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THE SHAPE OF DEFORMATION TWINS

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THE SHAPE OF DEFORMATION TWINS

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THE SHAPE OF DEFORMATION TWINS

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May 1964

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I. NOTATION

- s = magnitude of twinning shear.
- 2p = total number of dislocation loops or half-loops associated with a twin lamella.
- d = thickness of a twin lamella at its thickest point.
- a = interplanar spacing of the twin composition plane.
- l = length of the twin.
- G = shear modulus of elasticity.
- b = Burger's vector of a twinning dislocation ($|b| = as$).
- L = dimensions of the crystal containing the twin.
- ν = Poisson's ratio.
- P = force applied to the crystal to cause twinning.
- γ = specific surface energy of a twin boundary.
- h = spacing of twinning dislocations on a twin boundary.
- τ = applied shear stress.
- i, n, m - are integers.
- z = an axis parallel to the twinning shear with its origin at the crystal surface.
- β, θ - are defined in Fig. 4.

A few other, less important, symbols are defined in the text.

II. INTRODUCTION

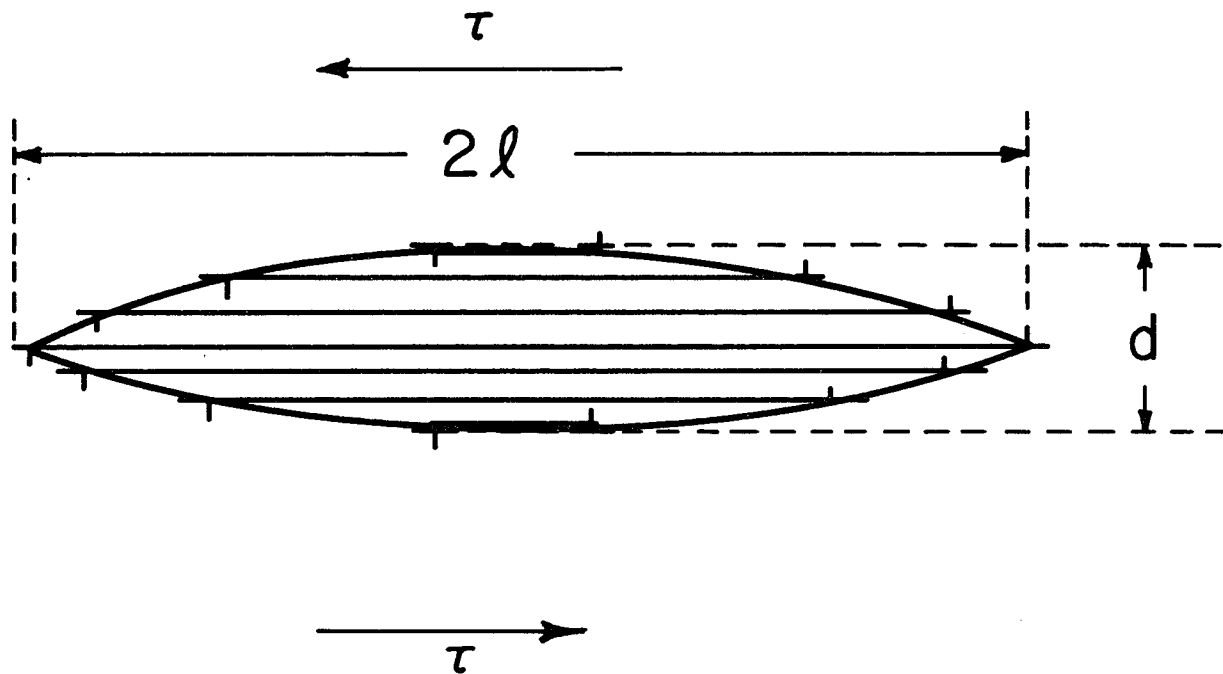
The twin shape most commonly found in metals is that known as lenticular. Using the usual metallographic sectioning and polishing techniques this three-dimensional shape appears as shown in Fig. 1.

The most important parameter required to specify such a shape as that shown in Fig. 1 is the ratio of thickness to length, $\frac{d}{2l}$. It has been pointed out by Cahn (1) that this ratio appears to depend on the magnitude of the twinning shear s . Thus for crystals of large shear (e.g., BCC metals, $s \sim 0.7$) twins are always very thin compared with their length while for metals of small shear (e.g., zinc, $s \sim 0.14$) twins are broad.

It is geometrically necessary for non-coherent twin boundaries to contain dislocation lines. This can be seen by considering Fig. 2 which shows a section of the lattice of a twinned calcite specimen, the plane of the section intersecting the twin composition plane. At any place where the twin boundary contains a "step" as it changes from one plane of atoms to another there will be a twinning dislocation. A non-coherent twin boundary can be considered to consist of a series of portions of coherent boundary connected by these mono-atomic "steps". Thus, there is a simple relationship between the size and shape of the twin and the number and distribution of the dislocations on its boundaries. The total number of dislocation associated with the twin lamella will be given by:

$$2 p = d/a$$

(See Chapter I for definition of the symbols.)



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Fig. 1. Schematic diagram of a lenticular twin.

