, MacDonald and Arkilic [5] and Ericksen [6].

The indicated invariance causes $\tilde{\phi}$ to have some unusual properties. Since G and $\bar{G}$ are not compact, one can pick any F in the domain of $\tilde{\phi}$, and find a sequence $H_n \in \bar{G}$ with FH_n unbounded as $n \rightarrow \infty$. Thus, the assumption that $\tilde{\phi} \rightarrow \infty$ when F grows large is untenable. Similarly, the invariance prevents $\tilde{\phi}$ from satisfying the Legendre-Hadamard condition for all kinematically possible values of F . These and other idiosyncracies are collected and discussed by

Fonseca [7], who includes relevant references. At least to those familiar to the calculus of variations, this might be enough to indicate that we face unusual difficulties, in trying to apply it.

To sketch one of the simplest problems, consider that of determining the stablest equilibrium configurations of an unloaded crystal, with T considered as a control parameter. Much the same problems arise, for crystals subject to an hydrostatic pressure. Mathematically, we should find the absolute minima of the functional

$$\int_{\Omega} \tilde{\phi}(F, T) \rho dv, \quad (2.14)$$

where ρ is a positive constant, the mass density, and Ω is the region occupied by a body in the reference configuration. Make Ω as simple and smooth as you like, assume $\tilde{\phi}$ very smooth, etc. to simplify matters as much as is possible. Here, there are no constraints on deformation, so we can begin by trying to minimize the integrand. This might well be possible. Suppose that for some constant $F = F_0$, with $\det F_0 > 0$, we have

$$\tilde{\phi}(F, T) > \tilde{\phi}(F_0, T), \quad (2.15)$$

for all F in the domain of $\tilde{\phi}$. This gives us, as a very simple minimizer, a homogeneous configuration with constant lattice vectors. Of course, with (2.13), we have an infinite collection of similar minimizers, with deformation gradients of the form

$$RF_0H. \quad (2.16)$$

Were $\mathcal{G}$ a continuous group, we might find a smooth inhomogeneous deformation, with F taking values in this set, but one can show that here, this is impossible. One could have additional minimizers not so related by invariance and, physically, this can happen at isolated temperatures, but we ignore this.

A complication is suggested by observations of twinning. Physically, it seems quite reasonable to regard twinned configurations as minimizers. Generalizing this idea, we should allow configurations for which F is piecewise continuous, as long as the displacement remains continuous. If $R_1 F_0 H_1$ and $R_2 F_0 H_2$ are two values in neighboring regions, meeting at a smooth surface with normal N in the reference configuration, the usual kinematical conditions of compatibility require that there exist a vector A satisfying

$$R_2 F_0 H_2 = R_1 F_0 H_1 (1 + A \otimes N). \quad (2.17)$$

One can normalize this by requiring that N be a unit vector, but I find it more convenient to use different normalizations in different cases. I will just assume that $A \otimes N = 0$ only if $A = 0$. With F_0 , the R 's and H 's constant, it is clear that A and N can be taken as constant so, where smooth, such surfaces are planes. As is discussed by James [8,9], one can deduce additional restrictions, if more than two such regions should meet. Briefly, there are many possibilities for so tacking together these homogeneous deformations and, to some extent, they depend on the function $\tilde{\phi}$, or at least on the values of its minimizers. What we would like to do is to get a good intuitive picture of all of the possibilities. Presently, I don't know how best to accomplish this, so we'll try to better understand some of the subsets.

