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THE PREFERRED HABIT OF A COHERENT THIN-PLATE INCLUSION IN AN ANISOTROPIC ELASTIC SOLID

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ABSTRACT

The work reported here was undertaken to find algebraic equations for the preferred habits of coherent thin-plate inclusions in anisotropic media on the assumption that the inclusion and matrix can be treated as linear elastic continua. The preferred habit minimizes the elastic energy, which depends on the elastic constants of the inclusion and the transformation strain connecting the lattices of the inclusion and the matrix. The paper presents four principal results concerning the preferred thin-plate habit. First, the mathematical conditions that determine the preferred habit are derived in compact form. Second, it is shown that these conditions are always satisfied when the transformation strain is dyadic and the habit is perpendicular to a vector of the dyad, reproducing a result that is given by Khatchaturyan [2] and included in the "crystallographic theory" of precipitate habits. Third, the extremal conditions are solved for orthorhombic symmetry, that is, when the elastic constants of the inclusion have orthorhombic symmetry with respect to the principal axes of the transformation stress. The results incorporate isotropic, cubic, hexagonal, and tetragonal (type II) symmetries. They are specialized to determine the minimum-energy habit as a function of the transformation strain for three classes of inclusions: isotropic inclusions, cubic inclusions with tetragonal transformation strains, and hexagonal inclusions with hexagonal transformation strains. Finally, it is shown by counter-example that there is no general algebraic solution for systems of arbitrary symmetry.

1. INTRODUCTION

It has been recognized since the work of Eshelby [1] that the state of a coherent inclusion in a crystalline solid can often be understood or predicted on the basis of a linear elastic model in which the matrix and inclusion are treated as elastic continua. The model has been successfully used to predict the energies, shapes, strains, and crystallographic habits of a variety of precipitates and structural transformation products [2].

A classic result of the linear elastic theory (first obtained by Khatchaturyan [3]) states that when the difference between the moduli

of the inclusion and the matrix can be ignored (the homogeneous case) the elastic energy of the inclusion is minimized when it has the form of a thin plate on a specific crystallographic plane. This plane is the preferred habit of the inclusion, at least in the limit of large size. The Khatchaturyan shape theorem offers an explanation for the frequent plate morphology of coherent precipitate phases and correctly identifies the preferred habits of many second-phase particles [2-10]. It incorporates the infinitesimal form of the "crystallographic theory" of precipitate habits [11,12] as a special case. While the Khatchaturyan shape theorem does not always hold when the inclusion and matrix have different moduli [6,14], the plate morphology is favored in a great many inhomogeneous systems of physical interest, as shown by numerical calculation [2,6,14] and experimental results [2-10].

The preferred habit of a thin-plate inclusion depends on the elastic constants of the inclusion and on the "transformation strain" that connects the lattices of the inclusion and the matrix. However, the dependence is sufficiently complex that the preferred habit planes are only known for simple symmetries. Khatchaturyan and Airapetyan [4] found the preferred habits for a cubic inclusion in a cubic matrix, and showed that they are identical to the habits predicted by Cahn [15] for spinodal decomposition waves in cubic solutions. Wen, Kostlan, et al. [7] determined the preferred habit planes for a pseudo-cubic inclusion with a tetragonal transformation strain. Less symmetric cases have been solved numerically; for example, Mayo and Tsakalakos [7] found the preferred habits for selected hexagonal precipitates in aluminum.

The present work was undertaken to find solvable algebraic expressions for the preferred habits of anisotropic, thin-plate inclusions. Four principal results are presented. First, the mathematical conditions that determine the preferred habits are derived in compact form. Second, it is shown that these conditions are always satisfied when the transformation strain is dyadic and the habit is perpendicular to a vector of the dyad, reproducing a result that is given by Khatchaturyan [2] and included in the "crystallographic theory" [11,12]. Third, the extremal conditions are solved for orthorhombic symmetry to obtain analytic expressions for the possible thin-plate habits. The results incorporate isotropic, cubic, hexagonal, and tetragonal (type II) symmetries. They are specialized to determine the minimum-energy habit as a function of the transformation strain for three particular classes of inclusions: isotropic inclusions, cubic inclusions with tetragonal transformation strains (the case treated in reference [7]), and hexagonal inclusions with tetragonal (or hexagonal) transformation strains. Finally, it is shown by counter-example that there is no algebraic solution for systems of arbitrary symmetry.

The results presented here are derived under the constraint that the inclusion has a thin-plate form. They hold whether or not the thin-plate morphology minimizes the elastic energy.

2. THE ELASTIC ENERGY OF A COHERENT, THIN-PLATE INCLUSION

The elastic energy of a system that contains a coherent elastic inclusion is derived in detail by Eshelby [1] and by Khatchaturyan

[2,3]. The derivation below roughly follows Khatchaturyan [2] and is included to establish several results that will be needed in the following. The derivation is based on the modified Eshelby cycle [1,2], that creates the inclusion through a series of imaginary operations that bring it into the correct final state.

A. The Eshelby Cycle

First, a volume (V) is cut out of the matrix (which has volume $V^T >> V$ and is free of stress) and transformed into an equivalent quantity of the inclusion phase. The transformation generally changes the size and shape of the extracted volume; this stress-free distortion defines the <u>transformation strain</u>, ε^*. Next, the inclusion is deformed by a surface traction that reverses the transformation strain. The resulting elastic stress within the inclusion is the negative of the <u>transformation stress</u>:

$$\sigma^0_{ij} = \lambda_{ijkl}\varepsilon^0_{kl} \tag{2.1}$$

where λ is the fourth-order tensor of isothermal elastic constants of the inclusion phase. Finally, the inclusion is replaced in the vacant hole in the matrix, welded to ensure coherency, and allowed to relax to equilibrium by deforming itself and the matrix around it. The relaxation introduces a displacement field, $\mathbf{u}(\mathbf{r})$ (measured with respect to the relaxed configuration of the matrix), with the associated strain field