The density of packing of dislocations on a twin boundary will be

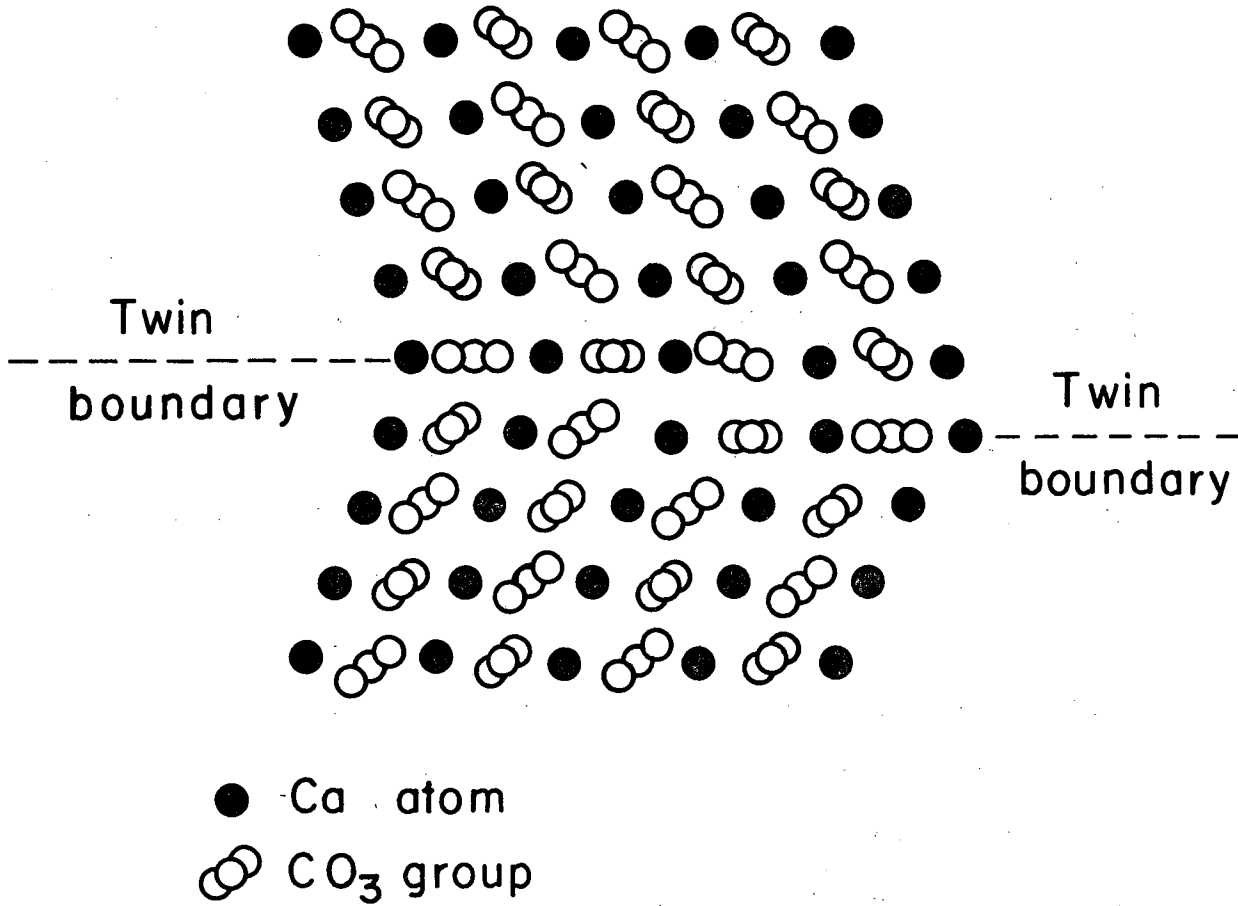
$$\frac{\partial P}{\partial \ell} = \frac{1}{a} \frac{\partial d}{\partial \ell} = \frac{1}{a} \tan \alpha'$$

where α' is the angle between the twin boundary and the twin composition plane at the point under consideration and $\frac{\partial P}{\partial \ell}$ is the number of dislocations per unit length resolved onto the twin composition plane.

In the case of a lenticular twin, then, the boundaries will contain loops of twinning dislocation all of the same sign, as shown in Fig. 1. The fact that a twin boundary must contain a loop of dislocation on every atomic plane provides the starting point for all dislocation theories of twin formation. These theories will not be considered here but it is clear that the twin shown in Fig. 1 can grow longer by dislocation glide but that for it to grow thicker new loops of dislocation must be formed.

III. STRESSES ASSOCIATED WITH TWINS.

Deformation twins are formed as a means of stress relief when some crystalline materials are subjected to external stresses. In forming they produce certain internal stresses which oppose twin growth and which in some cases lead to an equilibrium state in which the internal stresses balance the applied stress at all points in the material.



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Fig. 2. The appearance of a non-coherent twin boundary in calcite.

These internal stresses are:

(a) The surface tension of the twin boundary. This is due to the energy associated with the coherent component of the twin boundary. This energy is difficult to measure but an example can be given taken from the review paper by Chalmers (2). For copper (annealing twins) $\gamma = 12.8$ and 24 ergs/cm^2 , the best value being probably 18 ergs/cm^2 .

Later we shall consider the case of calcite twins in detail. No values for surface energy are available for this material but it may be quite high as the coherent twin boundary in calcite contains considerable misorientation of the CO_3 groups - see Fig. 2. A figure of $20\text{-}100 \text{ ergs/cm}^2$ may well be appropriate in this case. The surface area of a twin with approximately plane boundaries is affected only by movement of the dislocations at the twin tip. The surface tension therefore acts only on these dislocations.

(b) Line tension of the twinning dislocations.

The energy per unit length of a screw dislocation is

$$F_s \simeq \frac{Gb^2}{4\pi} \left\{ \ln \frac{L}{b} + 2 \right\} \simeq \frac{Gb^2}{2} \text{ ergs}$$

while that of an edge dislocation is slightly more being

$$F_\gamma = \frac{F_s}{(1-\nu)} .$$

This energy is numerically equal to the "tension" in the dislocation lines and this tension will produce stresses on the twin boundaries.

(c) Forces between dislocations.

The forces between two parallel edge dislocations of Burgers vector b and on the same glide plane is inversely proportional to the distance separating them and tends to push the dislocations

further apart. Thus this type of force tends to elongate the twin.

(d) The applied stress.

This acts so as to elongate the twin. It may or may not be uniform throughout the material. A non-uniform stress distribution with the stress at the twin tip lower than that at its thickest part can result in the formation of a stable wedge shaped twin such as is found in bending or in indentation experiments. A uniform applied stress however favors the formation of a parallel sided twin which fully traverses the specimen. This is the situation found in tensile experiments on single crystals, where wedge shaped twins are not found.

(e) "Friction" forces.

The motion of dislocations by glide is always opposed by forces of a frictional nature - Peierls Nabarro forces - even when the lattice is otherwise perfect. In a real crystal there may also be retarding forces due to impurity atoms, intersection with other dislocations, etc. During the formation of twins these frictional forces will oppose the growth of the twin. In calculations made in Chapter VI these forces will be assumed negligible - a reasonable assumption for calcite, as shown by the work of Garber (3).

