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A DISLOCATION MODEL FOR TWINNING AND FRACTURE AND ITS APPLICATION TO H.C.P. METALS*

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ABSTRACT

A dislocation model for deformation twinning and cleavage fracture is developed based on the dislocation theory of fracture and the anisotropic elasticity theory of dislocations. The extension of a Mode-I crack and a deformation twin is treated in a unified manner in terms of the surface energy, the twin boundary energy, and the applied stress state. A criterion is established for predicting twin nucleation or crack initiation and is applied to sixteen hexagonal metals.

INTRODUCTION

It is generally believed that deformation twinning, as one of the two principal modes of plastic deformation in crystalline solids, becomes prevalent only at high strain rates and/or low temperatures. In some b.c.c. alloys, however, the plastic flow by twinning is found to be very extensive over a wide range of temperature. Profuse twinning in Mo-35% Re (Hull, 1964) and continual twinning in Fe-Be (Richman, 1964) are two outstanding cases in point. In h.c.p. metals and alloys, the role deformation twinning plays in maintaining a generalized plastic flow of polycrystals is very important at all temperatures (Yoo, 1978). In fact, good ductility of Ti and Zr and their alloys may be attributed to the concurrent activities of a number of twinning modes; whereas the lack of additional twinning modes other than the common $\{10\bar{1}2\}$ twin in Zn and Be is a crucial factor in effecting poor ductility.

The purpose of the present paper is to develop a dislocation model for twinning and cleavage fracture and to apply this model to predict whether twin nucleation or crack initiation is favored under the applied stress. Example calculations are made for sixteen hexagonal metals, and the calculated results are discussed in terms of the surface energy, the twin boundary energy, and the varying degree of ductility reported for these metals.

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A DISLOCATION MODEL

Consider a region of high stress concentration within a stressed solid as depicted by Fig. 1. Take a two-dimensional problem (independent of x_3) such that the internal stresses, σ_{ij} , are biaxial, and assume that the internal stresses are homogeneous inside the region. The following conceptual probing experiment is useful: (a) insert a micro-crack of the size $2a$ inside the region and find the critical stress state for the crack extension, and likewise, (b) insert a micro-twin of the same size and find the critical stress state for the twin extension. If all the parameters that are involved in the equilibrium equations are known, then a simple comparison of the two separate critical stresses is sufficient to predict whether twinning or cracking is to occur.

Based on the dislocation theory of fracture (Bilby and Eshelby, 1968), the method of a double-ended pile-up of continuously distributed infinitesimal dislocations in an elastically anisotropic medium gives the crack extension force for a Mode-I crack as (Barnett and Asaro, 1972),

$$G_c = \pi a \sigma_{22} (B_{22} \sigma_{22} + B_{12} \sigma_{12}) , \quad (1)$$

Fig. 1. Crack and Twin Nucleation.

where B_{ij} is the symmetric second-rank tensor defined by Stroh (1958) that depends on the elastic constants and the orientation of the crack. By using Griffith's criterion for brittle fracture, $G_c \geq f_c$, where f_c is the total inelastic resistance against the crack extension including the surface energy contribution, one obtains

$$\frac{f_c}{\pi a} \leq B_{22}\sigma_{22}^2 + B_{12}\sigma_{12}\sigma_{22} . \quad (2)$$

Basal Cleavage and $\{10\bar{1}2\}$ Twin

For a Mode-I crack in the basal plane of hexagonal crystals, $B_{12} = 0$, therefore the critical stress for the crack extension is

$$\sigma_c = \sigma_{22}^* = \left(\frac{f_c}{\pi a B_{22}} \right)^{1/2} , \quad (3)$$

$$\frac{1}{B_{22}} = (\lambda^2 C_{33} + C_{11}) \left[\frac{C_{44}(\lambda^2 C_{33} - C_{13})}{C_{11}(\lambda^2 C_{33} + C_{13} + 2C_{44})} \right]^{1/2} , \quad (4)$$

where $\lambda^2 = (C_{11}/C_{33})^{1/2}$ and C_{ij} is the elastic stiffness constant. In an elastically isotropic material, $B_{22} = (1 - \nu)/\mu$, where μ and ν are the shear modulus and Poisson's ratio, respectively.

We will now calculate the critical stress for twin nucleation. As was pointed out recently by Yoo (1979), there are a couple of important distinctions between Mode-II slit cracks and deformation twins, namely, the finite thickness of a twin and the welded boundary condition for twin interfaces. In this paper, however, we will treat the micro-twin as a Mode-II slit crack for simplicity. In the case of a thin twin, as for the elastic twinning (Kosevich and Boiko, 1971) or for the micro-twins discussed here, one can regard all twin dislocations as distributed in a single plane, the twin plane (Indenbom, 1964). The calculated equilibrium distribution of twin dislocations under varying applied stresses obtained by Yoo and Loh (1970) are consistent with the view of thin twins.

