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THE CALCULATION OF HABIT PLANES FOR ELASTIC TRANSFORMATIONS BY MINIMIZATION OF THEIR ELASTIC STRAIN ENERGY

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ABSTRACT

By using Eshelby's method for the determination of the stresses and strains generated in a transformation, the shape and orientation of an ellipsoidal region of transformed phase that minimises the elastic strain energy accompanying the transformation are calculated together with the change in elastic strain energy. The orientation of minimum total energy describes the habit plane. The applicability of the approach is demonstrated by showing that the habit planes of twins in cubic crystals, and martensitic plates in In-20%Tl and Fe-31%Ni, which have been calculated by other methods, can alternatively be determined by this method. It is then used to calculate that the habit plane for martensitic plates in bulk, high density, oriented orthorhombic polyethylene should be $(\overline{4.67,1,0})_{\text{orthorhombic}}$.

As a consequence of these calculations it is shown that minimization of the total elastic strain energy must be the dominating factor in the nucleation event of transformed products in most metals.

1. Introduction

Modern phenomenological theories of martensitic transformation,(1-3) (reviewed for instance by Dunne and Wayman(4)) developed in the last twenty years, have been remarkably successful in inter-relating the crystallographic features of many martensites and in cases, such as certain Fe-C steels, have predicted the existence of very thin twins in the martensites prior to their observation in the electron microscope(5). These theories are all essentially based on the geometrically necessary operations required to describe the transformed crystal structure in terms of the parent structure. As such they can predict the interface or habit plane but cannot make any statement concerning the shape of the transformed region, or about the free energy change accompanying the transformation.

The purpose of this paper is to demonstrate that there is an alternative, but essentially equivalent, way of determining the habit planes, and at the same time, the shape of a transformed region and the energy change, one in which the formation of the transformation product is accomplished in order to minimize its total elastic strain energy. This approach is based on the methodology introduced in a series of papers by Eshelby(6,7,8), who wanted to calculate the stresses and strains produced when a region (the inclusion) within a body changes in shape and/or size. The relationship to the crystallographic theories is that the elastic strain energy of an oblate spheroid is a minimum when its long axes are parallel to a plane of invariant strain. This relationship is demonstrated by Christian.(9)

The stresses and strains created in both the inclusion and the surrounding material are shown by Eshelby to be proportional to the shape change of the inclusion that would have occured had the surrounding material not constrained the transformation of the inclusion. This shape change is denoted as the transformation strain tensor ε_{ij}^{T}. The elastic field created by the transformation, and the stored energy in the elastic field, were shown by Eshelby to be also dependent on the shape of the inclusion and its orientation with respect to the coordinate axes of the transformation strain. More recently, Brown and Clarke(10) have calculated these effects on the shear stress components of the elastic field, together with tabulating them for many of the more common inclusion geometries.

The approach adopted here is firstly to decide on a plausible transformation strain that will describe the change in crystal structure that occurs on transformation; secondly to calculate the stored elastic energy when an elipsoid has this strain, and to find the shape and orientation of the ellipsoid that will minimize this energy. The same approach has been employed independently by Shibata and Ono(11) to calculate successfully the habit planes for the bcc-hcp transformations in titanium.

In his 1957 paper, Eshelby used the idea that a transformation would occur in such a way as to minimize its total elastic energy, in order to deduce from Zener's(12) value of the heat of formation for martensite in iron that the martensite formed as discs with an aspect ratio of about 0.08. Later, Christian(13) in an attempt to relate the accommodation effects of a transformation to the Bowles and Mackenzie(14) dilatation parameter, applied Eshelby's method to the case of a thin ellipsoidal plate subjected to a general transformation strain. He showed that the accommodation, and hence the elastic energy, was minimized as the aspect ratio of the plate decreases.

Since it is based on Eshelby's method, the procedure used here is appropriate to any coherent shear transformation. For this reason section 3 is devoted to illustrating its applicability to a variety of transformation processes: a simple twinning reaction, the simple transformation in an indium-thallium alloy, the more complex martensitic transformation in an iron-nickel alloy, and the martensitic transformation in polyethylene crystals, where a habit plane has yet to be reported.

As the purpose of this paper is to demonstrate the calculation of habit planes and the shapes of the transformed products, rather than to present highly accurate calculations, the simplifications of linear isotropic elasticity and of an isotropic surface energy of the transformed inclusion are assumed. Indeed it is shown in section 4, that unless the transformed regions are very small ($\lesssim 10^{-21}\text{cm}^3$) the surface energy contribution to the total free energy is negligible compared with the elastic strain energy.

2. Background Theory

The problem that Eshelby tackled in his papers was how to calculate the elastic state of a body when an internal region underwent a change in shape or size, which in the absence of the constraining material could be described by a stress-free transformation strain, ε_{ij}^T.

Of the many results established by Eshelby, the one relevant here was that the energy stored in the elastic strain field caused by the transformation of an ellipsoidal inclusion could be expressed as:

$$E = -\frac{1}{2} V_I \, \sigma^I_{ij} \, \varepsilon^T_{ij} = -\frac{1}{2} V_I \, C_{ijkl} \, \varepsilon^I_{kl} \, \varepsilon^T_{ij} \qquad (1)$$

V_I is the volume of the ellipsoid, C_{ijkl} are the elastic constants and ε^I_{kl} is the strain within the inclusion. In this, and subsequent equations, the convention of summation over repeated suffixes is assumed.

The actual strain sustained by the inclusion is dependent only on the transformation strain and the shape of the inclusion. This relationship has been expressed in two equivalent ways depending on its usage, namely,

$$\varepsilon^I_{ij} = S_{ijkl} \, \varepsilon^T_{kl} - \varepsilon^T_{ij} = \gamma_{ijkl} \, \varepsilon^T_{kl} \qquad (2)$$

where S_{ijkl} are geometric coefficients introduced by Eshelby and γ_{ijkl} is an accommodation tensor. Tables of S_{ijkl} and γ_{ijkl} for a variety of commonly accuring inclusion shapes have been listed by Brown and Clarke (10). Eshelby prescribes how, for the general ellipsoid, the values of S_{ijkl} may be determined, and the reader is referred to his paper for details. They may alternatively be found for various aspect ratios from the graphs and tables of reference 15.

Two sets of orthogonal coordinate axes need to be defined in the calculation of the strain energy; the frame of the matrix phase and the frame of the transformed ("inclusion") region (Fig. 1). As shear transformations are considered in this paper, the matrix phase coordinate frame is defined by the crystallography of the parent phase with the x axis being the shear direction, the z axis being the shear plane normal, and the y axis being perpendicular to the other two in most of the examples given in section 3. The transformed region is defined in the inclusion frame and is assumed here to be a circularly symmetric ellipsoid about one axis, having a finite aspect ratio and intercepts along the axes of a, b and a. The aspect ratio, p, is given by the ratio b/a; when $b>a$ the inclusion is a prolate spheroid and when $b<a$ it is an oblate spheroid.