The forces opposing the formation of a twin can be large and in most materials which are capable of slip they are dissipated by this means while in some brittle materials they can be dissipated by cracking (e.g., "Rose's Channels" in calcite). In some cases, however, and under certain conditions, these opposing forces cannot be relieved and the twin will always be held in equilibrium such that there is

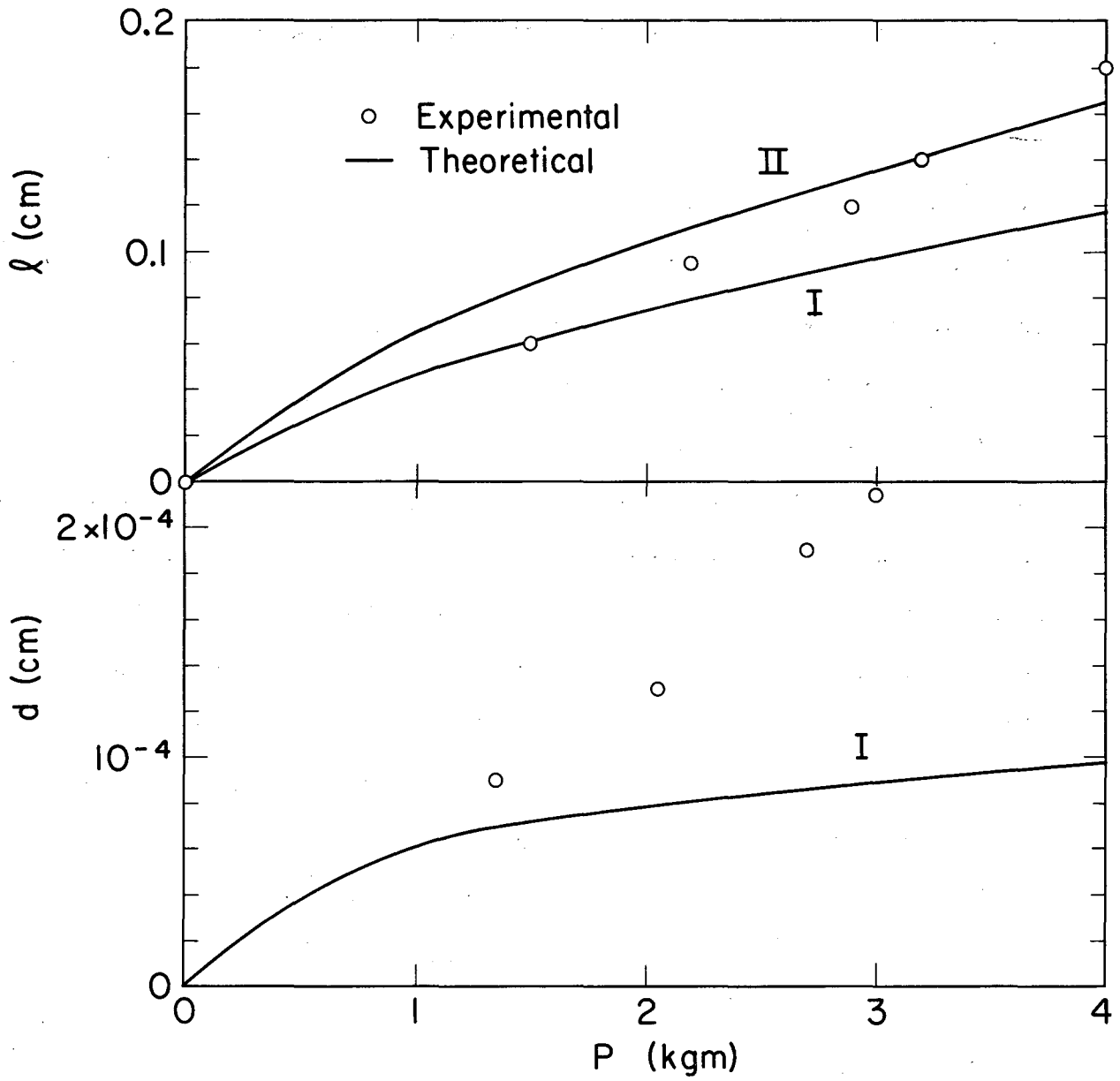
zero net force on every part of it. If the applied stress is then removed the unbalanced internal stresses will drive the twin out of the crystal leaving a more or less perfect crystal. This is the phenomenon of "elastic twinning" first investigated by Garber (3) in calcite (which does not form "Rose's Channels" under all conditions but probably mainly in the case of large twins) and in sodium nitrate. Antimony has since been shown to exhibit perfect elastic twinning while a number of other materials show vestiges of the phenomenon (see Cahn (1)).

Elastic twins, then, differ from other deformation twins only in being in equilibrium under a specific set of forces. They therefore represent an interesting phenomenon, being a direct link between an externally applied stress and a well defined array of dislocations. It should therefore be possible, in principle, to calculate the shape of such twins as the magnitudes of all the forces present can be calculated or measured. Calculations of this type will be considered in detail in Chapters V and VI.

IV. EXPERIMENTAL DETERMINATION OF THE SHAPE OF ELASTIC TWINS.

Few detailed results are available, the main ones being those of Garber (3) and Obreimov and Startsev (4) who all worked with calcite. Since calcite is transparent and doubly refracting it is particularly convenient for measurements of this type.

Obreimov and Startsev produced twins by the pressure of a hemispherical indenter on a polished surface which was perpendicular to the twinning shear vector. They measured the twin length and breadth directly and its thickness and shape by counting optical interference fringes set up within it. Their results show that the length, breadth and thickness all vary directly as the force applied to the indenter, the length and breadth being about equal and being about one thousand times as great as the thickness. (This large ratio of length to thickness is to be expected as the twinning shear s has the high value of 0.695). The twin as a whole presented the appearance of a surf board with the edges tapered down in a concave manner. Figure 3 gives an indication of the shape found. It is notable that the length, breadth and thickness all bear a constant relation to one another so that the twin shape is invariant as the applied force, and consequently twin size, are changed.



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Fig. 3. Obreimov and Startsev's experimental results and Vladimirskii's theoretical curves for twin shapes in calcite.

V. CALCULATIONS OF TWIN SHAPES - PREVIOUS WORK.

The first calculation of the shape of a twin was done by Vladimirskii (5) with particular reference to the case of calcite as described by Garber (3).

Vladimirskii made a very simple calculation of the total energy of a twinned specimen, the twin being considered to be a thin flat plate of uniform thickness. He considered these energy terms:

- a. the strain energy due to the twinning shear,
- b. surface energy of the twin, and
- c. work done on the specimen by the applied force.

By assuming that all these terms were of about the same magnitude he obtained, for minimum total energy:

$$l \simeq \left(\frac{P}{G} \right)^{2/3} a^{1/3}$$

$$d = \left(\frac{P}{G} \right)^{1/3} a^{1/3} .$$

Thus he predicted that $l \propto P^{2/3}$ and $d \propto P^{1/3}$ which does not agree with the experimental results (obtained some ten years later) of Obreimov and Startsev. Nevertheless on plotting these results together with Vladimirskii's calculated curves it can be seen (Fig. 3) that the discrepancy is not excessive. By a much more refined calculation Vladimirskii obtained a different expression for l :

$$l = \frac{P^{2/3} d^{2/3}}{G^{1/3} \gamma^{1/3}}$$

which is also plotted in Fig. 3 (curve II).

