DII-10

Plastic Accommodation at Micro Stress Concentrations

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Abstract

Plastic accommodation at the terminations of intense shear bands such as those occuring in MgO is studied by idealizing it as a linear array of continuously distributed edge dislocations. It is found that crack nucleation at the intersections of dislocation bands in MgO single crystals can be neither due to the high shear strength of the obstacle band, nor due to the stresses arising from the incompatible strains of the kinking mode of accommodation. Crack nucleation must be the result of a lag in the kinking accommodation in the obstacle band behind the widening of the intersecting band.

I Introduction

It has long been recognized that plastic deformation plays a critical role both in the generation and in the blunting of cracks. Argon and Orowan [1] have studied several relatively simple modes of plastic accommodation at dislocation band intersections in MgO in which this dual role of plastic deformation could be especially clearly observed. There it was found that plastic accommodation could not always prevent crack nucleation, partly on account of the incompatibilities of the strain in the primary band and the strain of accommodation kinking in the secondary band, and perhaps, partly on account of the higher shear strength of the secondary band undergoing accommodation kinking. Attempts at quantitatively describing the situation around such intersections have so far not been successful. A meaningful idealization of the situation which we shall discuss below leads to some interesting and not too obvious results. The approach which we shall use is the one introduced by Leibfried [2] utilizing the notion of a continuous distribution of dislocations, and applied to several problems of interest by Head and Louat [3] and more recently by Bilby, Cottrell, and Swinden [4]; Bilby, Cottrell, Smith, and Swinden [5]; and Bilby and Swinden [6].

II Formulation and Solution of the Problem

One of the frequently observed cases of plastic accommodation at dislocation band intersections studied by Argon and Orowan [1] (their

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Case II) is sketched in Fig. 1a. The edge dislocations of uniformly mixed sign in the left hand semi-infinite region have come from slip on planes parallel to the Y-Y plane at an earlier stage of deformation. As discussed by Argon and Orowan [7], when a limiting dislocation density is reached in a band after its interior undergoes a certain well defined shear strain γ, further deformation of the crystal occurs by widening of existing bands with no further deformation occuring inside previously deformed bands. The left hand half-space in Fig. 1a is taken to represent such a band which has reached its limiting shear strain. It has been observed earlier by Stokes, Johnston, and Li [8] that previously formed dislocation bands of a certain thickness become strong obstacles to dislocations in a conjugate slip system illustrated as the horizontal dislocation band in Fig. 1a. If the crystal were sectioned along the Y-Y plane and the right half-space were deformed freely the horizontal dislocation band would develop a slanted surface step of angle γ with the Y-Y plane, (as shown in Fig. 1b) displacing the upper vertical surface relative to the lower one by an amount $w\gamma$ in the positive x direction. When the crystal is intact the formation of such a step would be opposed by the deformed region of the left half-space as the dislocations of the horizontal band are blocked at the vertical boundary of the left half-space. Nevertheless the slanted surface step can be partially accommodated by the left half-space by slip in its vertical slip planes, i.e., by kinking. Such kinking requires further straining in an already hardened material and is therefore opposed by a higher dislocation friction stress than slip in a virgin area. Because of this, plastic accommodation is of limited amount and crack nucleation could not be postponed indefinitely as the horizontal band continues to widen and the relative displacement $w\gamma$ continues to increase. This is in fact what was observed by Argon and Orowan [1].

We will treat this problem below in the following idealized manner: When the horizontal band is of width w there will be a total concentration of dislocations with an integrated Burgers vector of magnitude $w\gamma$. Depending upon the degree of plastic accommodation these dislocations will be partly in the right hand and partly in the left hand region. We consider these dislocations continuously distributed in one plane in the fashion of Head and Louat [3]. The following quantities are introduced to complete the description (see Fig. 2): the crystal is under a positive shear stress σ; the dislocation friction stress in the left hand region is S_1 and in the right hand region S_2.

In view of the preceding argument for kinking accommodation the net applied stress $\sigma - S_1$ in the left half-space is negative, and $\sigma - S_2$ in the right half-space is positive; the extent of the dislocation distribution is a_1 and a_2 in the left and right half-spaces respectively.

If the dislocations on neighboring planes did not interact, it would not be permissible to consider all the dislocations with total Burgers vector $w\gamma$ in one plane. Stroh [9], however, showed that dislocation arrays on neighboring planes do interact in just such a may that all dislocations with total Burgers vector $w\gamma$ behave to a first order of approximation as if they were on one plane, provided the band width $w << a_2$.