$$\varepsilon_{ij}(\mathbf{r}) = (1/2)[u_{i,j} + u_{j,i}] \tag{2.2}$$

The stress field is

$$\begin{aligned}\sigma_{ij}(\mathbf{r}) &= [\lambda_{ijkl}\varepsilon_{kl}-\sigma^0_{ij}]\Theta(\mathbf{r}) + \lambda'_{ijkl}\varepsilon_{kl}[1-\Theta(\mathbf{r})] \\ &= [\Delta\lambda_{ijkl}\varepsilon_{kl}-\sigma^0_{ij}]\Theta(\mathbf{r}) + \lambda'_{ijkl}\varepsilon_{kl}\end{aligned} \tag{2.3}$$

where the fourth-order tensor λ' is the elastic modulus of the matrix, $\Delta\lambda$ is the modulus difference

$$\Delta\lambda_{ijkl} = \lambda_{ijkl} - \lambda'_{ijkl} \tag{2.4}$$

the Einstein summation convention is assumed, and $\Theta(\mathbf{r})$ is the shape function of the inclusion, equal to 1 when the position vector $\mathbf{r}$ falls within the inclusion and to 0 otherwise.

B. The Equilibrium Strain Field in the Thin-plate Limit

If we now introduce the assumption that the strain has a constant value, ε^*, within the inclusion, as we shall show that it does in the thin-plate limit, and define the "effective transformation stress",

$$\sigma^*_{ij} = \sigma^0_{ij} - \Delta\lambda_{ijkl}\varepsilon^*_{ij} \tag{2.5}$$

then the stress field can be written

$$\sigma_{ij}(\mathbf{r}) = -\sigma^*_{ij}\Theta(\mathbf{r}) + \lambda'_{ijkl}u_{l,k}(\mathbf{r}) \tag{2.6}$$

Mechanical equilibrium (Cauchy's First Law) requires that the divergence of the stress vanish. Hence

$$\sigma^*_{ij}\theta_{,j} = \lambda'_{ijkl}u_{l,kj} \tag{2.7}$$

whose Fourier transform is

$$- ik_j\sigma^*_{ij}\theta(\mathbf{k}) = \lambda'_{ijkl}k_k k_j u_l(\mathbf{k}) \tag{2.8}$$

The solution to this equation is

$$u_i(\mathbf{k}) = - i|\mathbf{k}|^{-2}\Omega'^{\mathbf{e}}_{ij}\sigma^*_{jk}k_k\theta(\mathbf{k}) \tag{2.9}$$

where the matrix elastic tensor $\mathbf{\Omega}'^{\mathbf{e}}$ is defined by its inverse:

$$[\Omega'^{\mathbf{e}}]^{-1}_{ij} = \lambda'_{iklj}e_k e_l \tag{2.10}$$

and $\mathbf{e}$ is a unit vector in the direction of $\mathbf{k}$. The deformation gradient is

$$\begin{aligned} u_{i,j}(\mathbf{k}) &= ik_j u_i(\mathbf{k}) \\ &= e_j\Omega'^{\mathbf{e}}_{ik}\sigma^*_{kl}e_l\theta(\mathbf{k}) \end{aligned} \tag{2.11}$$

In the thin-plate limit the inclusion is an arbitrarily thin plate whose orientation is specified by the normal vector, $\mathbf{n}$. The shape function, $\theta(\mathbf{k})$, vanishes unless $\mathbf{k}$ is almost parallel to $\mathbf{n}$. Since the factor modifying $\theta(\mathbf{k})$ depends only on the direction of $\mathbf{k}$, the reverse Fourier transform of equation (2.11) in the thin-plate limit is

$$u_{i,j}(\mathbf{r}) = n_j\Omega'^{\mathbf{n}}_{ik}\sigma^*_{kl}n_l\theta(\mathbf{r}) \tag{2.12}$$

Equation (2.12) shows that the displacement gradient, and hence the strain, is constant within the inclusion and zero outside. It can be recast in the form

$$Q^{\mathbf{n}}_{ikmn}u_{m,n} = n_k\Omega'^{\mathbf{n}}_{ij}\sigma^o_{jl}n_l \tag{2.13}$$

where the fourth order tensor $\mathbf{Q}^{\mathbf{n}}$ is

$$Q^{\mathbf{n}}_{ikmn} = \delta_{im}\delta_{kn} + n_k\Omega'^{\mathbf{n}}_{ip}\Delta\lambda_{pqmn}n_q \tag{2.14}$$

Using the identity

$$Q^{\mathbf{n}}_{ikmn}n_n\Omega^{\mathbf{n}}_{mj} = n_k\Omega'^{\mathbf{n}}_{ij} \tag{2.15}$$

where $\mathbf{\Omega}^{\mathbf{n}}$ is the elastic tensor of the inclusion phase in the direction $\mathbf{n}$, the constant strain within the inclusion can be written

$$\begin{aligned} u_{i,j} &= n_j\Omega^{\mathbf{n}}_{ik}\sigma^o_{kl}n_l \\ &= n_j q^{\mathbf{n}}_i \end{aligned} \tag{2.16}$$

where $q^{\mathbf{n}}_i$ is the <u>conjugate vector</u>

$$q_i^n = \Omega_{ik}^n \sigma_{kl}^o n_l \tag{2.17}$$

Equation (2.16) shows that the deformation gradient within the inclusion has a dyadic form that insures that there is no strain in the habit plane; the habit plane is an invariant plane of the crystallographic transformation that connects the relaxed state of the matrix to the strained state of the inclusion. The inclusion strain in the thin-plate limit is independent of the elastic constants of the matrix.