In terms of analyzing (2.17), there is no real loss of generality in setting $R_1 = H_1 = 1$, since F_0 is simply one of the set of minimizers. Looked at differently, if we set

$$\begin{aligned} R &= R_1^T R_2, \quad H = H_2 H_1^{-1} \\ \bar{A} &= H_1 A, \quad \bar{N} = H_1^{-T} N, \end{aligned} \quad (2.18)$$

(2.17) reduces to much the same thing, viz.

$$RF_0H = F_0(1 + \bar{A} \otimes \bar{N}). \quad (2.19)$$

I will assume that H belongs to the subgroup $\bar{G}^+$ of $\bar{G}$ defined by

$$\det H = 1 \iff \det m = 1, \quad (2.20)$$

there being no real loss of generality in doing this. Then, by taking determinants of both sides of (2.19), we find that

$$\det(1 + \bar{A} \otimes \bar{N}) = 1 \iff \bar{A} \cdot \bar{N} = 0 \quad (2.21)$$

By setting

$$a = F_0\bar{A}, \quad n = F_0^T\bar{N} \Rightarrow a \cdot n = 0, \quad (2.22)$$

we can rewrite (2.19) as

$$RF_0H = (1 + a \otimes n)F_0. \quad (2.23)$$

One can think of picking values of F_0 and H , and solving the latter for R , a and n , if possible. As is established by Ericksen [10], it is impossible unless

$$\det(JJ^T - 1) = 0, \quad (2.24)$$

where

$$J \stackrel{\text{def}}{=} F_0H^{-1}F_0^{-1}. \quad (2.25)$$

If (2.24) holds, then either

$$JJ^T = 1 \Rightarrow a = 0 \quad (2.26)$$

or there are two non-trivial solutions.* Given (R, a, n) for one, one can get corresponding values $(\bar{R}, \bar{a}, \bar{n})$ for the other by using the following prescriptions:

$$2\bar{a} = -\|n\|^2 a + n, \quad (2.27)$$

$$(\|a\|^2 \|n\|^2 + 4)\bar{n} = 4a + 2\|n\|^2 n, \quad (2.28)$$

Then, set

$$\bar{R} = \hat{R}R, \quad (2.29)$$

where

$$\hat{R} = (1 + \bar{a} \otimes \bar{n})(1 - a \otimes n). \quad (2.30)$$

It is straightforward to verify that $\hat{R}$ is a rotation, and that the prescriptions deliver the second solution. This does give one characterization of solutions, and a way of constructing numerous examples, but we would like some better way of picturing the possibilities.

At least for intuitive purposes and for making contact with works on crystallography, it can be useful to revert to the description in terms of lattice vectors, eliminating the rather arbitrary reference configuration. Set

$$e_a = F_0 E_a \quad (2.31)$$

and use (2.11) and (2.23) to get the equivalent

$$\begin{aligned} RF_0 H E_a &= RF_0^m E_a^b = Rm_a^b e_b \\ &= S e_a, \end{aligned} \quad (2.32)$$

* For this purpose, we count solutions obtained by multiplying a by a scalar, and dividing n by it, as the same.

where

$$S = 1 + a \times n. \quad (2.33)$$

That is, we can get lattice vectors on the other side of the plane by applying this simple shear to e_a , or we can get them by applying R and m as indicated. Some special cases are now well understood. Cases summarized in (2.26) translate to the condition that

$$R m_a^b e_b = e_a. \quad (2.34)$$

This means that R is an element of the crystallographic point group for these lattice vectors. In the terminology used by Ericksen [11], m belongs to the corresponding lattice group. From the theory of these groups, we know that they are finite, conjugate and different for different choices of e_a . Also, we must have

$$R^N = m^N = 1, \quad N = 1, 2, 3, 4 \text{ or } 6. \quad (2.35)$$

This covers the trivial solutions, involving no shear. There is another infinite set of solutions for which $R = 1$, so that

$$S e_a = m_a^b e_b. \quad (2.36)$$

There are the so-called lattice invariant shears, discussed in detail by Ericksen [4], things considered by metallurgists seeking to determine what deformations have taken place in certain phase transformations. For these, the x-ray crystallographer sees the lattice vectors as continuous, but one can need to consider them to analyze shapes of crystallites. Here, such m 's do not depend on the choice of e_a .