One serious error in Vladimírskii's first calculation is that he assumed the surface energy of the twin to be equal to the product of shear modulus and the lattice parameter. In the case of calcite this predicts that $\gamma \simeq 26,000$ ergs/cm² which is very much too large.

Friedel (6) has calculated the ratio $\frac{d}{2\ell}$ for a lenticular twin of the type shown in Fig. 1 using dislocation concepts. He first simplified the lenticular shape to that of a disk so that the twin is bounded by a set of concentric dislocation loops all of the same radius ℓ . Then each dislocation loop produces a stress at its center

$\tau_{\perp} = \frac{Gb}{4\ell}$ so that n loops will produce a shear stress

$\tau_n = \frac{nGb}{4\ell}$ and as $n = \frac{d}{a}$

$$\tau_n = \frac{dGb}{a4\ell} = \frac{Gsd}{4\ell} \quad (\text{as } b = as)$$

or
$$\frac{d}{\ell} = 4 \frac{\tau_n}{Gs} \quad [1]$$

Now τ_n is the stress necessary to force these loops into the prescribed array and is thus the shear stress necessary to form the twin. We see that the ratio of thickness to length of a lenticular twin varies inversely as the twinning shear s , which agrees with qualitative observations mentioned in Chapter I. The equation also predicts the magnitude of $\frac{d}{2\ell}$ fairly well.

It can be argued that this calculation may apply to materials in which plastic accommodation of the twin occurs. The process of twin formation is known to be rapid (of the order of microseconds) so that the applied stress τ need act only for a very short space of time in order to arrange the dislocation loops into the required array and

during this time stress relief by slip will not be likely to occur. Thus the applied stress to cause twinning, τ , can be equated to the opposing stress produced by the array of loops during this time interval. Plastic accommodation may relieve the stress due to the array of loops, and thus stabilize the twin, but will not be important during the short interval of time while the twin is being formed.

VI. DETAILED CALCULATIONS OF TWIN SHAPE

In this chapter the problem of calculating twin shapes will be considered for the case of an elastic wedge shaped twin which intersects the surface of a large block of crystal.

The calculation can be approached in two ways - from a consideration either of forces or of total energy.

A. Force Calculations.

In order that the twin shall be in equilibrium there must be zero net force on every dislocation on the twin boundaries. Under a given set of conditions (shear stress distribution in the specimen, surface energy, etc.) the twin will adjust its shape so that the above condition is fulfilled. Under some circumstances there will be no stable wedge shape and the twin will propagate fully across the specimen.

The problem is similar to the calculation of the form of a dislocation pile-up due to Eshlby et al (7). It is however more complex as there are more forces to consider. As an example consider the dislocation at the tip of the twin. The forces acting on unit length of this dislocation are:

(a) Surface tension: $F_{s.t.} = -\gamma$ dynes/cm of dislocation length.

(b) Repulsive forces between the dislocations:

$$F_{rep.} = 2 \times \frac{Gb^2}{2\pi(1-\nu)} \frac{1}{h} \sum_{n=1}^{n=p} \left(\frac{1}{n} \right) \approx \frac{Gb^2}{\pi(1-\nu)} \frac{8}{h}$$

for a uniform dislocation spacing h . (As for $p = 1000$ $\sum \approx 8$.)

For the dislocation at the tip of the twin the forces due to both boundaries have been considered and it has been assumed that the angle of the twin is small so that the dislocations can be assumed to be all in the same glide plane.

(c) Force due to the applied stress τ_l :

$$F_{a.s.} = \tau_l b$$

(d) Force due to dislocation line tension:

$$F_{l.t.} \approx -\frac{2Gb^2}{l} \text{ for a radius of curvature of } l,$$

where a positive force is taken to be one which tends to elongate the twin. Therefore, for the end dislocation to be in equilibrium:

$$\gamma + \frac{2Gb^2}{l} = \frac{Gb^2}{\pi(1-\nu)} \frac{8}{h} + \tau_l b \quad [2]$$

Now for calcite we can substitute approximate values:

$$\gamma \approx 20 \text{ ergs/cm}^2$$

$$G = \frac{1}{S_{44}} = 3.5 \times 10^{11} \text{ dynes/cm}^2$$

$$b \approx 5 \times 10^{-8} \text{ cm}$$

$$l = 0.1 \text{ cm}$$

$$v = 0.3 \text{ cm}$$

$$h \simeq 10^{-4} \text{ cm}$$

(a twin of length 0.1 cm is assumed to be 1.5×10^{-4} cm thick and therefore to contain 1000 dislocations per boundary).

Thus we find on substituting these numbers into the above equation that the force due to line tension is negligible compared with the other three forces and that the shear stress at the twin tip must be of the order of 10^8 dynes/cm² if it is to be directly effective in determining the actual position of the tip of the twin. Now, although we know that the length of the twin depends on the applied force and hence on the value of τ_ℓ , we cannot deduce from this that τ_ℓ is directly effective in determining the equilibrium of the tip of the twin. For instance the applied force may affect the equilibrium indirectly by determining the position of other dislocations along the twin boundary, which will thus determine the value of the repulsive forces on the end dislocation. Thus one cannot make any good estimate of the value of τ_ℓ except to say that it is probably not much more than 10^8 dynes/cm² ($\frac{G}{3500}$).

The value of the applied shear stress at the surface of the specimen, τ_0 , will be higher than τ_ℓ and may be in the range $\frac{G}{100}$ to $\frac{G}{1000}$. This stress level is sufficient to cause repeated nucleation of dislocation half-loops in order to cause twin thickening.

It has been shown then that there are three important types of force acting on the dislocations. A procedure can now be outlined for calculating the shape of a twin. One must estimate the magnitude of the stresses all along the twin from τ_0 to τ_ℓ . In arriving at these estimates other information such as the stress at which dislocation

nucleation is likely to occur (to obtain τ_0) can be used. Next consider the equilibrium equation for the twin tip.

Since the dislocation repulsion forces fall off inversely with distance the most important dislocations are those nearest to that under consideration. Thus although the expression for the total repulsion force was determined for a uniformly spaced array of dislocations it will apply quite well to a non-uniform array provided that the non-uniformity is not too severe near the point being considered. If we solve the equilibrium equation for h we obtain a good approximation to the average value of h at the point under consideration.

As an example, if we take $\tau_0 = 1 \times 10^8$ dynes/cm² and solve for h we obtain from Eq. [2]:

$$h \simeq 2 \times 10^{-4} \text{ cm}$$

and the angle of the twin wedge near its tip is 7.5×10^{-4} radians. At the thick end of the twin the analogous equation to Eq. [2] is:

$$\frac{4Gb^2}{\pi(1-\nu)h} = \tau_0 b$$

and if τ_0 is assumed to be 16×10^8 dynes/cm², $h \sim 2 \times 10^{-5}$ cm, the corresponding wedge angle being 7.5×10^{-3} radians. In this case the interactions of the dislocations in the other boundary have been neglected, halving the corresponding force term.