It is easily shown (and is physically obvious) that there is no traction on the habit plane:

$$\begin{aligned} \sigma_{ij}^n n_j &= - \sigma_{ij}^o n_j + \lambda_{ijkl} n_j n_k q_l^n \\ &= - \sigma^o{}_{ij} n_j + (\Omega^n)_{il}^{-1} q_l^n = 0 \end{aligned} \tag{2.18}$$

C. The Elastic Energy

Using the Eshelby cycle the elastic contribution to the Helmholtz free energy of the system can be written

$$\Delta F_{el} = \Delta F^o - \Delta F^1 \tag{2.19}$$

where ΔF^o is the <u>self-energy</u> of the inclusion, that is, the elastic energy stored in the inclusion when it is deformed to reverse the transformation strain, and ΔF^1 is the <u>relaxation energy</u>, the elastic energy recovered when the inclusion and matrix deform to relax the transformation stress. The self-energy is

$$\Delta F^o = (V/2)\sigma_{ij}^o \varepsilon_{ij}^o \tag{2.20}$$

Using equation (2.16) the relaxation energy of a thin plate with normal $\mathbf{e}$ can be written

$$\begin{aligned} \Delta F^1 &= (V/2)\sigma_{ij}^o u_{i,j} \\ &= (V/2)B^1(\mathbf{e}) \end{aligned} \tag{2.21}$$

where $B^1(\mathbf{e})$ is the <u>relaxation energy function</u>

$$\begin{aligned} B^1(\mathbf{e}) &= e_i \sigma_{ij}^o q_j^e \\ &= e_i \sigma_{ij}^o \Omega_{jk}^e \sigma_{kl}^o e_l \end{aligned} \tag{2.22}$$

Since ΔF^o is independent of the inclusion shape and habit, <u>the preferred thin-plate habits are those directions</u>, $\mathbf{n}$, <u>that maximize the relaxation energy function</u>, $B^1(\mathbf{e})$.

Note that $B^1(\mathbf{e})$ depends on the elastic constants of the inclusion, but is independent of the elastic constants of the matrix. The relaxation energy function depends on the matrix phase only through its structure: the transformation strain, ε^o, that determines σ^o provides a coherent connection between the matrix and the inclusion.

Also note that the symmetry of $B^1(\mathbf{e})$ with respect to orthogonal transformations of the vector, $\mathbf{e}$, is the joint symmetry of $\boldsymbol{\sigma}^{\mathbf{e}}$ and $\boldsymbol{\Omega}^{\mathbf{e}}$. The transformation stress tensor has at least orthorhombic symmetry with respect to its principal axes ($\mathbf{a}_i$, i=1,2,3), since

$$\boldsymbol{\sigma}^{\mathbf{e}} = \sigma^1\mathbf{a}_1\mathbf{a}_1 + \sigma^2\mathbf{a}_2\mathbf{a}_2 + \sigma^3\mathbf{a}_3\mathbf{a}_3 \tag{2.23}$$

where the σ^i are the three principal stresses. The symmetry group of $B^1(\mathbf{e})$ is at least the union of the orthorhombic group and the symmetry of the inclusion phase with respect to the principal axes of the transformation stress.

3. CONDITIONS GOVERNING THE MAXIMA OF $B^1(\mathbf{e})$

Our problem is to find the directions, $\mathbf{n}$, that maximize $B^1(\mathbf{e})$ for given $\boldsymbol{\lambda}$ and $\boldsymbol{\varepsilon}^{\mathbf{e}}$. Since

$$B^1(\mathbf{n}) = B^1(k\mathbf{n}) \tag{3.1}$$

for all non-zero constants k, there is no formal restriction on the magnitude of $\mathbf{n}$, which can be normalized after it is found. The maxima satisfy the relations

$$\partial B^1(\mathbf{n})/\partial n_i = 0 \tag{3.2}$$

$$\delta n_i H^{\mathbf{n}}_{ij}\delta n_j = \delta n_i[\partial^2 B^1(\mathbf{e})/\partial n_i\partial n_j]\delta n_j \leqslant 0 \tag{3.3}$$

where $\delta\mathbf{n}$ is an arbitrary vector and $\mathbf{H}^{\mathbf{n}}$ is the Hessian of $B^1(\mathbf{n})$.

A. The Extrema of $B^1(\mathbf{e})$

The extrema of $B^1(\mathbf{e})$ satisfy equation (3.2), from which we can obtain the following <u>theorem</u>:

If $\mathbf{n}$ extremizes $B^1(\mathbf{e})$ and $\mathbf{q}^{\mathbf{n}}$ is the vector conjugate to $\mathbf{n}$, then $\mathbf{q}^{\mathbf{n}}$ also extremizes $B^1(\mathbf{e})$ and $\mathbf{n}$ is the vector conjugate to $\mathbf{q}^{\mathbf{n}}$. Mathematically,

$$q^{\mathbf{n}}_i = \Omega^{\mathbf{n}}_{ij}\sigma^{\circ}{}_{jk}n_k \quad \Rightarrow \quad n_i = \Omega^{\mathbf{q}}_{ij}\sigma^{\circ}_{jk}q^{\mathbf{n}}_k \tag{3.4}$$

when $\mathbf{n}$ extremizes $B^1(\mathbf{e})$.

To prove the theorem we first differentiate $B^1(\mathbf{e})$:

$$dB^1(\mathbf{e}) = d(e_i\varepsilon^{\circ}_{ij}q^{\mathbf{e}}_j) = q^{\mathbf{e}}_j\varepsilon^{\circ}_{ji}de_i + e_i\varepsilon^{\circ}_{ij}dq^{\mathbf{e}}_j \tag{3.5}$$