The more common forms of twinning involve choices of m such that $m^2 = 1$. Then, as is discussed in detail by Pitteri [12], (2.31) can be solved for any

choice of e_a and solutions have the property that

$$m^2 = 1 \Rightarrow R^2 = 1. \quad (2.37)$$

Solutions can be of the form (2.34) or be non-trivial, depending on the choice of m and e_a . Pitteri also includes an interesting example showing that

$$R^2 = 1 \nRightarrow m^2 = 1, \quad (2.38)$$

pointing out that one will either have $m^2 = 1$ or m^N unbounded as $N \rightarrow \infty$, if $R^2 = 1$. Further, Pitteri has shown me a proof that, given any $m \in G$, with $\det m = 1$, we can find choices of e_a such that (2.13) can be satisfied or, equivalently, such that (2.24) holds, for the corresponding arguments.

A characterization of solutions possible with H similar to a rotation is given by Ericksen [10], who notes that this is equivalent to the assumption that

$$H^N = 1 \Leftrightarrow m^N = 1, \quad N = 1, 2, 3, 4 \text{ or } 6. \quad (2.39)$$

The case $N = 1$ is trivial and $N = 2$, covered by (2.36) is well understood, so cases with $N > 2$ are of more interest. At first, I thought that this might be a way of characterizing certain kinds of observed patterns, the "rotation twins" which are described by Barrett and Massalski [13, p. 406]. It is not, but there is some connection. Later, I will elaborate this. In the words of Barrett and Massalski, "Crystals are rotation twins if a two-, three-, four-, or six-fold rotation of one crystal about a twinning axis produces the orientation of the other. The rotation axis lies either in the twinning plane or normal to it and is not a symmetry element of the lattice of the individual crystals."

3. Examples

Here, I will present examples with $m^4 = 1$, most of which do not fit the aforementioned description of rotation twins. Pick any set of (linearly independent) lattice vectors e_a such that

$$\|e_1\| = \|e_2\| = 1, e_3 \cdot (e_1 + e_2) = 0, \quad (3.1)$$

and let e^a denote the corresponding reciprocal lattice vectors (the dual basis). Let e denote the unit vector given by

$$e = (e_1 + e_2) / \|e_1 + e_2\| = (e_1 + e_2) / \sqrt{2(1 + e_1 \cdot e_2)}. \quad (3.2)$$

One 180° rotation is defined by

$$R_1 = -1 + 2e \otimes e. \quad (3.3)$$

By an elementary analysis, one can verify that, with (3.1) we can also write

$$e = (e^1 + e^2) / \|e^1 + e^2\| = (e^1 + e^2) \|e_1 + e_2\| / 2, \quad (3.4)$$

thus, (3.3) is equivalent to

$$\begin{aligned} R_1 &= -1 + (e_1 + e_2) \otimes (e^1 + e^2) \\ &= -1 + (e^1 + e^2) \otimes (e_1 + e_2). \end{aligned} \quad (3.5)$$

This means that R_1 belongs to the point group for such e_a . Another 180° rotation is given by

$$R_2 = -1 + 2e_2 \otimes e_2. \quad (3.6)$$

Composing these, we obtain the rotation

$$R = R_2 R_1 \quad (3.7)$$

with axis parallel to the vector

$$(e_1 + e_2) \wedge e_2 = e_3. \quad (3.8)$$

The angle of rotation θ can be calculated, using the relation

$$\text{tr } R = 1 + 2 \cos \theta, \quad (3.9)$$

and, by using the definition of R , we find that

$$\cos \theta = e_1 \cdot e_2. \quad (3.10)$$

We can choose e_1 and e_2 , consistent with (3.1), to get any desired angle, excepting $\cos \theta = \pm 1$, which would contradict the requirement that the e_a be linearly independent.