The twin extension force for the micro-twin may be given as that for a Mode-II crack (Barnett and Asaro, 1972),

$$G_t = \pi a \sigma'_{12} (B'_{11} \sigma'_{12} + B'_{22} \sigma'_{22}) , \quad (5)$$

where σ'_{ij} is the transformed stress component with respect to the twin axes, x'_i , as depicted in Fig. 1, and

$$\sigma'_{12} = (\sigma_{22} - \sigma_{11}) \sin\theta \cos\theta + \sigma_{12} (\cos^2\theta - \sin^2\theta) , \quad (6)$$

$$\sigma'_{22} = \sigma_{11} \sin^2\theta - 2\sigma_{12} \sin\theta \cos\theta + \sigma_{22} \cos^2\theta , \quad (7)$$

and B'_{ij} is referred to the transformed coordinate, x'_i , also. Similarly as for Eq. (2), the critical condition for twin extension is

$$\frac{f_t}{\pi a} \leq B_{11}'(\sigma_{12}')^2 + B_{12}'\sigma_{12}'\sigma_{22}', \quad (8)$$

where f_t is the total resistance force of inelastic origin against the twin extension. This includes not only the lattice resistance to twin dislocations, but also the surface tension force due to the twin boundary energy. It is obvious that only the leading dislocation located at the end of the twin experiences the effect of such a surface tension force (Yoo and Wei, 1966). For a $\{10\bar{1}2\}$ $\langle 1011 \rangle$ twin, the most common type in h.c.p. crystals, the critical normal stress may be obtained from Eqs. (6-8) when $\sigma_{11} = \sigma_{12} = 0$ as

$$\sigma_t = \sigma_{22}' = \left[\frac{f_t(\gamma^2 + 3)^2}{3\pi a \gamma (\gamma B_{11}' + \sqrt{3} B_{12}')} \right]^{1/2}, \quad (9)$$

where $\gamma = c/a$, the axial ratio. For elastic isotropy $B_{12}' = 0$ and $B_{11}' = (1-\nu)/\mu$. It follows from Eq. (3) and Eq. (9) that the ratio of the critical stresses is

$$\frac{\sigma_t}{\sigma_c} = \alpha \left(\frac{f_t}{f_c} \right)^{1/2}, \quad (10)$$

where

$$\alpha = \left[\frac{(\gamma^2 + 3)^2 B_{22}'}{3\gamma (\gamma B_{11}' + \sqrt{3} B_{12}')} \right]^{1/2}, \quad (11)$$

In Eq. (10) the first term, defined in Eq. (11), is related to the material constants, and the second term is related to the imperfection parameters. For elastic isotropy, the former is reduced to $\alpha_0 = (\gamma^2 + 3)/\gamma\sqrt{3}$, which is essentially a constant $\alpha_0 \approx 2$.

Prismatic Cleavage and $\{10\bar{1}1\}$ Twin

Similarly for a $\{10\bar{1}1\}$ $\langle 10\bar{1}2 \rangle$ twin, when $\sigma_{12} = \sigma_{22} = 0$, the critical normal stress is

$$\sigma_t = \sigma_{11}' = \left[\frac{f_t(4\gamma^2 + 3)^2}{4\pi a \gamma^2 (3B_{11}' - 2\sqrt{3} B_{12}')} \right]^{1/2}, \quad (12)$$

and for a Mode-I crack in the prism plane $\{10\bar{1}0\}$ the critical normal stress is

$$\sigma_c = \sigma_{11}' = \left(\frac{f_c}{\pi a B_{22}'} \right)^{1/2}, \quad (13)$$

$$\frac{1}{B_{22}'} = (\lambda^2 C_{33} + C_{13}) \left[\frac{C_{44}(\lambda^2 C_{33} - C_{13})}{C_{33}(\lambda^2 C_{33} + C_{13} + 2C_{44})} \right]^{1/2}. \quad (14)$$

Hence, the ratio of the critical stresses is

$$\frac{\sigma_t}{\sigma_c} = \beta \left(\frac{f_t}{f_c} \right)^{1/2}, \quad (15)$$

$$\beta = \left[\frac{(4\gamma^2 + 3)^2 B_{22}}{4\gamma^2 (3B_{11} - 2\sqrt{3}\gamma B_{12})} \right]^{1/2}, \quad (16)$$

which becomes, for isotropy, $\beta_0 = (4\gamma^2 + 3)/2\sqrt{3}\gamma$.