The same principle can be applied at intermediate points along the twin, the force term changing gradually and in a rather complex manner from one end of the twin to the other as the dislocation forces on each side of the dislocation being considered rapidly cancel out and as the effect of the dislocations in the other boundary becomes more or less important. This analysis with its assumption of plane

boundaries does not explain the equilibrium of dislocations part way along the twin as these dislocations will be subjected to a shear stress of between 10^8 and 16×10^8 dynes/cm² but will have practically no net dislocation repulsion forces acting on them to oppose the applied stress.

The stability of these dislocations will be due to the fact that the boundaries are actually curved. Even a slight curvature can provide sufficient force to balance the applied stress as can be seen from the following calculation: consider a dislocation having on one side of it another at distance x and on its other side a dislocation at distance $x + \delta x$. Then the resultant force on the middle dislocation (considering nearest neighbors only) is

$$F = \frac{Gb^2}{2\pi(1-\nu)} \left[\frac{1}{x} - \frac{1}{x+\delta x} \right]$$

$$\approx \frac{Gb^2}{2\pi(1-\nu)} \frac{\delta x}{x} \quad \text{if } \delta x \ll x.$$

Thus for equilibrium $\tau b = \frac{Gb^2}{2\pi(1-\nu)} \frac{\delta x}{x}$ or $\frac{\delta x}{x} \approx 5 \times 10^{-3}$ (if $\tau = 4 \times 10^8$ dynes/cm² and figures for calcite as substituted). This corresponds to only a slight departure from a plane boundary.

We can see that the equilibrium of the dislocations defining the twin boundaries is determined primarily by the mutual forces between them and by the applied stress. The surface energy of the twin will only affect the shape near the tip of the twin. A low surface energy will favor a drawn out finely tapered twin tip while a high surface energy will favor a blunt rounded twin tip.

It can be seen that detailed calculation of the form which an elastic twin will assume requires more sophisticated mathematical methods than have been employed. Kosevich and Pastur (8,9 and 10) have approached the problem rigorously, replacing discrete dislocations by a continuous

dislocation density function which is not specified.

By this means they obtain an integral equation from which the shape of the twin may be deduced. The method has so far yielded no quantitative results although it is possible to see the qualitative shape which the twin will assume in certain situations, e.g., a dislocation barrier at the twin tip, a high "friction" force, etc.

B. Energy Calculations: *

In principle this calculation is similar to that of Vladimirskii but in this case instead of considering the twin to be simply a surface of discontinuity for elastic stresses the dislocation concept will be used, enabling more detailed calculations to be made.

The energy terms which will be considered are:

- (a) twin boundary energy,
- (b) mutual repulsion energy of the dislocations,
- (c) strain energy due to the applied stress,
- (d) dislocation line energy.

The twin will be assumed to be of infinite breadth and bounded by flat surfaces. It is therefore defined by two equally spaced rows of straight edge dislocations. The thickness of the twin will be taken as constant and the twin length, and hence spacing of the dislocations, is assumed to be free to assume the minimum energy value.

- (a) Twin boundary energy = $\gamma \times$ total area of boundary,
= $2\gamma h(p-1)/$ unit twin breadth,
 $\approx 2\gamma ph$ as p is usually $\gg 1$.

- (b) Dislocation repulsion energy.

For the i th dislocation interacting with the $(i+1)^{th}$ dislocation:

$$E_{i,i+1} = \frac{Gb^2}{2\pi(1-\nu)} \ln \frac{L}{h} = E_{i,i-1}$$

* See Reference Page.

assuming that for a spacing L which is equal to the dimensions of the crystal the interaction force will be zero,

and
$$E_{i,i+2} = \frac{Gb^2}{2\pi(1-\nu)} \ln \frac{L}{2h} = E_{i,i-2}, \quad \text{etc.}$$

therefore summing:

$$E_i = \frac{Gb^2}{2\pi(1-\nu)} \left\{ \sum_{n=1}^{n=p-i} \ln \frac{L}{nh} + \sum_{m=1}^{m=i-1} \ln \frac{L}{mh} \right\} .$$

The total interaction energy of all the dislocations will be:

$$E = \frac{1}{2} \sum_{i=2}^{i=p-1} E_i + 2 \sum_{m=1}^{m=p-2} \frac{Gb^2}{2\pi(1-\nu)} \ln \frac{L}{mh} .$$

The factor $\frac{1}{2}$ before the first sum is to allow for the fact that all the possible pairs of dislocations are counted twice during the summation. The limits of the first sum exclude the first and last dislocations in order to avoid including an energy term for the repulsion of a dislocation from itself. The second sum is included to describe the interaction energy of the first and last dislocations with all the others.

$$\therefore E = \frac{1}{2} \frac{Gb^2}{2\pi(1-\nu)} \left\{ \sum_{i=2}^{i=p-1} \left\{ \sum_{n=1}^{n=p-i} \ln \frac{L}{nh} + \sum_{m=1}^{m=i-1} \ln \frac{L}{mh} \right\} + 4 \sum_{m=1}^{m=p-2} \ln \frac{L}{mh} \right\} .$$

$$= \frac{1}{2} \frac{Gb^2}{2\pi(1-\nu)} \left\{ \sum_{i=2}^{i=p-1} \left\{ (p-i) \ln \frac{L}{h} - \ln(p-i)! + (i-1) \ln \frac{L}{h} - \ln(i-1)! \right\} \right.$$

$$\left. + 4 \left\{ (p-2) \ln \frac{L}{h} - \ln(p-2)! \right\} \right\} .$$

$$= \frac{1}{2} \frac{Gb^2}{2\pi(1-\nu)} \left\{ (p-1)(p-2) \ln \frac{L}{h} + 4(p-2) \ln \frac{L}{h} - \ln(p-2)! \right.$$

$$\left. - \sum_{i=2}^{i=p-1} \{ \ln(p-i)! + \ln(i-1)! \} \right\}$$

$$= \frac{1}{2} \frac{Gb^2}{2\pi(1-\nu)} \left\{ (p+3)(p-2) \ln \frac{L}{h} - [\ln(p-2)! + \sum_{i=2}^{i=p-1} (\ln(p-i)! + \ln(i-1)!)] \right\}$$

$$\approx \frac{1}{2} \frac{Gb^2}{2\pi(1-\nu)} \left\{ p^2 \ln \frac{L}{h} - K(p) \right\}$$

It has been assumed that there is no interaction energy between one twin boundary and the other but that the twin is reasonably thin so that the dislocations interact as if they are in the same glide plane.