Now, define $m \in G$ as follows:

$$\begin{aligned} m_1^a e_a &= -e_2, \\ m_2^a e_a &= e_1, \\ m_3^a e_a &= e_3, \end{aligned} \quad (3.11)$$

it being straight forward to show that

$$m^4 = 1. \quad (3.12)$$

By elementary calculations, we then find that

$$\begin{aligned} R m_1^a e_a &= e_1 - 2e_1 \cdot e_2 e_2, \\ R m_2^a e_a &= e_2, \\ R m_3^a e_a &= e_3 - 2e_1 \cdot e_3 e_2. \end{aligned} \quad (3.13)$$

We then have

$$Rm_b^a e_a = (1 + a \otimes n) e_b, \quad (3.14)$$

with

$$\begin{aligned} a &= 2e_2, \\ n &= e^2 - e_2. \end{aligned} \quad (3.15)$$

To have $n \neq 0$, we need

$$e^2 \neq e_2,$$

which will hold unless $e_1 \cdot e_2 = e_2 \cdot e_3 = e_1 \cdot e_3 = 0$, that is, unless the vectors are all orthogonal. If they are all orthogonal, (3.13) reduces to the form (2.34), R then being in the associated point group, the solutions becoming trivial. For one thing, the examples show that the analog of (2.37) does not hold, i.e.

$$m^4 = 1 \nRightarrow R^4 = 1. \quad (3.16)$$

From (3.10), we can have $R^4 = 1$, a 90° rotation, by assuming that

$e_1 \cdot e_2 = 0 \neq e_1 \cdot e_3$. Then n is orthogonal to e_1 and e_2 , hence parallel to e^3 which, from (3.8), is the axis of rotation. This particular case conforms to the description of rotation twins given by Barrett and Massalski [13, p. 406]. Another special case satisfies their description in part. By choosing e_1 and e_2 so that $2e_1 \cdot e_2 = -1$, we see from (3.10) that R will satisfy $R^3 = 1$. Their description also dictates that the axis of rotation, here e^3 , should be either parallel or perpendicular to n . Checking this, one finds that it is not parallel, and is perpendicular only if $e_1 \cdot e_3 = e_2 \cdot e_3 = 0$. Of course, one can pick e_a not satisfying these conditions. A somewhat similar

example is given by Pitteri [12], with $R^2 = 1$, with the axis of R neither parallel or perpendicular to n . As far as I know, nothing excludes the possibility that any lattice vectors might minimize some potential function $\tilde{\phi}$, and occur in nature.

4. Some Constructions

Here, we deduce some fairly general procedures for constructing examples of solutions fitting the aforementioned description of rotation twins. First, consider solutions of (2.32) with the special property that

$$Ra = a \neq 0, R \neq 1, \quad (4.1)$$

so that R has a unique axis parallel to a , hence perpendicular to n . Then, (2.32) is equivalent to

$$\begin{aligned} M &\stackrel{\text{def}}{=} m_a^b e_b \otimes e^a \\ &= R^T S \\ &= R^T + a \otimes n. \end{aligned} \quad (4.2)$$

Further, since n is perpendicular to a , the axis of R , there is a vector b such that

$$n = (R - 1)b \neq 0, b \cdot a = 0. \quad (4.3)$$

Let

$$\mathcal{T} = 1 + a \otimes b, \quad (4.4)$$

and we find that

$$\begin{aligned}
 \overline{S} R^T \overline{S}^{-1} &= R^T + a \otimes Rb - a \otimes b \\
 &= R^T + a \otimes n \\
 &= M,
 \end{aligned} \tag{4.5}$$

so M is similar to R^T . This implies that

$$M^N = R^N = 1, \quad N = 2, 3, 4 \text{ or } 6. \tag{4.6}$$

Briefly, taking traces gives

$$\begin{aligned}
 \text{tr } M &= m_a^a = \text{integer} \\
 &= \text{tr } R^T = 1 + 2 \cos \theta,
 \end{aligned} \tag{4.7}$$

where θ is the angle of rotation. Insert the possible integers, bearing in mind that M is similar to R^T , and you get (4.6), which is well known to crystallographers. It can be helpful to note that any rotation R is similar to its transpose: it is easy to verify that