Since the dislocation distribution $f(\xi)$ is uniform in sign and all in one plane, it must obey the integral equation [3]

$$\int_{-a_1}^{a_2} \frac{f(\xi)\, d\xi}{(x - \xi)} = \frac{P(x)}{A} \tag{1}$$

where P(x) is the net stress

$$P(x) = \begin{cases} -P_1 = \sigma - S_1 < 0 & \text{for } x < 0 \\ P_2 = \sigma - S_2 > 0 & \text{for } x > 0 \end{cases}$$

and $A = G/2\pi(1 - \nu)$ in isotropic elasticity. The formulation and solution of this problem is rather similar to the problem of the spreading of plastic yielding from a notch, investigated by Bilby et. al. [4]. The solution of the integral equation is readily obtained by Muskhelishvili's [10] inversion technique summarized by Head and Louat [3]. The dislocation distribution is given by the definite integral

$$f(x) = -\frac{\sqrt{(x + a_1)(x - a_2)}}{\pi^2 A} \int_{-a_1}^{a_2} \frac{P(\xi)\, d\xi}{(\xi - x)\sqrt{(\xi + a_1)(\xi - a_2)}} . \tag{2}$$

In addition for a solution to exist in this particular case the net stress must satisfy a second definite integral [9,3],

$$\int_{-a_1}^{a_2} \frac{P(\xi)\, d\xi}{\sqrt{(\xi + a_1)(\xi - a_2)}} = 0 \tag{3}$$

The evaluation of the condition integral (3) leads to an expression between the parameters a_1 and a_2 of the dislocation distribution and the net shear stresses P_1 and P_2.

$$\frac{2\sqrt{a_1 a_2}}{(a_2 - a_1)} = \frac{2\sqrt{m}}{m - 1} = \tan\frac{P_2\,\pi}{P_1 + P_2} = \tan\frac{\pi}{1 + n} = \frac{1}{K} \tag{4}$$

where $m = a_2/a_1$ and $n = P_1/P_2$. Solving (4) for m gives

$$m_{1,2} = (1 + 2K^2) \pm 2K\sqrt{1 - K^2} \tag{5}$$

Evidently only the root with the positive sign need be considered as only this solution leads to the correct limiting conditions for $n = 0$ and $n = \infty$. The change of m with n is plotted in Fig. 3.

Evaluation of the definite integral (2) now leads to the following solution

$$f(x) = -\frac{P_2(n + 1)}{\pi^2 A} \ln\left(\frac{(m - 1)x + 2a_2 - 2\sqrt{(a_2 - x)(a_2 + mx)}}{(m + 1)x} \right) \tag{6}$$

This leaves still the quantity a_2 undetermined. We determine a_2 from the condition that for a width w of the horizontal band the total integrated Burgers vector is $-w\gamma^*$, i.e.,

$$-w\gamma = \int_{-a_1}^{a_2} f(x)\, dx \qquad (7)$$

After some manipulation the integral is evaluated by standard techniques leading to a result of

$$a_2 = \frac{\pi A \gamma w \sqrt{m}}{P_2 (n+1)} \qquad (8)$$

In the limiting case where $a_1 \to 0$ the dislocation distribution approaches that for the Zener pile-up.

$$\lim_{a_1 \to 0} f(x) = \frac{P_2}{\pi A} \sqrt{\frac{a_2 - x}{x}} \qquad (9)$$

where the dislocations of total Burgers vector $-w\gamma$ are spread out over a length

$$a_2 = \frac{2Aw\gamma}{P_2} \qquad (10)$$

Both of these results have already been obtained by Head and Louat [3].

III Calculation of the Stresses due to the Dislocation Distribution

In order to determine how crack nucleation is influenced by the various distributions of a definite number $w\gamma/b$ of dislocations with a variation in the parameter n, it is necessary to find the nature of the singularity of the principal tensile stress at the origin. Since the local shear stress σ_{xy} is equal to the shear strength S_1 or S_2 of the material at every point along the dislocation distribution, it is not singular at the origin. Evidently, therefore, the stress σ_{xx} which has a singularity at the origin is a principal stress to first order quantities.