(c) Strain energy due to the applied stress:

An elementary slice of crystal at a depth z below the surface of the crystal and of thickness δz and parallel to this surface is considered. This slice is perpendicular to the twin length and the thickness of the twin at this depth z will be

$$d_z = d \left(1 - \frac{z}{l} \right)$$

The applied shear stress is assumed to decrease exponentially with z from a value τ_0 at the surface so that $\tau_z = \tau_0 e^{-\frac{\alpha}{l} z}$. Thus at the tip of the twin the shear stress is $\tau_l = \tau_0 e^{-\alpha}$. This variation of shear stress is assumed rather than a more precise analytical expression taken from elasticity theory in order to minimize the number of arbitrary constants which must be chosen in order to obtain numerical results from the final expression.

Hence the work done by the applied shear stress on this element of crystal will be

$$\delta w \simeq s \tau_z d_z \delta z .$$

This is a very approximate expression. Integrating after substituting the above expressions for τ_z and d_z we have

$$w = \int_{z=0}^{z=l} \delta w = 2 s \tau_0 a p^2 f(\alpha) h$$

where $f(\alpha) = \frac{1}{\alpha^2} (e^{-\alpha} - 1) + \frac{1}{\alpha}$. If $\alpha = 0$, $f(\alpha) \rightarrow 1$ and if α is large $f(\alpha) \rightarrow \frac{1}{\alpha}$.

(d) Dislocation line energy:

$$\begin{aligned} \text{line energy} &\simeq \frac{1}{2} G b^2 \times \text{total length of dislocation line} \\ &\simeq p G b^2 . \end{aligned}$$

As we are here considering a section of an infinitely wide twin the line energy will play no part as it depends only on the thickness of the twin and not on its length. In connection with the line energy of the dislocations there are, however, "image forces" attracting the dislocations to the surface of the crystal. These will change the energy from $G b^2 p$ to $\frac{G b^2 p}{4\pi(1-\nu)} \{ \ln \frac{h}{\delta} + \ln p - 1 \}$, where δ is the distance from the surface from which the image forces are integrated to obtain the true line energy.

For large values of p ($p \geq 1000$) the image forces have a negligible effect and the term can be taken to be $G b^2 p$. The total energy expression is thus:

$$\text{total energy} \simeq 2 \gamma p h + \frac{1}{2} \frac{Gb^2}{2\pi(1-\nu)} \left\{ p^2 \ln \frac{L}{h} - K(p) \right\} + 2 s \tau_o a p^2 f(\alpha) h + p G b^2$$

[3]

let us now take h to be variable and p constant:

$$\frac{\partial(\text{total energy})}{\partial h} = 2\gamma p - \frac{Gb^2}{2\pi(1-\nu)} p^2 \frac{1}{h} + 2 s \tau_o a p^2 f(\alpha)$$

For a maximum or minimum value of total energy, h is given by:

$$\frac{1}{h} = (\gamma + s \tau_o a p f(\alpha)) \frac{4\pi(1-\nu)}{Gb^2 p}$$

since $p \neq 0$. Taking d/l to be characteristic of the twin shape

$$\frac{d}{l} = \frac{2a}{h} = (\gamma + s \tau_o a p f(\alpha)) \frac{8\pi(1-\nu)a}{Gb^2 p}$$

[4]

The quantity $f(\alpha)$ can be evaluated for various values of α .

α	$f(\alpha)$	$\frac{\tau_l}{\tau_o} \quad (= e^{-\alpha})$
<u>0</u>	<u>1</u>	<u>1</u>
0.02	0.6	0.98
0.1	0.48	0.90
0.5	0.42	0.61
1.0	0.37	0.37
2.5	0.253	0.082
5.0	0.16	0.0067
10.0	0.09	4.5×10^{-5}

The value of $f(\alpha)$ is thus very sensitive to small changes of α near $\alpha=0$. This means that any slight departure from a uniform shear

stress will have a large effect on the value of d/l given by the above equation. This, however, is irrelevant as under a uniform shear stress (i.e., $\alpha=0$) a wedge-shaped twin will not be stable and so the above calculation does not apply for values of α near zero.

In Chapter VI-A the values of τ at different points along the twin were discussed. We assumed that $\tau_\ell = 10^8$ dynes/cm² = $\frac{G}{3500}$ and $\tau_0 \simeq 16 \times 10^8$ dynes/cm² = $\frac{G}{220}$. The ratio d/l can now be estimated from Eq. [4] as we can calculate α .

Substituting in suitable values for the other quantities ($s = 0.695$, $a = 7.5 \times 10^{-8}$ cm, $p = 10^3$, $b = 5 \times 10^{-8}$ cm), we find $s\tau_0 a p f(\alpha) \simeq 25,000$ ergs/cm² which means that γ in the numerator can be neglected.

We obtain:

$$\frac{d}{l} \simeq \frac{s\tau_0 a^2 8\pi(1-\nu)f(\alpha)}{Gb^2} = \frac{\tau_0}{Gs} 8\pi(1-\nu)f(\alpha) \quad [5]$$

This expression can be compared with that of Friedel for a lenticular twin (Eq. [1]). In both cases the ratio of twin thickness to length depends directly on the ratio of twinning stress to shear modulus and is inversely proportional to the twinning shear. The agreement is to be expected if γ is negligible as Friedel did not consider the effect of surface tension.

In the case of calcite Eq. [5] gives $d/l = 2.8 \times 10^{-2}$ (calculated) as compared with $d/l = 1.6 \times 10^{-3}$ (experimental).

This lack of agreement can be due to a variety of causes. Firstly, we have assumed the twin to have flat boundaries and secondly we have effectively considered only the two dimensional case. In addition the estimates of τ_0 and τ_ℓ and hence α may be in error. For instance, if one assumes $\tau_\ell = 2 \times 10^8$ dynes/cm² and $\tau_0 = 8 \times 10^8$ dynes/cm² then $f(\alpha) \simeq 0.34$. The calculated value of d/l is then 1.9×10^{-2} .

The two approaches both show, however, that the surface energy of the twin has little effect on the shape assumed by the twin.

It may also be that the term " $\sigma_0 \sin^2 \alpha$ " in Eq. [4] is an overestimate of the strain energy due to the applied shear stress as the method of calculation was very crude. If this term overestimates the strain energy contribution by a factor of ten then substituting values for calcite into Eq. [4] gives:

$$\frac{d}{l} = (20 + 2500) 1.5 \times 10^{-6} = 3.7 \times 10^{-3}.$$

Under these circumstances the value of γ still plays only small part in determining the twin shape but the calculated value agrees fairly well with the experimentally obtained value.