$$R^T = \tilde{R} R R^T, \tag{4.8}$$

where $\tilde{R}$ is a 180° rotation, with axis perpendicular to that of R . Thus, M is also similar to R . With (4.5) and (4.2), we have

$$M e_a = m_a^b e_b = \overline{S} R^T \overline{S}^{-1} e_a. \tag{4.9}$$

Let

$$\overline{e}_a = \overline{S}^{-1} e_a, \quad e_a = \overline{S} e_a, \tag{4.10}$$

and we have, as the equivalent of (4.9),

$$R m_a^b \overline{e}_b = \overline{e}_a. \tag{4.11}$$

Referring to (2.34), this means that m is in the lattice group for the lattice vectors $\bar{e}_a$, R being the corresponding element of the associated point group, also similar to m . To construct examples, we can pick any $m \in G$ such that

$$m^N = 1, \quad N = 2, 3, 4 \text{ or } 6. \quad (4.12)$$

As is discussed by Ericksen [11], this guarantees that there will exist vectors $\bar{e}_a$ and a rotation R satisfying (4.11), with $R^N = 1$. It is in fact fairly easy to determine them, given m . Then pick $a \neq 0$ parallel to the axis of R , $b \neq 0$ any vector perpendicular to it. With $\bar{S}$ then defined by (4.4), we can use (4.10) to determine e_a , satisfying (4.9). Use (4.3) to define n which, by the construction, will be perpendicular to a . Routine calculations then show that we have a solution of (2.32), satisfying (4.1).

With solutions of this kind, we can construct configurations consisting of symmetry-related wedges, fit together like the sections of an orange, special cases of the topological possibilities discussed by James [8,9]. Later, I will discuss this a bit more.

Much the same kind of analysis applies to solutions of (2.32) such that

$$Rn = n, \quad R \neq 1, \quad (4.13)$$

which also fit the description of rotation twins. Again define M as above. Instead of (4.2), we use

$$M^{-T} = R^T(1 - n \otimes a) = R^T - n \otimes a. \quad (4.14)$$

Here, we set

$$a = (1 - R)c, \quad c \cdot n = 0, \quad (4.15)$$

and similarly conclude that

$$M^{-T} = \bar{S} R^T \bar{S}^{-1}, \quad (4.16)$$

with

$$\bar{S} = 1 + n \otimes c, \quad (4.17)$$

or, equivalently,

$$M = \bar{S}^{-T} R^T \bar{S}^T. \quad (4.18)$$

Then, setting

$$\bar{e}_a = \bar{S}^T e_a, \quad (4.19)$$

we obtain, as the analog of (4.11),

$$R m_a^b \bar{e}_b = \bar{e}_a. \quad (4.20)$$

In a similar way, this can be read backwards to construct examples, and $\bar{S}^T$ is also interpretable as a simple shear. These solutions cannot be used to generate the "orange section" configurations referred to above, but do fit the description of rotation twins.

Bearing in mind (4.8), we note that, for all of these examples, M is similar to R . Suppose, conversely, that M is similar to R and

$$M = R^T (1 + a \otimes n). \quad (4.21)$$

In particular, we must have

$$\text{tr } M = \text{tr } R^T = \text{tr } R, \quad (4.22)$$

implying that

$$R^T a \cdot n = 0. \quad (4.23)$$

Also M^{-T} must be similar to R , and

$$M^{-T} = R^T(1 - n \otimes a), \quad (4.24)$$

similarly implying that

$$R^T n \cdot a = R a \cdot n = 0. \quad (4.25)$$

Of course, we must also have $a \cdot n = 0$.

By elementary reasoning, left to the reader, one finds that the three equations can hold only if at least one of the following four conditions holds:

$$R a = \pm a, \quad R n = \pm n. \quad (4.26)$$

If $R a = -a$, R is a 180° rotation, so $R^2 = 1$. With M similar, we also have $M^2 = 1$. These are then standard twinning solutions, referred to in (2.37). Similar remarks apply to the possibility that $R n = -n$. For all such twinning solutions, it is known that either $R a = a$ and $R n = -n$ or $R n = n$ and $R a = -a$. Thus, when M is similar to R , (4.26) reduces to the statement that either $R a = a$ or $R n = n$, the possibilities analyzed above.