The differential of $\mathbf{q}^{\mathbf{e}}$ can be found from equation (2.18)

$$\begin{aligned} 0 &= d(\sigma^{\mathbf{e}}_{ij}e_j) = (d\sigma^{\mathbf{e}}_{ij})e_j + \sigma^{\mathbf{e}}_{ij}de_j \\ &= \lambda_{ijkl}[e_k dq^{\mathbf{e}}_l + q^{\mathbf{e}}_k de_l]e_j + \sigma^{\mathbf{e}}_{ij}de_j \\ &= (\Omega^{\mathbf{e}})^{-1}_{il}dq^{\mathbf{e}}_l + (\lambda_{ijkl}e_j q^{\mathbf{e}}_k + \sigma^{\mathbf{e}}_{il})de_l \end{aligned} \tag{3.6}$$

from which

$$e_i\sigma^o_{ij}dq^e_j = -\ e_i\sigma^o_{ij}\Omega^e_{jl}(\lambda_{lmnp}e_m q^e_n+\sigma^e_{lp})de_p$$
$$= -\ q^e_j(2\sigma^e_{ji}+\sigma^o_{ji})de_i \tag{3.7}$$

Substituting equation (3.7) into (3.5),

$$dB^1(e) = -2(q^e_j\sigma^e_{ji})de_i \tag{3.8}$$

If $e=n$, an extremum of $B^1(e)$, then equation (3.8) must hold for arbitrary de_i. It follows that

$$\sigma^n_{ij}q^n_j = 0 = -\ \sigma^o_{ij}q^n_j + \lambda_{ijkl}q^n_j q^n_k n_l$$
$$= -\ \sigma^o_{ij}q^n_j + (\Omega^q)^{-1}_{ij}n_j \tag{3.9}$$

which establishes (3.4).

The relation (3.4) has the consequence that

$$B^1(n) = B^1(q) \tag{3.10}$$

Hence the habit specified by the conjugate vector q^n is degenerate with the habit specified by n. Equation (3.10) is automatically satisfied when the directions of n and q are related by a symmetry operation from the symmetry group of $B^1(e)$.

It is useful to distinguish three classes of extrema. Class 1: the conjugate vector, q^n, is proportional to n:

$$q^n = kn \tag{3.11}$$

for some non-zero constant k. In this case

$$(\lambda_{ijkl}n_j n_k)n_l = k^{-1}\sigma^o_{il}n_l \tag{3.12}$$

and n is an eigenvector of the tensor $\lambda_{ijkl}n_j n_k$. Class 2: the conjugate vector is not proportional to n. Class 3: the conjugate vector is zero. In this case

$$\sigma^o_{ij}n_j = 0 \tag{3.13}$$

and $B^1(n) = 0$. Habit planes of class 3 minimize $B^1(e)$ and need not be considered.

B. The Hessian Matrix

The Hessian matrix, H^n, of $B^1(n)$ can be found by differentiating equation (3.8) for $e=n$. The result is, after some algebra,

$$H_{ij} = 2[(\sigma^n_{ik}+\omega^{nT}_{ik})\Omega^n_{kl}(\sigma^n_{lj}+\omega^n_{lj}) - (\Omega^q)^{-1}_{ij}] \tag{3.14}$$

where we have used the symbols ω^n and ω^{nT} for the tensors

$$\omega^n_{ij} = \lambda_{iklj}n_k q^n_l \tag{3.15}$$

$$\omega_{ij}^{nT} = \lambda_{iklj} q_k^n n_l \tag{3.16}$$

When the vector $\mathbf{n}$ maximizes $B^1(\mathbf{e})$ the Hessian matrix is negative semi-definite [equation (3.3)].

4. THE PREFERRED HABIT WHEN ε^* IS DYADIC

As a first example let the transformation strain be dyadic

$$\varepsilon^* = (\varepsilon^0/2)[\mathbf{ln} + \mathbf{nl}] \tag{4.1}$$

where ε^0 is an arbitrary constant and $\mathbf{l}$ and $\mathbf{n}$ are arbitrary unit vectors. It is simple to show that, independent of the symmetry of the elastic constants, the preferred shape is a thin plate perpendicular to either $\mathbf{n}$ or $\mathbf{l}$ [2].

First let the plate have habit $\mathbf{n}$. Then, by the first of equations (3.4)

$$\mathbf{q}^n = \varepsilon^0 \mathbf{l} \tag{4.2}$$

The vector $\mathbf{n}$ satisfies the second of equations (3.4). It follows that $\mathbf{n}$ and $\mathbf{l}$ are degenerate extrema of $B^1(\mathbf{e})$. The extremal values are

$$B^1(\mathbf{n}) = B^1(\mathbf{l}) = \sigma_{ij}^0 \varepsilon_{ij}^0 \tag{4.3}$$

with which

$$\Delta F_{el} = 0 \tag{4.4}$$

Since ΔF_{el} cannot be negative, the habits $\mathbf{n}$ and $\mathbf{l}$ minimize the elastic energy.

Equation (4.4) generates the "crystallographic theory" of inclusion habits [7,8] in the linear case. When the inclusion is a thin plate with the habit $\mathbf{n}$ or $\mathbf{l}$ the total strain within it is

$$\mathbf{N} = (\varepsilon^0/2)[\mathbf{nl} + \mathbf{ln}] - \varepsilon^* = 0 \tag{4.5}$$

It follows that $\mathbf{n}$ and $\mathbf{l}$ are invariant planes of the transformation connecting the lattices of the inclusion and the matrix. The preferred habits can be found directly from ε^* by identifying its invariant planes.

Reversing the analysis, any invariant plane connecting the matrix and inclusion lattices is a strain-free habit for a thin-plate inclusion. Hence, as emphasized by Christian [16], the crystallographic theory remains valid when the transformation strain is large and the linear elastic model does not hold.

5. THE PREFERRED HABIT OF AN ORTHORHOMBIC INCLUSION

The most general situation for which we have found algebraic solutions for the extremal habits is when $B^1(\mathbf{e})$ has orthorhombic symmetry.

Let the relaxed state of the inclusion be referred to orthogonal axes that coincide with the principal axes of the transformation stress, σ^*. Let the elastic constants of the inclusion phase be referred to the same axes. Our solution is valid when the rotated matrix of elastic constants has at least orthorhombic symmetry, that is, when λ_{ijkl} is zero unless i=j and k=l or i=k and j=l. The symmetry of $B^1(\mathbf{e})$ is always at least orthorhombic when the inclusion has orthorhombic or higher symmetry and the principal axes of the transformation stress coincide with its crystal axes. $B^1(\mathbf{e})$ is at least orthorhombic when the inclusion is isotropic.