The transformation strain and the elastic strain energy density are defined in the matrix coordinate frame, whereas the S_{ijkl} coefficients are presented by Eshelby and by Brown and Clarke in the inclusion frame. In the general case of the matrix frame and the inclusion frame not being coincident, the S_{ijkl} coefficients required in equation (2) can be found from those defined in the inclusion frame S^{IF}_{mnop} by the usual tensor relationship

$$S_{ijkl} = a_{im}\, a_{jn}\, a_{ko}\, a_{lp}\, S^{IF}_{mnop}$$

where a_{ij} is the matrix relating the two coordinate frames (Fig. 1).

The method of determining the minimum energy position is to calculate, for each relative position in space of the two frames, values of the S_{ijkl} coefficients in the matrix frame and hence values of the elastic energy from equations 2 and 1. This is a complicated set of calculations and is best manipulated using a computer. The position of minimum energy can then be identified.

For most cases of importance the spheroidal ellipsoid is a versatile enough approximation to the true shape. When it is not, equation 1 must be replaced by its integral over the volume of the shape.

3. Applications

3.1 Twinning in Cubic Crystals

Twinning in cubic crystals is a particularly simple transformation process because the crystal structure of the twinned region is related to the parent structure by a single pure shear. In addition the transformation is well characterised; in fcc metals a (tensor) shear strain of $\frac{1}{2\sqrt{2}}$ in the $[11\bar{2}]$ direction describes both the macroscopic shear and the lattice reorientation of a twin on a (111) plane, and in bcc metals the same value of shear strain in the $[\bar{1}\bar{1}1]$ direction on a (112) plane describes the twin. Because of this simplicity of lattice reorientation and the ample experimental observations and verifications, it is of interest to show that the observed twinning modes correspond to minima of the strain energy accompanying the twinning transformation.

Using the directions $[\bar{1}\bar{1}1]$, $[1\bar{1}0]$ and $[112]$ to form an orthogonal set of coordinate axes in the bcc parent phase, the transformation strain that describes the atomic adjustments occuring during twinning can be written as

$$\varepsilon^{T}_{ij} = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 0 & S \\ 0 & 0 & 0 \\ S & 0 & 0 \end{pmatrix}$$

$$\text{where } S = \frac{1}{\sqrt{2}}$$

The same strain describes the twinning transformation in fcc structures, provided the coordinate axes are chosen as $[11\bar{2}]$, $[\bar{1}10]$ and $[111]$. These axes correspond to the shear direction, the normal to both the shear direction and the shear plane normal, and the normal to the shear plane, respectively. This expression for the twinning strain is only approximate. The complete strain tensor required to describe the crystallography of twinning contains terms in s^2, and as the value of s is not small these terms cannot strictly be neglected. However, since the transformation elasticity equations used throughout this paper are only valid for a linear elasticity, it is probably not worthwhile to use the complete strain tensor and so the less accurate infinitesmal-strain approximation is used. One result of this approximation is to make the transformation strain symmetrical to the Ox and the Oz axes rather than to the conventionally denoted η_1 and η_2 axes. It should be symmetrical to the latter since a twin and its conjugate represent equivalent deformations differing only by a pure rotation.

Following the method of calculation described in the introduction, the elastic strain energy per unit volume for twinned regions with this transformation strain is found to vary with both the orientation and the aspect ratio of the twinned region. It is found to be smaller when the twinned region is an oblate spheroid than if it were a prolate spheroid. Furthermore, it has a minimum at two positions in a bcc parent phase, when the normal to the spheroid is either [112] or $[\bar{1}\bar{1}1]$. The second minimum position is a result of the approximate transformation strain used with its symmetry with respect to the 111 and 112 bcc axes. As this symmetry doesn't exist, as explained above, this minimum is fictitous.

The sharpness of the elastic energy minima is portrayed in Fig. 2, which is a plot of the variation in calculated stored elastic strain energy density of an oblate spheroid twin for different positions of its normal in the plane whose normal is $[110]_{bcc}$. The aspect ratio of this particular spheroid is 0.01, and even for this ratio there is a very large variation of the strain energy calculated - almost two orders of magnitude. The sharpness of the minima probably indicates why there is very little scatter in the composition planes determined experimentally.

In Fig. 3, the elastic strain energy density is plotted as a function of the aspect ratio of the spheroid. The curve shows that a transforming twin can minimise its elastic strain energy by forming as an oblate spheroid with as small an aspect ratio as possible, and in the limit tending asymptotically to being infinitely small. This is the deduction that Christian(13) made.

3.2 Martensitic Transformation in In-20.4%Tl.

The martensitic transformation in indium-thallium is one of the classic transformations; the transformation interfaces can be made to sweep reversibly through a crystal and the fcc and fct lattices are so nearly alike that the choice of lattice correspondence is clear. In addition as the fct martensites are twin-related lamallae, the prediction of the {110} habit plane was relatively straightforward.(16)

The reason for considering this transformation here is to demonstrate the applicability of the transformation approach to one of the simplest martensitic transformation, and to calculate both the habit plane and elastic strain energy change involved.

On cooling, at about 60°C, a fcc indium 20.4 atomic percent Thalium alloy transforms to a face-centered-tetragonal martensite by contracting along two <001> directions and expanding along the other. The values of the lattice parameters of this alloy are approximately $a_{fcc} = 4.740$, $a_{fct} = 4.710$ and $c_{fct} = 4.787\text{Å}$ (Fig. 3 of a paper by Moore et al.,(17)).

Referred to a coordinate system where the x,y and z axes are [100], [010] and [001] respectively in the fcc phase, the transformation strain in the approximation of linear elasticity, is:

$$\varepsilon_{ij}^{T} = \begin{pmatrix} -0.0633 & 0 & 0 \\ 0 & 0.0099 & 0 \\ 0 & 0 & -0.0633 \end{pmatrix}$$

Computation of the elastic strain energy density involved during this transformation shows that the minimum energy orientation corresponds to an oblate spheroid having a habit plane within 1/2° of $(1\bar{1}0)$. This agrees very closely with the observed {110} habits. As with the twinning transformation, the minimum is sharply defined and the energy is calculated to decrease with decreasing aspect ratio (Fig. 3). The elastic strain energy accompanying the transformation of a spherical region of In-Tl is given in Table I.