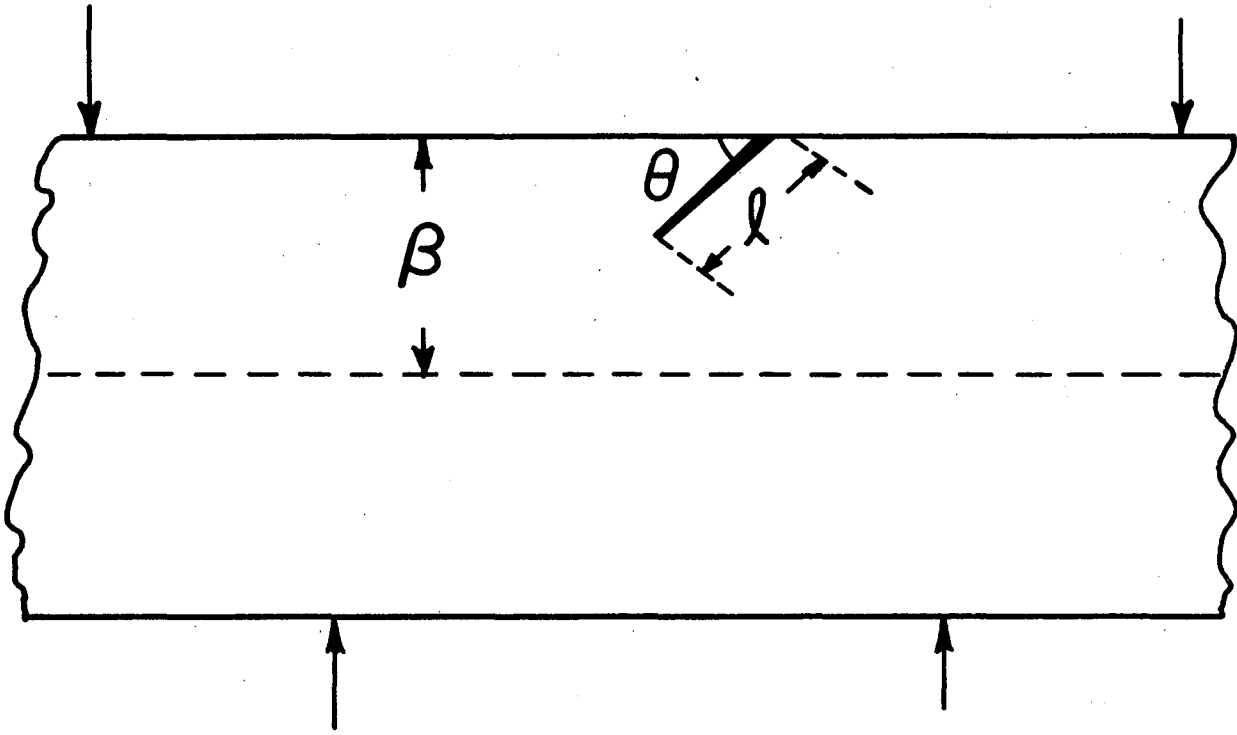
C. Behavior Under a Bending Stress.

A similar calculation based on energy considerations can be made for a bending stress applied so that the twin plane corresponds with the plane of maximum shear stress (Fig. 4). This situation corresponds to that found on applying a bending stress to a cleaved bar of zinc with the neutral plane parallel to the basal plane.

Again choosing the z axis parallel to the twinning shear vector the shear stress is given by:

$$\tau_z = \tau_0 \left(1 - \frac{z}{\beta} \operatorname{cosec} \theta\right)$$

where $\theta \sim 45^\circ$,



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Fig. 4. Twinning of zinc under a bending stress.

and the twin is assumed wedge-shaped as before so

$$d_z = d_o \left(1 - \frac{z}{l}\right) .$$

$$\therefore \text{strain energy } w = \int \delta w \simeq \int_{z=0}^{z=l} \left(1 - z \frac{\operatorname{cosec} \theta}{\beta}\right) \left(1 - \frac{z}{l}\right) dz$$

$$= s\tau_o d \left\{ \frac{l}{2} - \frac{l^2}{6\beta} \operatorname{cosec} \theta \right\} .$$

The total energy expression becomes:

$$\text{Total energy} = \frac{Gb^2}{2\pi(1-\nu)} \left\{ p^2 \ln \frac{L}{h} - K(p) \right\} + 2\gamma ph + 2s\tau_o ap \left\{ \frac{ph}{2} - \frac{p^2 h^2}{6\beta} \operatorname{cosec} \theta \right\} .$$

$$\frac{\partial(\text{total energy})}{\partial h} = - \frac{Gb^2}{2\pi(1-\nu)} p^2 \frac{1}{h} + 2\gamma p + s\tau_o ap^2 - \frac{2}{3} \frac{s\tau_o ap^3 h}{\beta} \operatorname{cosec} \theta$$

For maximum or minimum total energy:

$$h^2 \frac{2}{3} \frac{s\tau_o ap^2 \operatorname{cosec} \theta}{\beta} - h(2\gamma + s\tau_o ap) + \frac{Gb^2 p}{2\pi(1-\nu)} = 0$$

There are therefore in general two real values of h which correspond to maximum or minimum energy twin shapes.

Substituting suitable numbers for zinc we find:

$$\gamma \simeq 20 \text{ ergs/cm}^2 \text{ and } s\tau_o ap \simeq 2000 \text{ ergs/cm}^2 .$$

Thus even if the term " $s\tau_o ap$ " should be divided by 10 as is suggested in Chapter VI-B the surface energy term can still be neglected to a first approximation. Thus we find:

$$h = \frac{1 \pm \left(1 - \frac{4}{3} \frac{Gbp \operatorname{cosec} \theta}{\beta \pi (1-\nu) \tau_0} \right)^{\frac{1}{2}}}{\frac{4}{3} \frac{p \operatorname{cosec} \theta}{\beta}}$$

We can therefore see that as p and β are the only important variables there is a maximum value of p/β above which there can be no real value of h corresponding to a minimum energy twin shape. This critical value is given by

$$\frac{p}{\beta} = \frac{\frac{3}{4} \pi (1-\nu)}{\frac{G}{\tau_0} b \operatorname{cosec} \theta} \approx 5 \times 10^3 \text{ (for zinc).}$$

The value of β determines the maximum possible twin length ($\ell_{\max} = \beta \sin \theta$) and therefore

$$\left(\frac{p}{\ell} \right)_{\max \text{ crit}} \approx 7 \times 10^3$$

and as d is related to p , we have $\left(\frac{d}{\ell} \right)_{\text{crit}} \approx 3.5 \times 10^{-4}$. Thus there can be no minimum energy configuration if $\frac{d}{\ell} > 3.5 \times 10^{-4}$ which corresponds approximately to $h > \frac{\beta}{p}$, i.e., a twin stretching from the surface to beyond the neutral plane. Thus we obtain the expected, though rather, trivial, result that the minimum energy twin configuration must be such that the twin does not extend beyond the neutral plane. Any twin which does extend beyond this plane will be unstable.