To obtain the stress σ_{xx} across the positive part of the Y-Y plane as a function of the distance r from the origin, it is necessary to integrate the effects of all of the dislocation distribution from $-a_1$ to a_2, i.e.,

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* We use the notation where an edge dislocation with its positive direction parellel to the positive z axis and its extra half plane coincident with the $y \geq 0$ part of the y - z plane has a Burgers vector pointing in the positive x direction.

$$\sigma_{xx}(x=0) = -A \int_{a_1}^{a_2} f(x) \frac{r(3x^2 + r^2)}{(x^2 + r^2)^2}\, dx \qquad (11)$$

This integral can be written in two parts as follows:

$$\sigma_{xx} = Ar \int_{a_1}^{a_2} f(x)\, d\left(\frac{x}{x^2 + r^2}\right) - Ar \int_{a_1}^{a_2} f(x)\, d\left(\frac{2}{r} \tan^{-1} x/r\right) \qquad (11a)$$

The first integral which can be readily evaluated, shows no singularity at the origin. The second integral, however, cannot be integrated in closed form. Since it is primarily desired to establish the correct singularity of the stress on the distance r, the inverse tangent in the second integral will be replaced by a function chosen for its ease of integration and for similar behavior at x = 0 and at x = ∞. Such a function replacing $\tan^{-1}(x/r)$ is

$$\tan^{-1}(x/r) \to \begin{cases} -\dfrac{\pi}{2} \dfrac{x}{x - \pi r/2} & \text{for } x \leq 0 \\ \dfrac{\pi}{2} \dfrac{x}{x + \pi r/2} & \text{for } x \geq 0 \end{cases} \qquad (12)$$

The integration can now be carried out without any further difficulty and leads to the following result:

$$\sigma_{xx} \simeq \frac{2P_2(n+1)}{\pi} \ln \frac{8a_2}{\pi r(m+1)} \qquad (13)$$

in the neighborhood of the origin.

The approximation given in (12) leads in the limiting case for the length ratio $m \to \infty^*$ to the stress

$$\sigma_{xx} \simeq P_2 \sqrt{\frac{a_2 \pi}{2r}} \qquad (14)$$

in the vicinity of the origin. On the other hand direct integration of the distribution of the Zener pile-up given by (9) leads to a normal stress

$$\sigma_{xx} = \frac{3P_2}{2} \sqrt{\frac{a_2}{2r}} \qquad (15)$$

in the neighborhood of the origin. Comparison of (14) and (15) shows that the approximation of (12) leads in the limiting case of the Zener pile-up to the correct stress dependence around the origin and differs from the exact solution by a numerical factor of only 1.15. Because of this, we will accept the result given by (13) as a very close approximation of the normal stress due to the dislocation distribution of (6).

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* This value cannot be obtained by arbitrarily letting $m \to \infty$ in the solution of (13) since the nature of the dislocation distibution f(x) changes for very large m, and requires separate integration of (11a) for large m, with the approximation of (12).

IV Condition of Crack Nucleation

With increasing width of the obstructed horizontal band the stress will rise logarithmically until it is high enough to nucleate a crack across the interface between the two regions. Since our consideration is meant to apply only to a brittle type crack nucleation in which the only mode of plastic accommodation is the one discussed above, it is natural to adopt the criterion of Stroh [9]. Stroh proposed that a brittle crack will be nucleated at a stress singularity when the elastic energy released by the crack to be nucleated equals the energy of the crack surfaces. We proceed by calculating the elastic energy released by a crack of length of 2c nucleating from the stress singularity. According to Stroh [11] the released elastic energy can be written as,

$$W_e = \frac{\pi(1-\nu)}{G}\int_0^1 (\tau'^2 + \tau''^2)\mu \, d\mu \tag{16}$$

$$\tau' = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} \sigma_{xx}(\mu\sin\theta)\,d\theta \tag{17}$$

$$\tau'' = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} \sigma_{xx}(\mu\sin\theta)\sin\theta\,d\theta\ , \tag{18}$$

and the origin is chosen at the center of the crack, and all lengths μ, are represented in units of the half crack length c. Then evaluation of (17) and (18) gives

$$\tau' = \frac{C}{\pi}\ \ell n \frac{2Ba_2}{c(1+\sqrt{1-\mu^2})} \tag{17a}$$

$$\tau'' = \frac{C}{\pi}\left(\frac{1-\sqrt{1-\mu^2}}{\mu}\right) \tag{18a}$$

where $C = \frac{2P_2(n+1)}{\pi}$, and $B = \frac{8}{\pi(m+1)}$.