To facilitate the solution we express the elastic constants in the Voigt form:

$$c_{mn} = \lambda_{ijkl} \tag{5.1}$$

where the symmetric pairs (ij) and (kl) are changed into m and n by the relations (11)->1, (22)->2, (33)->3, (23)->4, (13)->5, (12)->6. The 6x6 matrix of the c_{mn} is symmetric. When the system is orthorhombic the matrix $[c_{ij}]$ is [17]

$$[c_{ij}] = \begin{vmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{55} & 0 \\ & & & & & c_{66} \end{vmatrix} \tag{5.2}$$

The matrix is symmetric across the diagonal. The matrix (5.2) incorporates the isotropic, cubic, hexagonal, and type II tetragonal symmetries (two two-fold or mirror plane axes perpendicular to the four-fold axis).

The solution to the orthorhombic problem follows with the aid of the following <u>theorem</u>:

If $B^1(\mathbf{e})$ has orthorhombic or higher symmetry and the direction $\mathbf{n}$ provides an extremum of $B^1(\mathbf{e})$, then the elements of the conjugate vector, $\mathbf{q}^{\mathbf{n}}$, satisfy the relations

$$q_i/|\mathbf{q}| = \pm n_i \tag{5.3}$$

Hence the direction $\mathbf{q}/|\mathbf{q}|$ is related to $\mathbf{n}$ by a symmetry operation of the orthorhombic system.

To prove this theorem we define the second order tensor $\mathbf{n}^{\mathbf{M}}$ by the relations

$$n^M_{ij} = n^i \delta_{ij} \tag{5.4}$$

where the superscript index i is not summed, and define the vector

$$\mathbf{n}^2 = \mathbf{n}^M \cdot \mathbf{n} = n_1^2 \mathbf{e}_1 + n_2^2 \mathbf{e}_2 + n_3^2 \mathbf{e}_3 \tag{5.5}$$

When σ^o is diagonal the symmetry relation

$$q_i^n \sigma_{ij}^o n_j = n_i \sigma_{ij}^o q^n{}_j \tag{5.6}$$

implies the three conditions

$$q_{ij}^M \sigma_{jk}^o n_k = n_{ij}^M \sigma_{jk}^o n_k \tag{5.7}$$

which become, after substituting equations (3.4),

$$q_{ij}^M (\Omega^n)_{jk}^{-1} q_k - n_{ij}^M (\Omega^q)_{jk}^{-1} n_k = 0 \tag{5.8}$$

Equation (5.8) is equivalent to the the matrix equation

$$\begin{vmatrix} 0 & -c_{55} & c_{66} \\ c_{44} & 0 & -c_{66} \\ -c_{44} & c_{55} & 0 \end{vmatrix} \cdot [\mathbf{q}^2 \mathbf{x} \mathbf{n}^2] = 0 \tag{5.9}$$

which holds only if $[\mathbf{q}^2 \mathbf{x} \mathbf{n}^2]$ vanishes or of it is parallel to the vector $(c_{55}c_{66})\mathbf{e}_1 + (c_{44}c_{66})\mathbf{e}_2 + (c_{44}c_{55})\mathbf{e}_3$. But the latter has only positive components, and hence cannot parallel the vector product of two vectors that both have positive components. It follows that

$$[\mathbf{q}^2 \mathbf{x} \mathbf{n}^2] = 0 \tag{5.10}$$

Equation (5.10) shows that when $B^1(\mathbf{e})$ is orthorhombic all of its extrema satisfy the relation

$$q_i^n = \pm k n_i \tag{5.11}$$

where k is a constant, which establishes equation (5.3).

Since the sign of k and choice of n_3 are arbitrary the two classes of extrema identified in Section 3 reduce to the two cases

$$[q_1^n, q_2^n, q_3^n] = k[n_1, n_2, n_3] \tag{5.12}$$

$$[q_1^n, q_2^n, q_3^n] = k[-n_1, -n_2, n_3] \tag{5.13}$$

The other extrema of class 2 can be found by adjusting the sign and re-indexing.

It is useful to divide the extrema into three types: (1) the extrema [100], [010], and [001], each of which is a solution to the orthorhombic form of (3.4); (2) extrema of the type [hkl], h,k,l non-zero; (3) extrema of the type [h0l], h,l non-zero (the [hk0] and [0kl] extrema can be found by re-indexing). Given orthorhombic symmetry the direction $\mathbf{n}'$ with components $n_i' = \pm n_i$ maximizes $B^1(\mathbf{e})$ if $\mathbf{n}$ does. It therefore suffices to consider the octant of positive components.

We require algebraic expressions for the extrema of types [hkl] and [h01], each of which may be of class 1 (5.12) or class 2 (5.13).

A. Extrema of the Type [hkl]

Since σ^{o} is diagonal we define the vector

$$\sigma^{v} = \sigma^{1}e_1 + \sigma^{2}e_2 + \sigma^{3}e_3 \tag{5.14}$$

where the σ^{i} are the principal stresses. Using this notation the equation

$$\Omega^{n}_{ij}\sigma^{o}_{jk}n_k = \Omega^{n}_{ij}n^{M}_{jk}\sigma^{v}_{k} = q^{n}_{i} \tag{5.15}$$

has the solution

$$\sigma^{v}_{i} = \{(n^{M})^{-1}_{ij}(\Omega^{n})^{-1}_{jk}(n^{M})^{-1}_{kl}\}n^{M}_{lm}q^{n}_{m} \tag{5.16}$$

where the elements of the matrix $G^{n}_{il} = \{(n^{M})^{-1}_{ij}(\Omega^{n})^{-1}_{jk}(n^{M})^{-1}_{kl}\}$ are

$$G^{n} = \begin{vmatrix} [c_{11}+c_{66}n_2^2/n_1^2+c_{55}n_3^2/n_1{}^2] & c_{12}+c_{66} & c_{13}+c_{55} \\ c_{12}+c_{66} & [c_{22}+c_{66}n_1^2/n_2^2+c_{44}n_3^2/n_2^2] & c_{23}+c_{44} \\ c_{13}+c_{55} & c_{23}+c_{44} & [c_{33}+c_{55}n_1^2/n_3^2+c_{44}n_2^2/n_3^2] \end{vmatrix} \tag{5.17}$$