Thus, we have a rather nice characterization of a subset of the rotation twins, at least. There might or might not be other solutions fitting their description. I have not made a careful study of this question, but do not know of any examples.

5. Composition

Suppose that we have two solutions of (2.32) for the same choice of e_a , say

$$S e_a = (1 + a \otimes n) e_a = R m_a^b e_b \quad (5.1)$$

and

$$\overline{S}e_a = (1 + \overline{a} \otimes \overline{n})e_a = \overline{R} \overline{m}_a^b e_b. \quad (5.2)$$

One way of composing these is obtained by noting that

$$\begin{aligned} Rm_a^b(\overline{S}e_b) &= R\overline{S}R^T(Rm_a^b e_b) \\ &= R\overline{S} R^T(S e_a) \\ &= R\overline{R}m_a^b \overline{m}_b^c e_c \\ &= R\overline{R}m_a^b \overline{m}_b^c (R^T S m_c^{-1} e_d). \end{aligned} \quad (5.3)$$

In particular, we then have

$$\tilde{S}(Se_a) = \tilde{R}m_a^b (Se_b). \quad (5.4)$$

with

$$\begin{aligned} \tilde{S} &= R\overline{S}R^T = 1 + (R\overline{a}) \otimes (R\overline{n}), \\ \tilde{R} &= \overline{R}R^T, \\ \tilde{m} &= \overline{m}m^{-1} \in G. \end{aligned} \quad (5.5)$$

So, (5.1) links e_a by an admissible discontinuity to lattice vectors Se_a . With (5.4) we link the latter by a similar discontinuity to lattice vectors $\tilde{S}(Se_a)$. One can similarly compose to link the latter to a fourth set, etc. This is a first step toward building configurations involving several regions tacked together. It needs to be supplemented by considerations such as are discussed by James [8,9], relevant when the various planes of discontinuity intersect.

In particular, nothing prevents us from taking the two solutions indicated by (5.1) and (5.2) to be the same, iterating this as many times as we desire. This gives a sequence of the form

$$Se_a = Rm_a^b e_b$$

$$RSR^T(Se_a) = Rm_a^b(Se_a)$$

$$R^2 S(R^T)^2 (RSR^T S)e_a = Rm_a^b (RSR^T S)e_a,$$

the Nth step giving

$$\begin{aligned} R^N S(R^T)^N e_a^{N-1} &= Rm_a^b e_b^{N-1} \\ &= R^{N+1} (m^{N+1})_a^b e_b^{N-1}, \end{aligned} \quad (5.6)$$

with

$$e_a^{N-1} = \prod_{M=0}^{N-1} R^M S(R^T)^M e_a. \quad (5.7)$$

Here, (5.6)₂ follows immediately from (5.3)₃ for $N = 1$ and is easily established by induction for $N > 1$.

Sometimes, after a finite number of steps, this iteration will return the lattice vectors to their original values, the condition for this being that, for some $N = V < \infty$,

$$R^V (M^V)_a^b e_b = e_a. \quad (5.8)$$

One can continue the iteration, reproducing the collection e_a^{N-1} in a periodic fashion, so I call these periodic solutions.

Recalling (2.33), we see that (5.8) implies that m^V is in the lattice group for e_a , with R^V in the corresponding point group. These groups are finite and conjugate, so we have

$$R^V \text{ similar to } m^V \text{ similar to } M^V, \quad (5.9)$$

with M defined as in (4.2). That these groups are finite also implies that there are smallest integers P and Q such that