Substitution of (17a) and (18a) into (16) followed by integration gives the released elastic energy in two parts.

$$W_e^{(1)} = \frac{c^2C^2\pi^2(1-\nu)}{G}\left(\frac{1}{2}\left(\ell n\frac{2Ba_2}{c}\right)^2 + \frac{9}{2}\ell n\frac{2Ba_2}{c} - \frac{4E\varepsilon_c}{C} - 6\ell n2 + \frac{1}{4}\right) \tag{19a}$$

$$W_e^{(2)} = \frac{\pi(1-\nu)E^2\varepsilon_c^2B^2a_2^2}{2G}\exp(-2E\varepsilon_c/C) \tag{19b}$$

the first part $W_e^{(1)}$ is the elastic energy released by the crack from the Hookean elastic region outside $r = \varepsilon$ while the second part $W_e^{(2)}$ is the elastic energy released from the non-Hookean region inside $r = \varepsilon$ .It is assumed that in the Hookean region the stress is given by (13) and in the non-Hookean region inside $r = \varepsilon$ the stress remains constant at a value

of $E\varepsilon_c$, where E is the Young's modulus and ε_c the uniaxial ideal normal strain to fracture.

For crack nucleation the total elastic energy released by the nucleated crack of length 2c must equal the enrgy of the crack surfaces, i.e.,

$$W_e = W_e^{(1)} + W_e^{(2)} = 4\alpha c \tag{20}$$

where α is the specific surface energy of the brittle solid. Since in all cases of interest $W_e^{(1)} >> W_e^{(2)}$, we neglect $W_e^{(2)}$. The condition for crack nucleation then becomes

$$\delta\left(\frac{w}{c}\right) = \frac{1}{2}\left(\ell n\beta\frac{w}{c}\right)^2 + \frac{9}{2}\ell n\ \beta\frac{w}{c} - \frac{2\pi}{(n+1)}(E\varepsilon_c/P_2) - 6\ell n2 + \frac{1}{4} \tag{21}$$

where

$$\delta = \frac{1}{(n+1)^2}\frac{\alpha\pi G}{(1-\nu)P_2^2 w}$$

$$\beta = \frac{8\gamma G\sqrt{m}}{\pi(1-\nu)P_2(n+1)(m+1)}$$

For a solution of (21) to exist, w/c must also satisfy the first derivative of (21), i.e.,

$$\delta\frac{w}{c} = \ell n\ \beta\frac{w}{c} + \frac{9}{2}\ ,$$

which requires further that $w/c = 1/\delta$ (22)

Substitution of (22) into (21) now gives the final fracture condition as

$$\ell n\ \frac{8}{\pi^2}\left(\frac{n+1}{\sqrt{m}}\right)\left(\frac{m}{m+1}\right)\left(\frac{P_2w\gamma}{\alpha}\right) = \frac{-9+\sqrt{120.3+(16\pi/n+1)(E\varepsilon_c/P_2)}}{2} \tag{23}$$

Equation (23) gives the band width w as a function of the ratio n of the net shear stresses in the two regions. This relation is plotted in Fig. 4 with $E\varepsilon_c/P_2$ as a parameter.

It is interesting to apply these results to the crack nucleation mode of Argon and Orowan [1] discussed above. As grown MgO crystals of commercial quality have lower yield stresses σ of the order of 0.75×10^9 dyne/cm^2 for strain rates of say 10^{-4} per sec. [12]. In the absence of definite information for MgO, we will assume that the ratio of the stress S_2 at which dislocations begin to move with an inifinitesimally small velocity to the lower yield stress σ is the same as in LiF, i.e., about 2/3 [13, 14] giving for $P_2 = 0.25 \times 10^9$ dyne/cm^2. The surface energy of MgO, measured by cleavage experiments is 1200 ergs/cm^2 [15]. For 1/E, 1/G, and ν we will take $s_{11} = 4.01 \times 10^{-13}$ cm^2/dyne, $s_{44} = 6.46 \times 10^{-13}$

* In the condition obtained from the Norton Co. of Worcester, Mass. U.S.A.

cm^2/dyne, and $-s_{12}/s_{11} = 0.23$ respectively [16]. The critical uniaxial strain to fracture ε_c, may be taken to be 0.05 [17], and the limiting shear strain $\gamma = 0.1$ [7].