Given equation (5.17), (5.16) can be written in the form

$$k^{-1}\sigma^{v}_{i} = L_{ij}n^{M}_{jk}n_k \tag{5.18}$$

where L is a 3x3 matrix. The solution of equation (5.18) is

$$\begin{aligned} n_i^2 &= k^{-1}L^{-1}_{ij}\sigma^{v}_{j} \\ &= k'^{-1}L^{c}_{ji}\sigma^{v}_{j} \end{aligned} \tag{5.19}$$

where L^{c} is the cofactor of L and the constant k′ can be used to normalize n.

For the [hkl] extremum of of class 1,

$$L = \begin{vmatrix} c_{11} & a_3 & a_2 \\ a_3 & c_{22} & a_1 \\ a_2 & a_1 & c_{33} \end{vmatrix} \tag{5.20}$$

where

$$a_1 = c_{23} + 2c_{44} \tag{5.21}$$

$$a_2 = c_{13} + 2c_{55} \tag{5.22}$$

$$a_3 = c_{12} + 2c_{66} \tag{5.23}$$

The solution is

$$n_1^2 = k'^{-1}\{[c_{22}c_{33}-a_1^2]\sigma^1 + [a_1a_2-c_{33}a_3]\sigma^2 + [a_1a_3-c_{22}a_2]\sigma^3\}$$
$$n_2^2 = k'^{-1}\{[a_1a_2-c_{33}a_3]\sigma^1 + [c_{11}c_{33}-a_2^2]\sigma^2 + [a_2a_3-c_{11}a_1]\sigma^3\} \qquad (5.24)$$
$$n_3^2 = k'^{-1}\{[a_1a_3-c_{22}a_2]\sigma^1 + [a_2a_3-c_{11}a_1]\sigma^2 + [c_{11}c_{22}-a_3^2]\sigma^3\}$$

For the [hkl] extrema of class 2,

$$L = \begin{vmatrix} -c_{11} & -a_3 & c_{13} \\ -a_3 & -c_{22} & c_{23} \\ -c_{13} & -c_{23} & c_{33} \end{vmatrix} \qquad (5.25)$$

and the solution is

$$n_1^2 = k'^{-1}\{[c_{23}^2-c_{22}c_{33}]\sigma^1 + [c_{33}a_3-c_{13}c_{23}]\sigma^2 + [-c_{23}a_3-c_{13}c_{22}]\sigma^3\}$$
$$n_2^2 = k'^{-1}\{[c_{33}a_3-c_{13}c_{23}]\sigma^1 + [c^2{}_{13}-c_{11}c_{33}]\sigma^2 + [-c_{13}a_3+c_{11}c_{23}]\sigma^3\} \qquad (5.26)$$
$$n_3^2 = k'^{-1}\{[-c_{13}c_{22}+c_{23}a_3]\sigma^1 + [-c_{11}c_{23}+c_{13}a_3]\sigma^2 + [c_{11}c_{22}-a_3^2]\sigma^3\}$$

In both cases the normalizing constant k' is obtained by summing the bracketed terms on the right hand side to ensure that

$$n_1^2 + n_2^2 + n_3^2 = 1 \qquad (5.27)$$

The solution only has physical meaning when $0 \leqslant n_i^2 \leqslant 1$ for all i.

B. Extrema of the Type [h01]

Equations (5.15-19) still apply, but

$$\mathbf{n}^M = n_1\mathbf{e}_1\mathbf{e}_1 + n_3\mathbf{e}_3\mathbf{e}_3 \qquad (5.28)$$

so L and L^c can now be written as (2x2) matrices. Choosing k so that $q_3^n = kn_3$, $q_1^n = \pm kn_1$ (positive for class 1, negative for class 2) there are two solutions.

For the [h01] extrema of class 1,

$$L = \begin{vmatrix} c_{11} & a_2 \\ a_2 & c_{33} \end{vmatrix} \qquad (5.29)$$

and the solution is

$$n_3^2 = 1 - n_1^2 = k'^{-1}\{-a_2\sigma^1 + c_{11}\sigma^3\} \qquad (5.30)$$

where, as before, k' is chosen to normalize **n**,

$$k' = (c_{11}-a_2)\sigma^3 + (c_{33}-a_2)\sigma^1 \qquad (5.31)$$

and the solution is only relevant when $0 \leqslant n_3^2 \leqslant 1$.

For the [h01] extrema of class 2

$$L = \begin{vmatrix} c_{11} & -c_{13} \\ c_{13} & -c_{33} \end{vmatrix} \tag{5.32}$$

and

$$n_3^2 = 1 - n_1^2 = k'^{-1}\{-c_{13}\sigma^1 + c_{11}\sigma^3\} \tag{5.33}$$

where

$$k' = (c_{11}+c_{13})\sigma^3 - (c_{33}+c_{13})\sigma^1 \tag{5.34}$$

6. EXAMPLES

To illustrate the application of the formulae in Section 5 we consider three specific examples: (1) isotropic inclusions with arbitrary transformation strains; (2) cubic inclusions with tetragonal transformation strains (equivalent to the case considered by Wen, et al. [7]); and (3) hexagonal inclusions with hexagonal transformation strains (incorporating the examples treated by Mayo and Tsakalakos [8]).