$$R^P = 1, \quad m^Q = M^Q = 1. \quad (5.10)$$

Also, it implies that there exists a rotation $\hat{R}$ such that

$$M \text{ is similar to } \hat{R} \Rightarrow \hat{R}^Q = 1. \quad (5.11)$$

First, suppose that $P = Q$, in which case we can take $R = \hat{R}$, giving us the solutions discussed in §4. For example, we might pick one with $Ra = a$, $P = Q = 3$. The iteration generates the three directions, n , Rn and R^2n , making 120° angles with each other. Clearly, we can construct three half planes whose normals have these directions, their edges meeting on a line with direction a . In the wedges thus formed, we can assign lattice vectors e_a , $Rm_a^b e_b$ and $R^2(m_a^2)^b e_b$, and have all the desired jump conditions satisfied on the planes of discontinuity. Clearly, (5.8) holds, with $M = 3$. Such triplets are called by some "trills". Clearly, one can construct similar solutions with four or six wedges, resembling the structure seen in oranges. If one uses the solutions with $Rn = n$, one gets parallel planes, so one can't form such wedges, but one can put together any number of strips, with the lattice vectors changing in a periodic fashion, as one traverses them. The width of the strips can be assigned arbitrarily. Such patterns of plane defects often occur in parts of real crystals. Frequently, these are the standard twins, described by (2.37) but, clearly, they need not be. From casual observation, one might be misled into thinking that they are, when they are not. The aforementioned description of rotation twins does serve to warn us against making this mistake, to look closely at the crystal structure.

There are the remaining possibilities, with $P \neq Q$. In §3, we encountered examples with $P = 3, Q = 4$, enough to indicate that we are not discussing the null set. From (5.8)-(5.11) we must have

$$\begin{aligned} \text{tr } R &= 1 + 2 \cos(2\pi/P), \\ \text{tr } M &= \text{tr } \hat{R} = 1 + 2 \cos(2\pi/Q) = \text{integer}. \end{aligned} \quad (5.12)$$

and

$$\cos(2V\pi/P) = \cos(2V\pi/Q). \quad (5.13)$$

If $P = 1$, the only solutions of (5.1) are the lattice invariant shears noted in (2.36), and none of these satisfy (5.10). Similarly, $Q = 1$ yields no non-trivial possibilities. As is discussed by Pitteri [12], possibilities consistent with (5.10) are such that $P = 2 \Rightarrow Q = 2$ and vice versa. The remaining possible values of P and Q are 3,4 and 6. From (5.13), we must have

$$V(1/P - 1/Q) = \text{integer}, \quad (5.14)$$

so it is straightforward to find the smallest possible values of V . With (2.18), we easily find that

$$\begin{aligned} (P,Q) &= (3,4) \text{ or } (4,3) \Rightarrow V = 12, \\ (P,Q) &= (3,6) \text{ or } (6,3) \Rightarrow V = 6, \\ (P,Q) &= (4,6) \text{ or } (6,4) \Rightarrow V = 12. \end{aligned} \quad (5.18)$$

In all these cases, (5.8) is satisfied in the trivial way, by having $R^V = m^V = 1$. Since all solutions with $m^Q = 1$ are fairly well characterized by Ericksen [10], one might better characterize the (proper) subset satisfying (5.10), with $P \neq Q$, and determine the kinds of patterns which they can generate. Here, I'll not pursue this.

These rather naive and elementary analyses give us snapshots of what some of our minimizers can look like, a means of constructing certain kinds of examples, but not enough to give us a good picture of the whole set. To some degree, metallurgy is the art of controlling these and more complex morphologies, albeit imperfectly. Clearly, we have a long way to go, to develop mathematical theory to apply to such problems.

Some observations of rotation twins, grown from solution, are discussed by Aoki and Nakamuta [14]. Their analysis of them is in some conflict with ideas presented here. Mario Pitteri has shown me a different analysis which almost, but not quite is consistent with the ideas presented here, and agrees about as well with the measurements. It is possible that a still different analysis would be consistent. My knowledge of such growth twins is very limited, so I am reluctant to say more about this.

Acknowledgment. This material is based on work supported by the National Science Foundation under Grant No. MEA-8304750. Also, I thank Dr. Mario Pitteri for helpful comments.

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