3.3 Martensitic Transformation in Fe-31%Ni Steels

Of the very many martensitic transformations in steels that have been analysed, the one chosen here to illustrate the applicability of the transform method to complex transformations is the one that occurs in Fe-31%Ni. This is because it is one of the few transformations for which there is a crystallographic explanation for the observed orientation relationship.

It is not at all clear what strain tensor should be used to describe the transformation as there is no information as to what the detailed atomic movements accompanying the transformation are. However, in the absence of such data the crystallographic mechanism originally proposed by Nishiyama seems reasonable as it does at least lead to the observed orientation relationship. Although the mechanism cannot be entirely correct, since it doesn't predict the extensive {121} twinning within the martensitic plates observed by electron microscopy, it is nevertheless used here as an approximation to the actual transformation mechanism.

Nishiyama$^{(18)}$ observed that in the Fe-31%Ni alloy the orientation relationship between the austenite (γ) and martensite (α') phases was $\{111\}_\gamma$ // $\{110\}_{\alpha'}$ and $\langle 211\rangle_\gamma$ // $\langle 110\rangle_{\alpha'}$.
As a result he proposed that the transformation occurred by a shear parallel to $\{111\}_\gamma$ in the direction $\langle 211\rangle_\gamma$ through an angle of 19°28', followed by lineal adjustments to enlarge the basal angle of 60° to 70°32' and to satisfy the measured interplanar spacings. Although this leads to the correct orientation relationship the mechanism implies the habit plane to the $\{111\}_\gamma$ and as this is at variance to the observed habit, the Nishiyama mechanism has been discarded. Later, the phenomenological crystallographic theories showed that the observed habit could be tolerably predicted by a Bain distortion and a lattice invariant shear strain in the $\langle 111\rangle_{\alpha'}$ direction on a {121} plane, derived from a {110} austenite plane. A better agreement was later obtained by the incorporation of a small dilatation parameter$^{(14)}$.

Despite the shortcomings of the Nishiyama mechanism it can be shown that a minimum energy position is predicted close to the observed habits.

Choosing the matrix coordinate frame to be described by the austenite directions $[\bar{2}11]$, $[0\bar{1}1]$ and $[111]$, the necessary transformation strain required to describe the Nishiyama mechanism becomes

$$\varepsilon_{ij}^{T} = \begin{pmatrix} -0.07556 & 0 & 0.17673 \\ 0 & 0.1321 & 0 \\ 0.17673 & 0 & -0.01945 \end{pmatrix}$$

when the lattice parameters for the austenite and martensite are a_γ = 3.591 and $a_{\alpha'}$ = 2.875Å respectively.(19)

In Figure 4 the position of minimum elastic energy for an oblate spheroid of aspect ratio 0.01 is plotted in a stereographic triangle, together with some of the more recently reported precision habit planes determinations, for Fe-31.1%Ni and Fe-30.9%Ni taken from Fig. 3b of Breedis and Wayman.(19) As can be seen the predicted habit plane is quite close to the reported habits and falls within 2° of the median position. This agreement is unexpectedly good since the transformation strain used does not include any terms appropriate to the observed internal {121} twinning of the martensite produced. The closeness is probably rather fortuitous.

Also plotted are contours of energy corresponding to the minimum energy plus one percent and five percent, to give an indication of the possible variation in habit planes produced if the minimum energy criterion is not exactly fulfilled. The large variation encompassed by the five percent contour is of particular interest because the simplifications of isotropic elasticity used in calculating the energies will probably introduce an error of typically five to ten percent for most metals. The five percent contour is of further interest since comparison with the positions of habits reported for Fe-Ni alloys with varying Ni content from 30.9 to 34.8% (Reed,(20) and Figure 22 of reference 21) strikingly shows that they too are encompassed by the contour. Thus relatively large variations in alloy content can lead to significant variations in habit, whilst only changing the elastic energy by a small amount. Although the energy minimum is relatively shallow, the variation in elastic energy between the minimum energy and the maximum energy positions is large. Naturally this variation increases as the aspect ratio decreases but even for an aspect ratio of 0.01 it is large; minimum energy density and maximum energy density are computed to be 4.2×10^{-2} and 1.3×10^{-1} μV respectively. As a result it is not surprising that the habit planes are located near to (259).

As with the previous examples, the strain energy density decreases with decreasing aspect ratio (Fig. 3) from the value given in Table I for a spherical region, but this does not markedly affect the predicted habit plane, which is that shown in Fig. 4, provided that the aspect ratio is smaller than about 0.3.

3.4 Martensitic Transformation in Bulk Polyethylene

Having established in the previous examples the viability of the transformation method, we now use it to predict what the habit plane in high density, oriented crystalline polyethylene should be.

Young and Bowden(21) have reported that when bulk oriented, high density polyethylene is deformed in compression at right angles to the molecular chains, it undergoes a martensitic orthorhombic to monoclinic transformation resulting in an orientation relationship of the type Tl_2. This is the designation of one of the orientation relationships proposed by Bevis and Crellin(23) that might geometrically occur as a consequence of a transformation in polyethylene. The Tl_2 relationship corresponds to the $(110)_o$ and $(010)_m$ planes being inclined to each other by 7°, and an angle of 44° separating the $(220)_o$ and $(220)_m$ planes. The subscripts o and m refer to orthorhombic and monoclinic respectively. Young and Bowden show that the orientation relationship they observe can be obtained if the orthorhombic crystal transforms by a shear on a plane $(\overline{4.667}, 1, 0)_o$. This is shown diagramatically in Fig. 3 of reference 22.

Defining the molecular chain orientation, $[001]_o$ to be the z axis, the c_1 orthorhombic axis, [100], to be the x axis and the c_2 axis, [010], to the y axis, the transformation can be described by the strain

$$\varepsilon^T_{ij} = 0.1005 \begin{pmatrix} \sin 2\theta & \cos 2\theta & 0 \\ \cos 2\theta & -\sin 2\theta & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

where θ, the angle the shear plane makes with the $(100)_o$ plane, is 171.87 degrees. Since the transformation is independent of position along the molecular chains (z axis), the predicted habit must also be perpendicular to the z axis.

Although the martensitic transformation is stress induced, the applied stress will not affect the orientation assumed by the monoclinic phase. This is because the elastic energy due to the interaction of the applied stress field and the transforming inclusion is independent of the shape or orientation of the inclusion.(6-8)

By analogy with the case of cubic twinning, where the transformation strain also describes a pure shear, it is to be expected that the predicted habit plane will coincide with the plane of shear, namely $(\overline{4.667},1,0)_o$.

When this transformation strain is used and the minimum energy configuration found, the predicted habit plane normal is indeed at right angles to the polyethylene chains and is the same as the shear plane. Its position is shown on the (001) orthorhombic stereographic projection, of Fig. 5, together with the 120% of the minimum energy density contour. As yet it cannot be compared to any experimental determination as none has been reported.