A. The Isotropic Inclusion

When the inclusion is isotropic the orthorhombic elastic constants reduce to the set

$$c_{11} = c_{22} = c_{33} = \alpha_1 = \alpha_2 = \alpha_3 = 2\mu(1-\upsilon)(1-2\upsilon)^{-1} \tag{6.1}$$

$$c_{12} = c_{13} = c_{23} = 2\mu\upsilon(1-2\upsilon)^{-1} \tag{6.2}$$

$$c_{44} = c_{55} = c_{66} = \mu \tag{6.3}$$

where μ is the shear modulus and υ is Poisson's ratio. It can easily be shown that the extrema of types [hkl] and [h01] are either imaginary or zero. The only relevant extrema are the habits [001], [010], [100]:

$$\mathbf{n} = \mathbf{e}_i \quad (i = 1,2,3) \tag{6.4}$$

where the $\mathbf{e}_i$ are the orthogonal principal axes of the stress.

In an isotropic system the tensor $\Omega^{\mathbf{n}}$ is [2]

$$\Omega^{\mathbf{n}}_{ij} = \mu^{-1}\delta_{ij} - [2\mu(1-\upsilon)]^{-1}n_i n_j \tag{6.5}$$

The values of $B^1(\mathbf{e})$ for the three habits specified by equation (6.4) are

$$\begin{aligned} B^1(\mathbf{e}_i) &= (\sigma^i)^2\Omega^{\mathbf{e}}_{11} \\ &= c_{11}^{-1}(\sigma^i)^2 \end{aligned} \tag{6.6}$$

where σ^i is the principal stress along $\mathbf{e}_i$. Choosing $|\sigma^1| \leqslant |\sigma^2| \leqslant |\sigma^3|$, the preferred habit of a thin-plate inclusion is

$$\mathbf{n} = \mathbf{e}_3 \quad \Rightarrow \quad |\sigma^3| = \max\{|\sigma^i|\} \tag{6.7}$$

If $\sigma^2 = \sigma^3$ then $B^1(\mathbf{e})$ is isotropic in the plane containing $\mathbf{e}_2$ and $\mathbf{e}_3$, and the habit can lie anywhere in the plane. If $\boldsymbol{\sigma}^\bullet$ is spherical the thin-plate habit is arbitrary.

B. Cubic Inclusion with a Tetragonal Transformation Strain

When the inclusion is cubic the orthorhombic elastic constants reduce to the set

$$c_{11} = c_{22} = c_{33} \tag{6.8}$$

$$c_{12} = c_{23} = c_{13} \tag{6.9}$$

$$c_{44} = c_{55} = c_{66} \tag{6.10}$$

moreover,

$$\alpha_1 = \alpha_2 = \alpha_3 = c_{12} + 2c_{44} \tag{6.11}$$

$$c_{11} - \alpha_1 = c_{11} - c_{12} - 2c_{44} = c_{44}\Delta \tag{6.12}$$

where Δ is the <u>anisotropy factor</u>. If $\boldsymbol{\varepsilon}^\bullet$ is tetragonal and $\mathbf{e}_3$ is the tetragonal axis then $\boldsymbol{\sigma}^\bullet$ is also tetragonal with principal stresses $\sigma^1 = \sigma^2 \neq \sigma^3$.

The type 1 extrema [100] and [010] are degenerate. The extremum [001] is unique. The type 2 ([hkl]) solutions are:

(1) for $\mathbf{q} = k\mathbf{n}$

$$n_3^2 = [(c_{11}+\alpha)\sigma^3 - 2\alpha\sigma^1]/[\Delta c_{44}(2\sigma^1+\sigma^3)] \tag{6.13}$$

(2) for $[q_1,q_2,q_3] = k[n_1,n_2,-n_3]$

$$n_3^2 = [(c_{11}+\alpha)\sigma^3-2c_{12}\sigma^1]/[\Delta c_{44}(c_{11}-c_{12}+2c_{44})\sigma^3-2(c_{11}+c_{12})\sigma^1] \tag{6.14}$$

In both cases

$$n_1^2 = n_2^2 = (1/2)[1-n_3^2] \tag{6.15}$$

The extrema (6.13) and (6.14) are, respectively, the extrema L_2 and L_1 identified in reference [7] for the habits of type [hhl]. Together with the extrema [100] and [001] they govern the preferred habit when $\Delta > 0$.

The type 3 ([h01]) solutions are:

(1) for $\mathbf{q} = k\mathbf{n}$

$$n_3^2 = [c_{11}\sigma^3-\alpha\sigma^1]/[\Delta(\sigma^1+\sigma^3)] \tag{6.16}$$

(2) for $[q_1,q_2,q_3] = k[-n_1,0,n_3]$

$$n_3^2 = [c_{11}\sigma^3-c_{12}\sigma^1]/[(c_{11}+c_{33})(\sigma^3-\sigma^1)] \tag{6.17}$$

In both cases

$$n_1^2 = 1 - n_3^2 \tag{6.18}$$

These are, respectively, the extrema L_2 and L_1 identified in reference [7] for habits of the type [h01]. The extremum L_2, equation (6.16), minimizes $B^1(\mathbf{e})$. When $\Delta \leqslant 0$ the preferred habit is determined by the the extremum L_1, equation (6.17), together with the extrema [100] and [001].

The preferred habits are identified in reference [7] as a function of the anisotropy factor and the tetragonality of the transformation strain.

C. Hexagonal Inclusion with a Hexagonal Transformation Strain

When the inclusion is hexagonal the orthorhombic elastic constants reduce to the set

$$c_{11} = c_{22} \neq c_{33} \tag{6.19}$$

$$c_{13} = c_{23} \neq c_{12} \tag{6.20}$$

$$c_{44} = c_{55} \tag{6.21}$$

$$c_{66} = (1/2)[c_{11}-c_{12}] \tag{6.22}$$

where $\mathbf{e}_3$ is the hexagonal axis. The hexagonal system has the property that $B^1(\mathbf{e})$ is isotropic in the basal plane of the hexagon. When ε^* is hexagonal or tetragonal on the same axes it is also isotropic in the basal plane. Then all directions in the basal plane are equivalent, and the extremal habits have the form [h01] where the direction of the axis $\mathbf{e}_1$ is arbitrary.