CALCULATED RESULTS AND DISCUSSION

The coefficients α and β defined by Eqs. (11) and (16), respectively, for the two cases discussed above were calculated for sixteen hexagonal metals, and the results are shown in Table 1. The results are all for room temperature except for Zr and Ti for which the absolute temperature is given in parenthesis. Calculations of B_{ij} were made by using the numerical method developed by Yoo and Loh (1971) and the elastic constants compiled by Simmons and Wang (1971). Since the range of the calculated values of α and β is 1.41–2.46, which is minor compared to a presumable range of variation of f_t/f_c in Eqs. (10) and (15), the important factor determining whether fracture or twinning occurs should be the actual value of f_t/f_c . If the inelastic contribution such as Peierl's force on twin dislocations is neglected, the ratio of twin boundary energy to surface energy is the determining factor, i.e., $f_t/f_c \approx \Gamma_t/\Gamma_s$.

TABLE 1 The Coefficients α and β Calculated from Eqs. (11) and (16) for h.c.p. Metals

Metal	α	β	Metal	α	β
Cd	1.88	1.53	Gd	1.64	2.00
Zn	1.90	1.41	Ti(4)	1.68	2.05
Mg	1.66	2.02	Ti(298)	1.70	2.11
Co	1.65	2.11	Ti(1156)	1.80	2.33
Re	1.65	2.05	Ru	1.63	2.01
Tl	1.87	2.46	Hf	1.67	2.04
Zr(4)	1.70	2.10	Dy	1.61	1.95
Zr(298)	1.72	2.16	Y	1.60	1.87
Zr(1133)	1.82	2.39	Er	1.60	1.87
Sc	1.62	1.98	Be	1.47	1.87

In the case of Cd and Zn ($\gamma > \sqrt{3}$), $\{10\bar{1}2\} \langle 10\bar{1}1 \rangle$ twinning does not occur under σ_{22} tensile stress. Therefore the basal cleavage will take place when $\sigma_{22} > \sigma_c$. In all other hexagonal metals ($\gamma < \sqrt{3}$), the likelihood of basal cleavage vs $\{10\bar{1}2\} \langle 10\bar{1}1 \rangle$ twinning under σ_{22} tensile stress depends on the relative values of $\{10\bar{1}2\}$ twin boundary energy, Γ_t , and the basal surface energy, Γ_s . For example, for Mg and Ti $\{10\bar{1}2\} \langle 10\bar{1}1 \rangle$ twinning is favored if $\Gamma_t < 0.38 \Gamma_s$, and basal cleavage fracture is favored if $\Gamma_t > 0.38 \Gamma_s$. The critical ratio for Be is $\Gamma_t/\Gamma_s = 0.5$.

An analogous argument can be made also for comparing prismatic cleavage and $\{10\bar{1}1\} \langle 10\bar{1}2 \rangle$ twinning. Under σ_{11} tensile stress the critical ratio, below which $\{10\bar{1}1\} \langle 10\bar{1}2 \rangle$ twinning is favored over the prismatic cleavage, is $\Gamma_t/\Gamma_s = 0.35, 0.25, 0.22$, and 0.29 respectively for Zn, Mg, Ti, and Be. Since $\{10\bar{1}1\} \langle 10\bar{1}2 \rangle$ twinning does not occur in Zn and Be (Yoo, 1978), it may be rationalized that $\Gamma_t > 0.35 \Gamma_s$ in Zn and $\Gamma_t > 0.29 \Gamma_s$ in Be.

Since the plastic flow by slip deformation at the crack tips or at the twin tips

was not considered in the present analysis, the criterion for cleavage and twinning developed here is applicable only for the nucleation of micro-cracks and micro-twins, but not for the growth stage of cracks and twins. All the example calculations in this paper were based on the uniaxial tensile stress, either σ_{11} or σ_{22} . The critical stress state for the twin extension under a combined stress of σ_{11} , σ_{22} , and σ_{12} may be obtained from Eqs. (6), (7), and (8). Only the surface tension contribution to the resistance force on twin dislocations has been considered in discussing the calculated results. The lattice resistance to twin dislocation mobility, Peierl's force, should depend on the specific twin mode. This is due to the atomic shuffling that occurs in the core region of zonal twin dislocations (Yoo and Loh, 1970) in a double lattice such as is associated with h.c.p. structure. An analysis of a crack with two symmetric twins joining each crack tip may offer valuable information on the role of twinning in crack propagation.

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