It is to be expected that the polyethylene crystal will be highly anisotropic elastically, having maximum stiffness parallel to the molecular chains in the crystal, i.e. along the $[001]_o$ direction. Whilst such elastic anisotropy hasn't been included in these calculations, it is anticipated that its inclusion, for this particular transformation, would not alter the calculated habit. This is because the calculated habit plane already includes both the expected elastically stiff direction and the shear direction between the chains; any other habit plane would result in greater distortion in the hard direction thereby increasing the strain energy.

4. The Total Free Energy Change

In the previous section the habit planes were calculated on the basis that they were determined by the minimization of the elastic strain energy alone. However, if the material undergoes an equilibrium shear transformation, it is the minimization of the total free energy that determines the shape and orientation of the transformed product. It is the purpose of this section to deduce that the overwhelming orientation dependent contribution to the free energy change comes from the elastic strain energy. In general there will be five main contributions to this free energy change: the "chemical" contribution, the elastic energy stored in the strain field created by the transformation, the surface energy of the product, the energy associated with any elastic interactions, and lastly, the energy associated with the image strain field.

The "chemical" contribution is the free energy change which would occur if the inclusion transformed by its stress free strain in the absence of any matrix. As such, the elastic transformation theory can make no statement concerning this contribution, but it will of course be independent of orientation. The elastic interaction energy has two parts; the elastic interaction between any applied stress field and the transforming inclusion, and the interaction between the individual products distributed throughout the volume of the parent phase. The first part is of no consequence as Eshelby has shown it to be independent of the shape of the transformed region.$^{(6-8)}$

The second part would be the most difficult to calculate since it depends on a knowledge of the spatial distribution of the product phase. However, it does not seem necessary to calculate it. If it were isotropic it would be a constant additive term independent of orientation. If it were anisotropic it would be manifested by the product phase being oriented more often on one of a set of planes than on the others in the same crystallographic set, and as such preferential orientations are rarely seen the anisotropic component of the elastic interaction energy must be small in comparision to the other energy contributions. The energy stored in the image strain field has been determined by Eshelby$^{(8)}$ who showed that it depends on both the transformation strain, and the image strain field as well as on the volume fraction of the transformed product present. The calculation of the image strain field presents few problems$^{(10,24,25)}$ but the evaluation of its associated energy has not been included here because of the lack of experimental data on the variation of volume fraction of transformed product as transformations proceed. As the image field exists in order to render the tractions at the surface zero, the contribution is zero for an infinite body, so these calculations are strictly for infinite body materials.

Since the elastic strain energy of an ellipsoid of unit volume decreases with a decreasing aspect ratio, Fig. 3, it would appear to be energetically favourable for the transformed product to form in as thin a plate as possible(13). However, for small aspect ratios and small volumes, the contribution from the surface energy term becomes significant. An ellipsoid of revolution has a surface energy given by the equation

$$E_s = \gamma_s \left(\frac{V}{P}\right)^{2/3} 2\pi \left(\frac{3}{4\pi}\right)^{2/3} \left\{1 + \frac{p^2}{\sqrt{1-p^2}} \log \left[\frac{(1-p^2)^{1/2} + 1}{P}\right]\right\}$$

(assumed to be isotropic), where γ_s is the interphase surface energy per unit area/ V is the volume of the ellipsoid and p is its aspect ratio.* For all but very small volumes (less than about 10^{-23}cm^3) the surface energy contribution is small in comparison with the elastic strain energy, since the interphase surface energy per unit area is very much smaller than the shear modulus; γ_s is typically of the order of 10 ergs cm^{-2} whereas μ is of the order of 10^{11} dynes cm^{-2}. However, for small volumes, the rapid increase in surface energy with aspect ratio counters the relatively slow decrease in elastic strain energy with aspect ratio.

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* For extremely small particles, the expression used by Orowan(26) for the surface energy is probably more realistic than this, as it takes into account the area of the atomic steps forming the surface. However, the difference between the two expressions is small for ellipsoids of small aspect ratio.

It might be thought then that two regimes may be identified. One, where the volume is large, and the habit plane and shape are determined by a desire to minimise the elastic strain energy, the surface energy being insignificant. Two, where the volume is small and the habit and shape are determined by a minimisation of the combined surface and strain energies. If the interphase surface energy is isotropic the habit plane will be unaffected and the only effect of the surface energy will be to determine the aspect ratio of the transformed product for its particular volume. However, for most transformations the surface energy contribution will be negligibly small for physically realistic volumes of material. This is illustrated by the values, listed in Table II, of the aspect ratios, thicknesses, surface energies and strain energies calculated for five different plates of martensite in the Fe-31%Ni alloy when they are of minimum combined surface and strain energy. An isotropic inter-phase surface energy, γ_s, of 15 erg cm^{-2} and shear modulus for Fe-31%Ni of 1.52×10^{12} dynes cm^{-2} (27) were used in the calculation. Quite clearly, plates of such sub-atomic thicknesses as predicted by the minimization of the combined surface and elastic strain energies, cannot possibly exist. What probably occurs is that the transformed phase grows into a thin disc or plate by spreading out in an attempt to minimise its strain energy density until it is prevented from growing out any further by meeting an impediment, for instance a grain boundary, another growing plate of product phase, or an inclusion. Then according to whether it is energetically favourable or not for the whole material, the transformation proceeds by the plate growing thicker or by other plates continuing to spread out. Similar values to those in Table II are obtained for the other transformations, so the conclusion that the transformation cannot physically attain a minimum value of combined surface and elastic strain energy, is also valid for them.

This leads back to the nucleation of the transformed product and although the elastic energy approach elaborated here can not say anything about the nucleation event, it can legitimately be used to estimate the product size below which the elastic strain energy of the transformation has no influence on the particle orientation. Assuming at this critical size, the maximum elastic strain energy is equal to the minimum surface energy, and the shape of the product is clearly a sphere. The energy balance is then

$$4/3\ \pi a^{*3} \mu\ E_p = 4\pi a^{*2} \gamma_s \quad \text{leading to} \quad a^* = \frac{3\gamma_s}{\mu E_p}$$

where E_p is the elastic strain energy density constant and is related to the total elastic strain energy, E, by $E = \mu V E_p$. For the Nishiyama transformation, using the energy density constant for a sphere given in Table I leads to a critical radius, a^*, of $\sim 2\gamma_s \times 10^{-3}$Å. Because any anisotropic corrections are unlikely to be greater than a factor of two, and the interphase surface energy is probably not more than an order of magnitude greater than about 20 ergs cm^{-2}, the minimization of elastic strain energy must be an important factor in the nucleation phenomenon. Also, clearly, whatever the nucleation process the subsequent growth will be determined by a minimization of the elastic strain energy, unless the transformation is an exceedingly non-equilibrium process.

