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The Equilibrium Shape of Deformation Twins

A number of metals and non-metals exhibit the phenomenon of elastic twinning[1] due to lack of accomodation of stresses which oppose the formation of the twin lamella. Since such accomodation normally occurs by slip the phenomenon is seen only in materials which slip is difficult under the conditions of observation.

By making various simplifying assumptions it has been found possible to calculate the equilibrium shape of such elastic twin lamellae. The method used is to obtain an expression for the total energy of the twinned specimen and to find the equilibrium shape by differentiation of this expression. Dislocation friction forces are assumed negligible.

A force concentrated along a line on the surface of a block of crystal of infinite breadth and of length and height L is considered. This force leads to the formation of a twin which is assumed to be a flat faced wedge of infinite breadth and of length ℓ and of maximum thickness d, where d, $\ell \ll L$.

The energy terms considered are:

(i) twin boundary energy,
(ii) twinning dislocation interaction energy and,
(iii) the elastic strain energy due to the applied force,
(iv) dislocation line energy.

In terms of forces acting, these energy terms correspond to (i) the twin boundary surface tension, which acts on the dislocations at the twin tip; (ii) the mutual repulsion forces between the twinning dislocations making up the non-coherent twin boundaries; (iii) the forces on the dislocations due to the applied shear stress, which varies along the length of the twin, and (iv) dislocation line tension.

Twin boundary energy.

This is equal to γ x total boundary area

$$= 2\gamma h(p-1)$$

where γ = specific surface energy (in this case per unit breadth),

h = spacing between neighboring dislocations in a twin boundary,

and p = total number of dislocations in a boundary.

Since p is large for optically observable twins the expression can be written

$$\text{twin boundary energy} \simeq 2\gamma ph/\text{unit breadth.}$$

Dislocation interaction energy.

As the twin has flat faces and is of infinite breadth the twinning dislocations form an array of uniformly spaced parallel edge dislocations. If one considers the interaction of every dislocation with every other dislocation one obtains, for two twin boundaries:

$$E \simeq \frac{Gb^2}{2\pi(1-\nu)} \left\{ p^2 \ell n \frac{L}{h} - K(p) \right\}/\text{unit breadth}$$

where $K(p) = \ell n\ (p-2)! + \sum_{i=2}^{i=p-1} \{ \ell n\ (p-i)! + \ell n\ (i-1)! \}$

and

G = elastic shear modulus,

b = Burgers vector of a twinning dislocation,

ν = Poisson's ratio.

It has been assumed that any pair of dislocations will have zero interaction energy when separated by a distance L. It has also been assumed that the twin is reasonably thin compared with its length so that the dislocations behave as if all in the same glide plane but that there is no interaction between one boundary and the other.

Strain energy due to the applied stress.

Considering an elementary slice of crystal of thickness δz at a depth z below the surface of the crystal and parallel to this surface: then the thickness of the twin at this depth z will be

$$d_z = d(1-z/\ell)$$

the shear stress is assumed to decrease exponentially with z from a value τ_o so that $\tau_z = \tau_o e^{-\frac{\alpha}{\ell}z}$. [This variation is chosen rather than one found in elasticity theory, such as the Boussinesq solution, in order to minimize the number of arbitrary constants which must be chosen to obtain numerical results from the final expression.] Hence the work done by the applied shear stress on this element of crystal is found to be

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

where s = twinning shear. Integrating, we obtain $w = 2\,s\tau_o a p^2 f(\alpha) h$ where a = interplanar spacing of the twin composition plane and

$$f(\alpha) = \frac{1}{\alpha^2}(e^{-\alpha} - 1) + 1/\alpha \quad .$$

If $\alpha = 0$, $f(\alpha) = 1$; if α is large $f(\alpha) \to 1/\alpha$.

Dislocation line energy.

Line energy $= 2p\cdot 1\cdot \frac{1}{2}\,Gb^2 = pGb^2$/unit breadth.

The total energy expression can then be obtained by addition.

By considering a twin of given thickness (p = constant) the total energy expression can be differentiated with respect to h to give the value of h corresponding to a minimum energy configuration. We obtain:

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

and, characterizing the twin shape by the ratio d/ℓ:

$$d/\ell \simeq (\gamma + s\tau_o apf(\alpha)) \frac{8\pi(1-\nu)a}{Gb^2 p} .$$

Since γ is negligible compared with $s\tau_o apf(\alpha)$ we have

$$d/\ell \simeq \frac{8\pi(1-\nu)\tau_o f(\alpha)}{Gs}$$

Comparison with the experimental results of Obreimov and Startsev[2] for twins in calcite shows that if τ_o is chosen to be $\frac{G}{1000}$ and α =10 (chosen so that the shear stress at the twin tip due to the applied force is very much less than that necessary for dislocation glide) then:

$$d/\ell \text{ (calculated)} \simeq 2.5 \times 10^{-3}$$

$$d/\ell \text{ (observed)} \simeq 1.6 \times 10^{-3} .$$

Further, if $\alpha = 0$ we have $d/\ell \simeq \frac{4\tau}{Gs} \cdot 2\pi(1-\nu)$ which can be compared with Friedel's[3] calculation of the shape of a disk shaped twin in equilibrium under a uniform shear stress τ which states:

$$d/\ell \simeq \frac{4\tau}{Gs} .$$

[In comparing the equation for a wedge shaped twin of length ℓ with a lenticular twin the diameter of the lenticular twin has been taken as 2ℓ.]

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