Since zinc twins suffer plastic accommodation, Rosenbaum (11), the calculation of twin shapes for this metal under a bending stress cannot strictly be compared with experimentally observed shapes. However, such a calculation can readily be done giving, for $p = 10^3$ and $\beta = 1$ cm.

$$h \approx 1 \times 10^{-3} \text{ cm} \quad \text{or} \quad h \approx 2 \times 10^{-6} \text{ cm}$$

the larger value corresponding to the minimum energy configuration and the smaller to that of maximum energy. These values correspond to

$$\frac{d}{l} \simeq 10^{-4} \text{ (minimum energy)}$$

and

$$\frac{d}{l} \simeq 5 \times 10^{-2} \text{ (maximum energy)}$$

Calculations of forces acting on dislocations along the length of the twin can be made as in Chapter VI-A. The value of τ_0 assumed will be 6×10^8 dynes/cm² (the highest resolved shear stress for twinning of zinc under uniform stress conditions found by Bell and Cahn (12) was 5.3×10^8 dynes/cm²), and $\tau_l \simeq 2 \times 10^8$ dynes/cm². Then applying Eq. [2] we find that $h \simeq 4 \times 10^{-3}$ cm near the twin tip corresponding to a twin wedge angle at that point of about 2.5×10^{-3} radians.

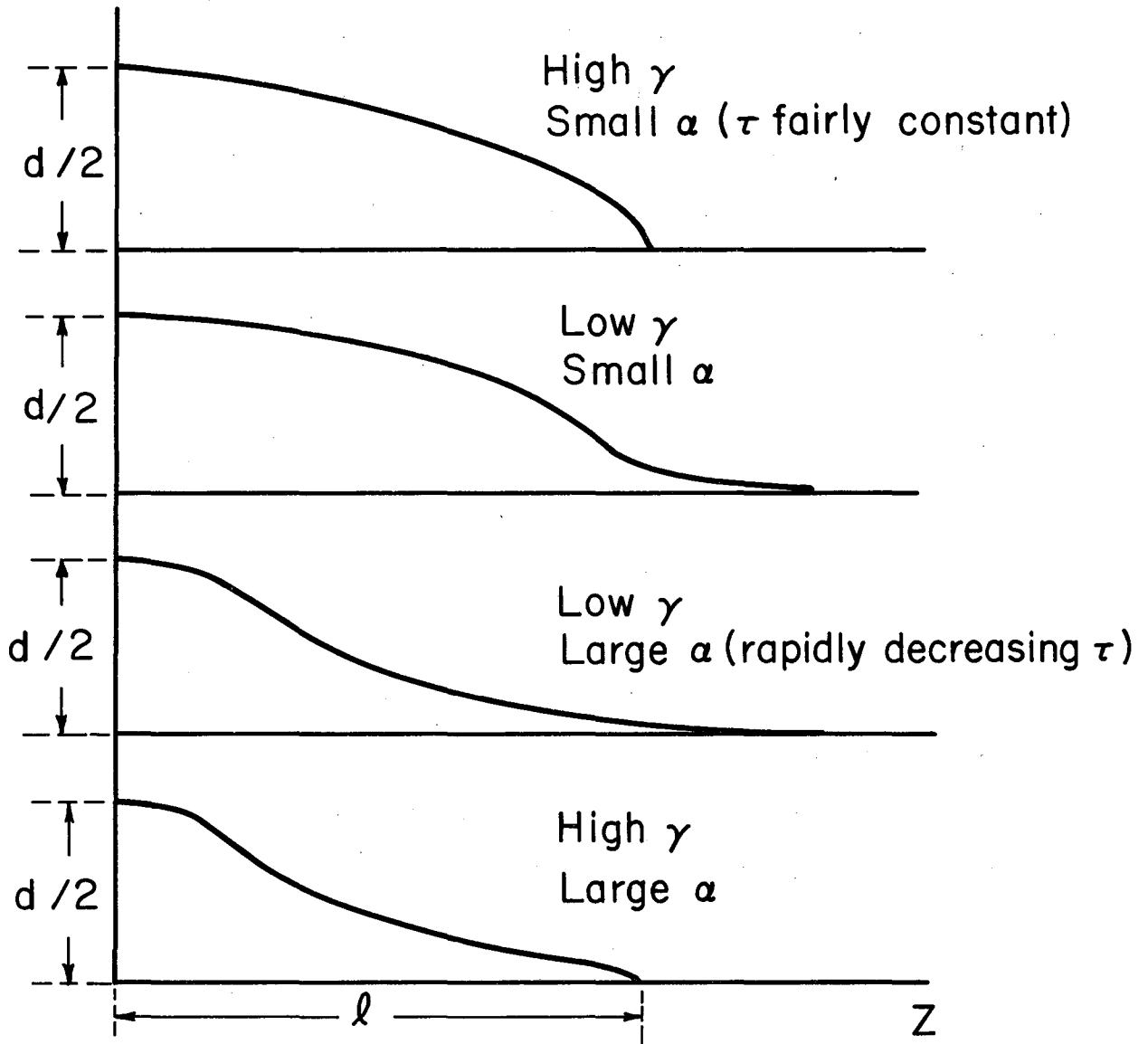
VII. CONCLUSIONS

In this paper the factors which influence the shape of deformation twins have been considered. The case of wedge shaped elastic twins has been examined in detail from two points of view - force and energy - and under two types of stress variation. The method involving the calculation of forces acting on individual twinning dislocations can give more information about precise twin shapes and even in the simple form as developed here it shows the way in which the dislocation density varies along the twin length. The results obtained by this method, however, depend on an accurate knowledge of the magnitude of the shear stress along the whole length of the twin.

It appears that the shape assumed by a twin depends primarily upon the magnitude of shear stress necessary to form it and the way in which this shear stress varies along the length of the twin. The surface energy determines only the shape near the tip of the twin. Figure 5 summarises this behavior in the form of sketches of twin profiles.

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Fig. 5. Schematic twin shapes.

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* Footnote, p. 15.

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