The conclusions of the previous paragraph are based on the assumption that at the critical nucleus size the elastic strain energy is equal to the surface energy. It is likely, however, that at certain orientations, such as those corresponding to the cusp in surface energy, asymmetric growth may occur even though this may be unfavourable elastically, in which case the above estimates would have to be modified. In such circumstances the determination of the habit and critical nucleus shape is a difficult problem, compounded by the absence of detailed measurements on the variation of surface energy with orientation, which is beyond the limited objectives of this particular paper. To complete the picture, a fully rigorous approach would also have to assess the probability of occurrence for surface versus elastically dominated shapes.

5. Discussion

The inherent limitation of the minimization of elastic strain energy approach is that it can say nothing about the path of the atoms undergoing the transformation; a transformation strain must be supplied. Furthermore unless the transformation mechanism chosen is the same as that which actually occurs, the predicted habit planes and shapes will not necessarily be the same as those observed. As such part of the usefulness of the strain energy approach is in differentiating between proposed possible atomic mechanisms, and in relating mechanisms to energy changes experimentally measured on transformation. Unfortunately the reverse is not possible. Furthermore, as with all energy minimization techniques, the existence of a minimum total energy configuration is only a necessary condition for the occurrence of that configuration, and the sufficiency condition are determined by the nucleation and kinetics of the reaction.

In addition to these fundamental limitations there are others which are not inherent; the use of isotropic linear elasticity, isotropic surface energies and identical elastic constants in parent and product phases. The simplification of isotropic elasticity can be easily removed by the use of the appropriate anisotropic equations using the work of Walpole(28) who extended Eshelby's formulation to anisotropic materials. The use of anisotropic surface energies also presents no problem, but their use is restricted by the dearth of the necessary measurements. Similarly, the lack of experimental data on the elastic moduli of the transformed product phases precludes, for most materials, allowance for the two phases having different elastic constants. The case of the transformation product being inhomogeneous has been treated in isotropic elasticity by Eshelby(6-8) and in anisotropic elasticity by Walpole(28).

One advantage of the energy minimization formulation is that it leads quite naturally to the possibility of a variability, or scatter, of the habit planes, since there will inevitably be several sources of perturbation preventing the transformed product forming at the exact position of minimum energy. The positional energy contours shown in Fig. 4 and 5 show that even a relatively small perturbation (1 to 20%) can cause wide variation in possible habits.

Although only diffusionless transformations have been considered in this paper, Eshelby's method can equally be applied to diffusion controlled transformations by the use of an appropriate transformation strain. For instance, it has been used to describe the generation of stresses and strains produced by precipitation from a super-saturated solid solution(29), and in the calculation(30) of the diffusional stress relief during elastic deformation of copper containing particles of silica.

The curves of Fig. 3 and the strain energy values of Table I can be used in two ways in estimating the strain energy contribution to the free energy change accompanying a transformation event. Firstly, if the volume fraction of product phase and its aspect ratio are known, then the contribution may be calculated directly and compared to the experimentally measured heat change. Alternatively, as the strain energy density is a maximum for a spherical particle, an upper bound may be placed on the strain energy contibution by multiplying the value for a sphere by the volume fraction of the product phase. The fact that in Fig. 3 the curves for polyethylene and twinning are identical is simply due to the choice of a pure shear to describe the transformation for both materials. As such the curves for the two materials are in direct proportion to the magnitudes of their shear transformation strain and after scaling only the geometrical effect of the aspect ratio remains. Similarly, the curves for the Fe-31%Ni and In-20%Tl are nearly alike, since their transformation strains consist of a pure shear and a dilatation and although the relative values of the shear to dilatation for the two transformations are slightly different, the two curves are so similar after scaling that they are covered by the same line.

The particular form of energy minimization adopted in this paper, based as it is on the Eshelby analysis, applies only to coherent transformations that are homogeneously nucleated. It is assumed here that the martensite and twinning transformations are indeed both coherently and homogeneously nucleated. Whilst this does conflict with some experimental evidence suggestive of heterogeneous nucleation, the controversy over the nucleation of these transformations remains such an open issue that this assumption is reasonable. A consequence of such a homogeneously nucleated coherent transformation is that the dislocation mechanism, by which the glide and climb of suitable interfacial dislocations produces, respectively, the shear and dilatational components of the transformation strain, cannot be correct. The dislocation structures observed must therefore be a result of the transformation mechanism occurring, for instance to accommodate local strains produced by non-relaxed stresses created during the transformations, rather than representing the causal mechanism itself. The actual mechanism might then originate in lattice vibration modes as suggested for martensite by Wasilewski(31) and so successfully applied to the omega transformation by Cook, et al.(32) and the phase transformations in barium titanate following the method described by Cochran.(33)

An important question is what reliance should be placed on the predictions made using the energy minimization formulation, since the prediction of the minimum energy may be computed as accurately as desired given a transformation strain that describes the lattice reorientation. If the transformation also occurs in thermodynamic equilibrium, then the predictions should be exact. However, the position is in practice limited by the inaccuracies and uncertainties of the reported lattice parameters, elastic constants and surface energies. In addition, it has been assumed that the nucleation event, if one exists, does not affect the subsequent growth of the product. These factors, together with any inhomogeneity in the material, probably determine how far from the exact position of minimum energy the product phase forms. As such the predictions of the habit plane, its variation with perturbations, and the value of the elastic strain energy involved in the transformation, are probably very reliable. If precise lattice parameters, orientation relationships, elastic constants and thermal expansion coefficients were available, it should be possible to determine the effects of composition and temperature on habit planes. Furthermore, given reliable information on the percentage of transformed material as a function of temperature the stored energy could be related to the energy change measured.

Conclusions

The minimization of the elastic strain energy has been shown to be an alternative calculational procedure to the crystallographic theories for the calculation of habit planes of a wide variety of coherent transformation products. The method also enables an estimate to be made of the shape of the product, and of the free energy change accompanying the transformation, it should be of particular value when used in conjunction with the crystallographic theories of transformations.

In particular, as well as reproducing the known composition plane for twinning in cubic crystals and the habit plane for the martensitic transformation in In-20%Tl, the method has been used to show that Nishiyama's mechanism for the martensitic transformation in the Fe-31%Ni alloy does lead to a habit plane close (within 2°) to the experimental determinations. Although this close agreement is unrealistic, since no account was taken of the observed internal twinning of the martensite plates, it is probably indicative that the Nishiyama mechanism does form a basis for the atomic motions taking place during the transformation.