The relevant extrema are [001], [100], and the two extrema of type [h01]. Defining the parameter

$$\alpha = \alpha_2 = c_{13} + 2c_{44} \tag{6.23}$$

the extrema can be written:

(1) for $\mathbf{q} = k\mathbf{n}$

$$n_3^2 = 1 - n_1^2 = [c_{11}\sigma^3-\alpha\sigma^1]/[(c_{33}-\alpha)\sigma^1+(c_{11}-\alpha)\sigma^3] \tag{6.24}$$

(2) for $[q_1,q_2,q_3] = [-n_1,0,n_3]$

$$n_3^2 = 1 - n_1^2 = [c_{11}\sigma^3-c_{13}\sigma^1]/[(c_{11}+c_{13})(\sigma^3-\sigma^1)] \tag{6.25}$$

The extremum (6.21) minimizes $B^1(\mathbf{e})$. The general solution for the preferred thin-plate habit can be found by comparing the value of

$B^1(e)$ at the extremum given by (6.21) to its values at [100] and [001]. The transformation strain is, in dyadic form,

$$\varepsilon^0 = \varepsilon^0[e_1e_1 + e_2e_2 + (1+\eta)e_3e_3] \tag{6.26}$$

where ε^0 is the constant strain in the basal plane, η is the "tetragonality factor" [7],

$$\eta = [\varepsilon_{33}-\varepsilon^0]/\varepsilon^0 \tag{6.27}$$

and ε_{33} is the strain along the hexagonal axis. We can set $\varepsilon^0=1$ without loss of generality. The principal stresses are then

$$\sigma^1 = (c_{11}+c_{12}+c_{13}) + c_{13}\eta \tag{6.28}$$

$$\sigma^3 = (c_{33}+2c_{13}) + c_{33}\eta \tag{6.29}$$

The preferred habit is given as a function of η by the relations

$$\begin{aligned} n_3^2 &= [c_{11}\sigma^3-c_{13}\sigma^1]/[(c_{11}+c_{13})(\sigma^3-\sigma^1)] && (\eta\leqslant\eta^0) \\ &= 0 && (\eta^0\leqslant\eta\leqslant\eta^1) \\ &= 1 && (\eta^1\leqslant\eta) \end{aligned} \tag{6.30}$$

where

$$\eta^0 = [c_{13}(c_{11}-c_{12}-c_{13})+c_{11}c_{33}]/[c_{13}^2-c_{11}c_{33}] \tag{6.31}$$

$$\eta^1 = [c_{13}(c_{11}+c_{13}-c_{12})-c_{12}c_{33}]/[c_{13}^2-c_{11}c_{33}] \tag{6.32}$$

Equations (6.30) include the results of Mayo and Tsakalakos [8] for the habits of hexagonal precipitates in aluminum as a special case.

7. UNSOLVABILITY OF THE TRICLINIC PROBLEM

While the problem of determining the preferred thin-plate habit is solvable for orthorhombic and higher symmetries, it is not algebraically solvable in general. To establish this we show that the problem cannot always be solved for the particular case of an isotropic transformation stress in a triclinic inclusion.

Khatchaturyan and Airapetyan [4] showed that for a spherical transformation stress the ⟨111⟩ directions maximize the relaxation energy of a cubic crystal with positive anisotropy. In this case all the absolute maxima of $B^1(e)$ occur at non-trivial solutions to equation (3.12):

$$\lambda_{ijkl}n_jn_kn_l = n_i/k \tag{7.1}$$

If we perturb the elastic constants slightly we can produce a neighborhood (in the 21-dimensional space of triclinic elastic constants) of almost cubic elastic constants, all with the property that the absolute

maxima of the relaxation energy fall at solutions to (7.1).

By analytic continuation, if an algebraic formula for solving (7.1) exists and works for the perturbed set of elastic constants described above then the same formula applies when the elastic constants are replaced by complex constants. However, there are admissable sets of complex constants for which equation (7.1) cannot be solved.

For example, consider the set

$$\lambda_{1111} = 2\lambda_{3333} = 2$$

$$\lambda_{1112}=\lambda_{1121}=\lambda_{1211}=\lambda_{2111}=\lambda_{3323}=\lambda_{3332}=\lambda_{3233}=\lambda_{2333} = i(2/3)^{1/2} \qquad (7.2)$$

$$\lambda_{ijkl} = 0 \qquad \text{(otherwise)}$$

Using these constants and setting $n_3=1$ (recall that **n** need not be a unit vector) the vector equation (7.1) reduces to the simultaneous equations

$$\begin{aligned} 2n_1^3 + 3(2/3)^{1/2} i n_1^2 n_2 &= [1+3(2/3)^{1/2} i n_2] n_1 \\ (2/3)^{1/2} i n_1{}^3 + (2/3)^{1/2} i &= [1+3(2/3)^{1/2} i n_2] n_2 \end{aligned} \qquad (7.3)$$

The solution is

$$n_1^5 - (3/2)n_1 + 1 = 0 \qquad (7.4)$$

which can be shown to be irreducible (for example, by Kronecker's method [18]). A classic result of Galois theory [18] states that an irreducible quintic of the form x^5+px+q is solvable if and only if its resolvent sixth degree equation,

$$(y^3-5py^2+15p^2y+5p^3)^2 = (2^8p^5+5^5q^4)y \qquad (7.5)$$

has at least one rational solution. But for $p=-(3/2)$ and $q=1$ this equation has no rational roots.

It follows that the problem of determining the preferred thin-plate habit has no general algebraic solution when $B^1(\mathbf{e})$ has triclinic symmetry. Note that triclinic symmetry my result either from the crystal symmetry of the inclusion or from the mismatch between the crystal axes of the inclusion and the principal axes of the transformation stress.

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