When the procedure is applied to the stress-induced martensitic transformation in oriented high-density polyethylene, a habit plane of $(\overline{4.67},1,0)_{\mathrm{orthorhombic}}$ is predicted to occur.

By consideration of the elastic strain energy generated by a transformation it is deduced that orientation to minimise the elastic strain energy contribution must be an important factor in the nucleation of a transformed structure in most metals.

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TABLE I

Elastic strain energy of a spherical region of transformed material.

Transformation	Energy units of μV
Cubic Twinning	2.67×10^{-1}
In-20%Tl	1.74×10^{-4}
Fe-31%Ni	8.90×10^{-2}
Polyethylene	2.16×10^{-2}

TABLE II

The Surface Energy and Elastic Strain Energy Contributions of a Martensitic Plate of Minimum Total Energy

Volume of Ellipsoid cm^3	Aspect Ratio	Diameter of Ellipsoid (a) cm	Thickness of Ellipsoid cm	Surface Energy ergs	Elastic strain energy stored ergs
10^{-15}	1×10^{-3}	1.2×10^{-4}	1.2×10^{-7}	3.6×10^{-7}	621×10^{-7}
10^{-18}	5×10^{-3}	7.2×10^{-6}	3.6×10^{-8}	1.2×10^{-9}	63×10^{-9}
10^{-21}	2×10^{-2}	4.6×10^{-7}	9.2×10^{-9}	4.9×10^{-12}	67×10^{-12}
10^{-23}	4×10^{-2}	7.8×10^{-8}	3.0×10^{-9}	1.5×10^{-13}	7.2×10^{-13}
10^{-24}	6×10^{-2}	3.2×10^{-8}	1.9×10^{-9}	2.4×10^{-14}	7.6×10^{-14}

FIGURE CAPTIONS

Fig. 1. The relationship between the inclusion and matrix coordinate frames, together with the transformation matrix relating them.

Fig. 2. The variation in the elastic strain energy density of a twinned ellipsoid in a cubic crystal as a function of the orientation of its normal in the plane whose normal is [$1\bar{1}0$]. The minimum energy density positions are marked for a bcc lattice; the equivalent fcc positions are given in the text. The aspect ratio used was one tenth.

Fig. 3. The variation of the elastic strain energy density with aspect ratio, for ellipsoids of Fe-31%Ni and polyethylene. The curve for the twinning transformation is identical to that for the polyethylene and that for the In-Tl is very similar to that for the Fe-31%Ni. The curve corresponds to the minimum energy density orientation of the ellipsoid having the aspect ratio shown. Note, the scales have been normalised so that the elastic strain energy density of a sphere is unity.

Fig. 4. Stereogram depicting the predicted habit plane (∇ - close to 5, 13, 18) and the 101% and 105% (dashed line) of minimum energy contours calculated for Fe-31%Ni using an aspect ratio of 0.05. Also shown (in dots) are the martensite mid-rib plane determinations made by Breedis and Wayman(19) on Fe-30.9%Ni and Fe-31.1% Ni specimens.

Fig. 5. The predicted habit plane [∇ - close to $(\overline{4.67},1,0)_o$] for the martensitic transformation in polyethylene, together with the 120% of minimum energy contour An aspect ratio of 0.05 was used in the calculations.

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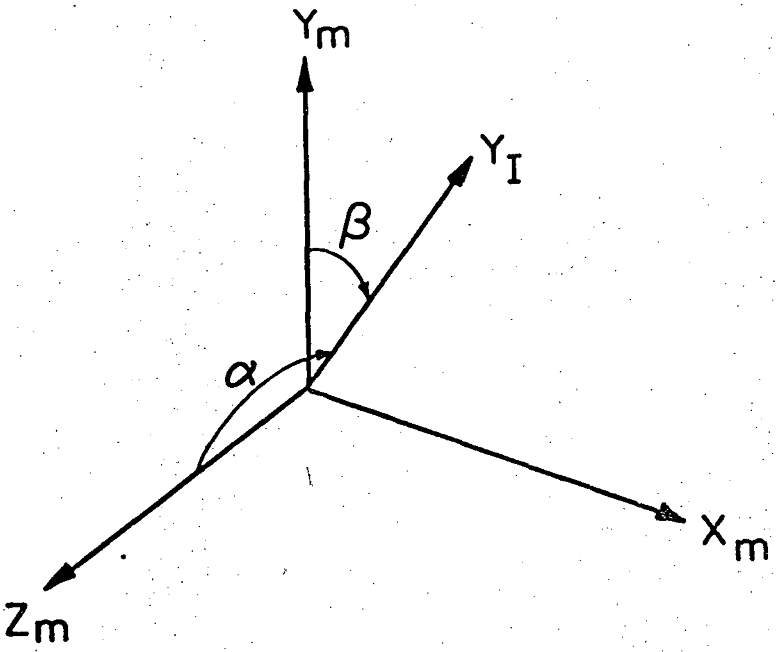


$$a_{ij} = \begin{pmatrix} \sqrt{C} & \sqrt{1-C} & 0 \\ -\cos\beta\sqrt{\frac{1-C}{C}} & \cos\beta & \frac{-\cos\alpha}{\sqrt{C}} \\ -\cos\alpha\sqrt{\frac{1-C}{C}} & \cos\alpha & \frac{\cos\beta}{\sqrt{C}} \end{pmatrix}$$

$$C = \cos^2\alpha + \cos^2\beta$$

XBL 756-6615

Fig. 1.

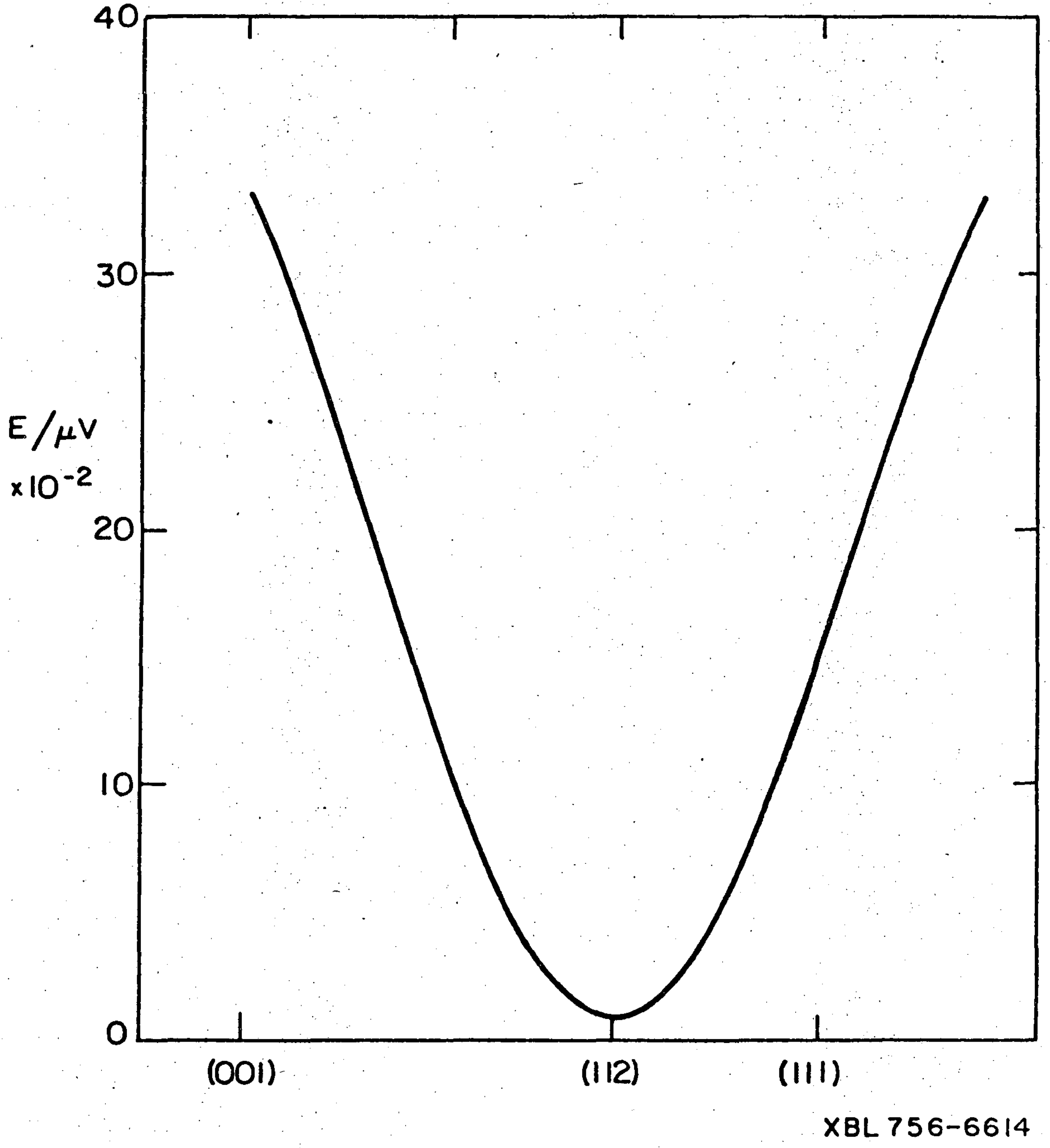
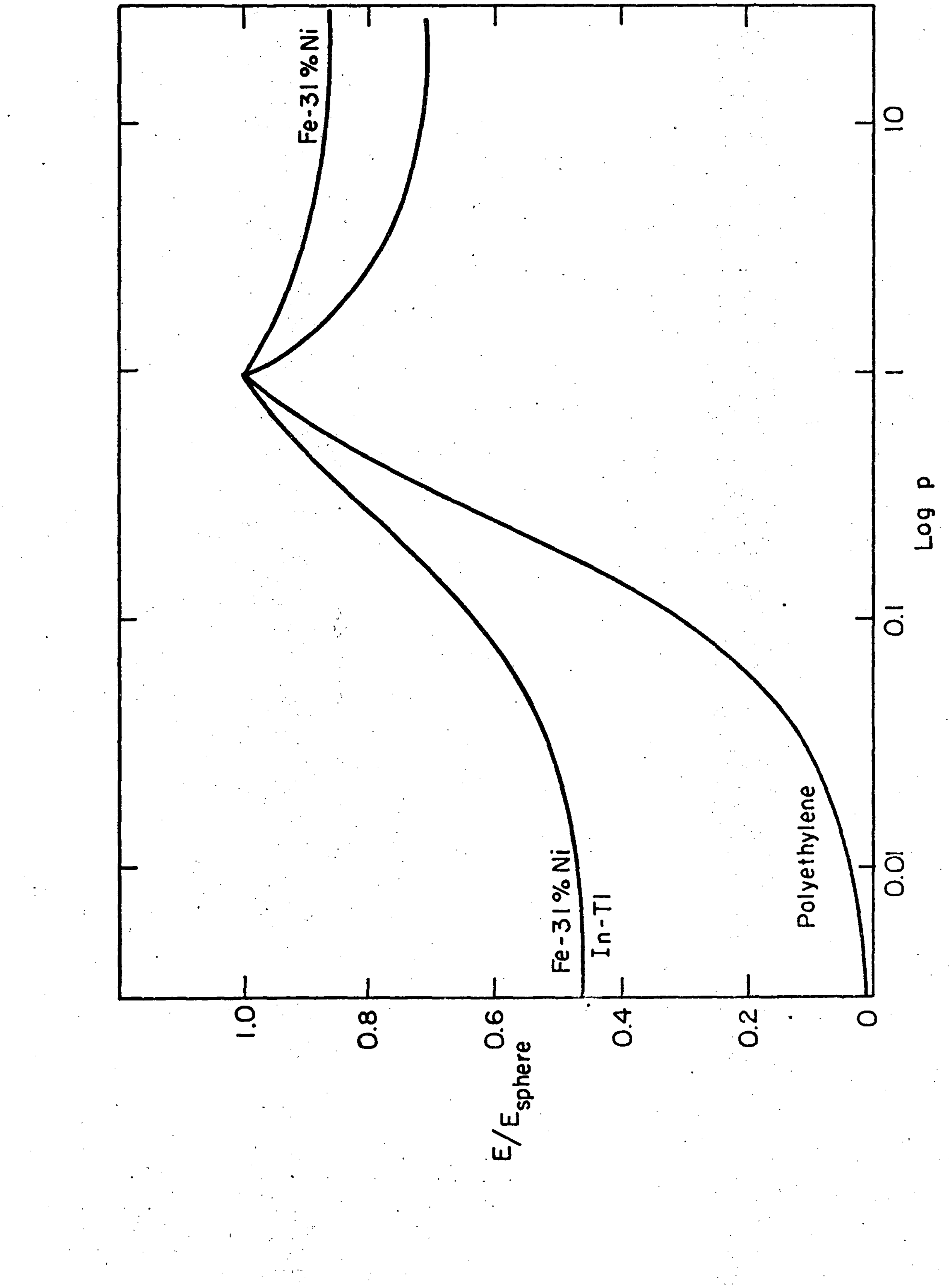


Fig. 2.



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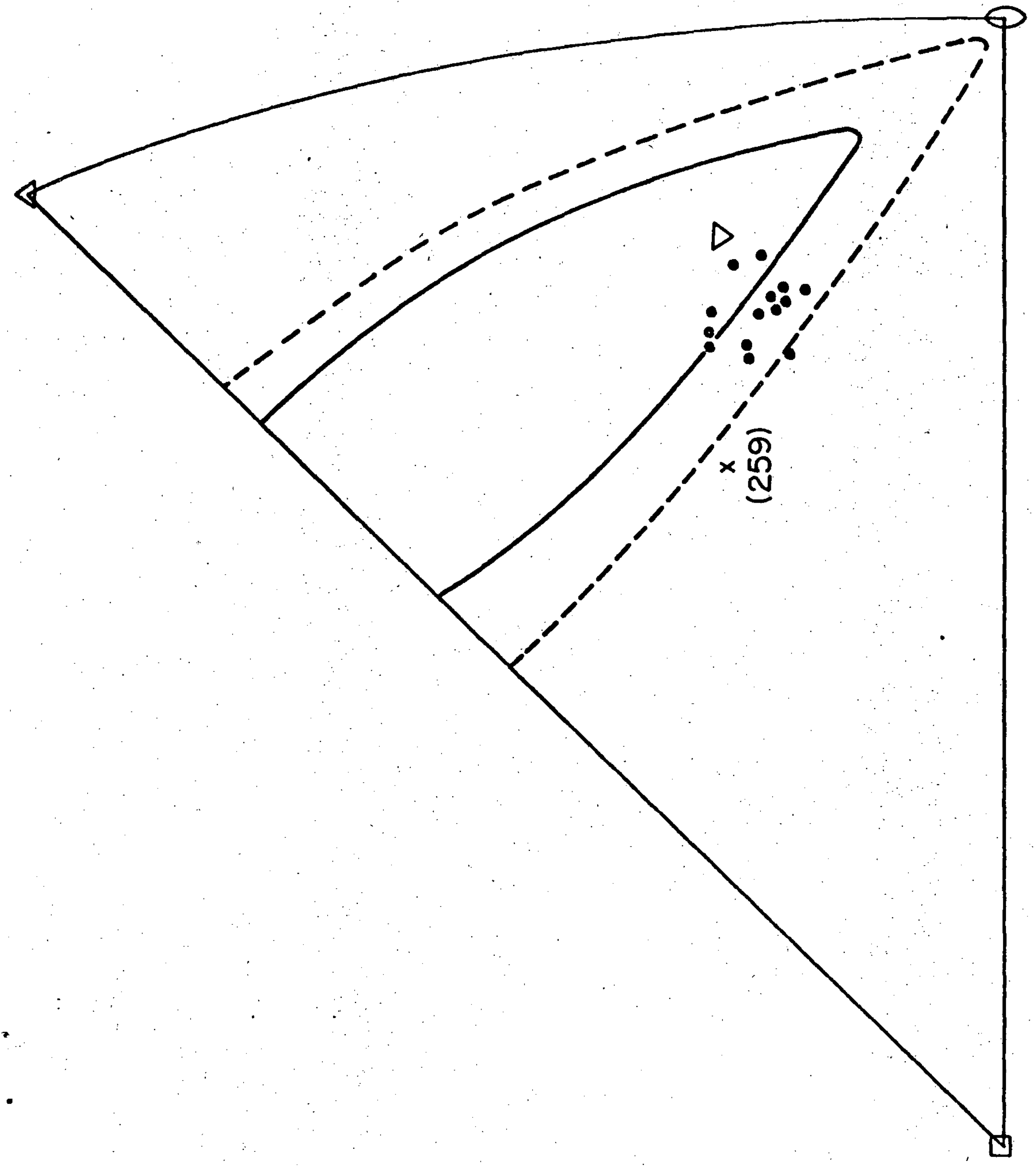

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Fig. 4.

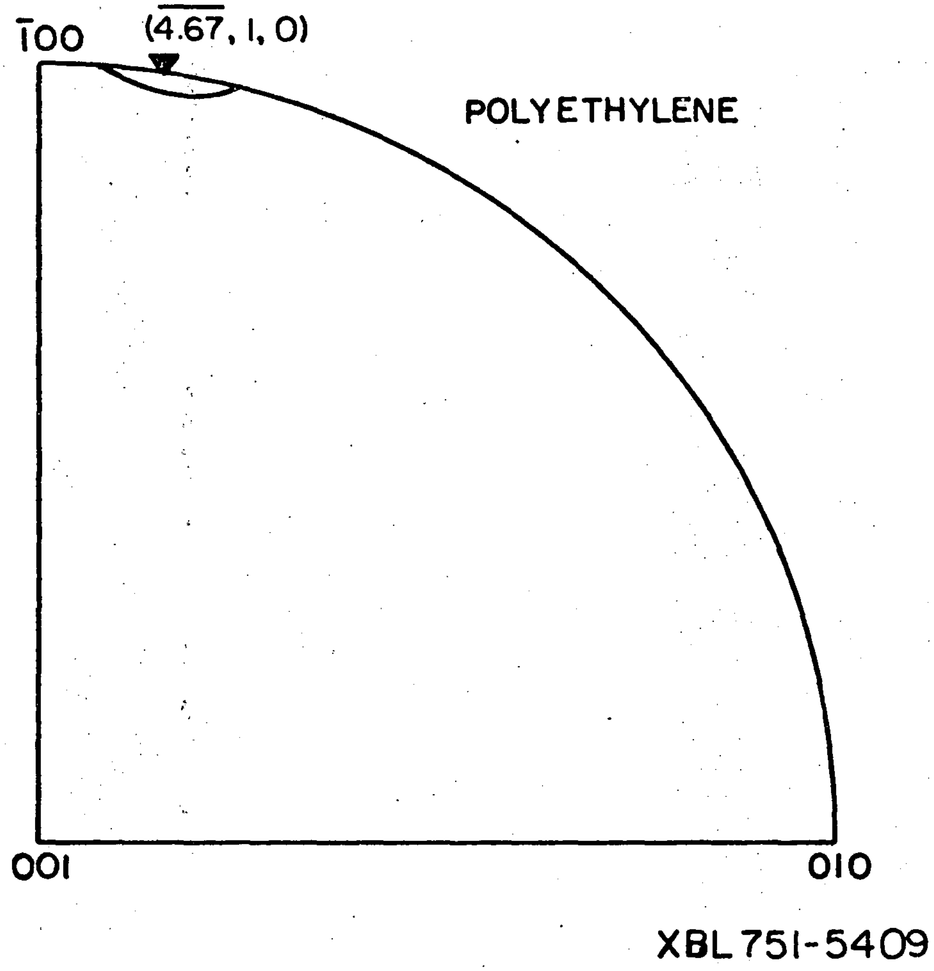

Fig. 5.

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