In the crack nucleation mode of Argon and Orowan [1], the width w of the band at crack nucleation varied greatly; but, if the value of 10^{-2} cm of Fig. 5 is taken, $P_2 w\gamma/\alpha \approx 200$. In this case $E\varepsilon_c/P_2 \approx 500$, and we obtain from Fig. 4, n = 90, which would mean a shear strength of 2.25×10^{10} dyne/cm^2 in the hardened band, i.e., about 45 times higher than the shear strength of the active band. Since it is unlikely that the shear strength of the hardened inactive band exceed the shear strength of the active band by more than 100%, we must conclude that crack nucleation could not have occured in this quasi-static mode of accommodation.

V Discussion of Results

It has been generally accepted that even a small amount of plastic accommodation at stress concentrations is effective in reducing the danger of crack nucleation. Figure 4 shows that as the ratio of the shear strengths decreases to decrease n, the band width w, to nucleate a crack increases steeply.

The solution given above is based on considering all dislocations in the band on the slip plane. Once the ratio w/a_2 becomes of order 0.1, however, the mutual interaction of dislocations on parallel planes should decrease, and the normal stress should reach an asymptotic value. If cracks cannot be nucleated up to that time the material would survive indefinitely. The critical condition for this, when w/a_2 becomes of order 0.1 is (for large n):

$$\frac{w}{a_2} \approx \frac{P_2 \pi (1-\nu)}{G\gamma} < 0.1 \quad . \tag{24}$$

In MgO this condition is never reached, and the stress continues to rise steadily with increasing band width.

In single crystals where the ratio of the shrear strengths of the obstacle band to that of the active band is not likely to exceed 2, and the ratio $E\varepsilon_c/P_2 \approx 500$, the critical band width for crack nucleation is found to be about 50 cm. From this we must conclude again that in MgO single crystals the observed cracks of the type which we have been discussing could not have been due to a quasi-static expansion of an active dislocation band against an inactive dislocation band.

Two possibilities for crack nucleation in MgO now remain. First it is possible that crack nucleation is due to the stress resulting from the incompatible strains of the kinking type of accommodation. These stresses were not considered in the above model. This possibility, however, must be ruled out for three reasons. First, the maximum kink non-accommodation stress acts across the kink boundaries shown in Fig. 5, with

the stress across the boundary AB (in Fig. 1) being only a Poisson stress of one third of this value [7]. Second, this stress is of a geometrical origin: it is set up because the boundary AB (in Fig. 1) usually is not symmetrically arranged between the latice planes of the two parts of the crystal which it separates, and therefore, does not change much in magnitude as the horizontal, active band grows [7]. Third, when a_1/a_2 is of order unity the boundary AB is approximately symmetrically arranged between the two parts of the crystal, and therefore, no significant kink non-accommodation stress is actually set up: the case being considered comes close to this. The second and only remaining possibility is that the kinking mode of plastic accommodation lags behind the growth of the horizontal, active band. If the two kink boundaries shown in Fig. 5 cannot be moved apart as rapidly as the horizontal band widens, rather large stresses could be set up momentarily by the non-accommodated margins of the horizontal band, producing a crack. This is perhaps the reason why crack nucleation has been observed with bands of widely different widths. A similar conclusion has also been reached by Clarke and co-workers [18, 19], based on birefringence and cinematographic studies of MgO crystals during deformation.

It is likely that a lag of plastic accommodation behind the production of a stress concentration is a widespread mechanism responsible for the notch brittleness of many strain rate and temperature sensitive materials. It is perhaps no accident that face centered cubic metals showing little temperature and strain rate sensitivity are not susceptible to notch brittleness while most body centeredcubic metals, which are strongly temperature and strain rate sensitive, are also notch brittle.

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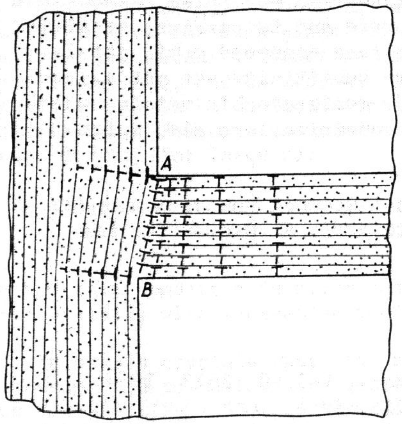

Fig. 1a

Sketch of the mode of plastic accommodation by partial kinking observed by Argon and Orowan. The dots represent a homogeneously mixed plus and minus population of edge dislocations. The "T"'s represent excesses of one kind over the other.

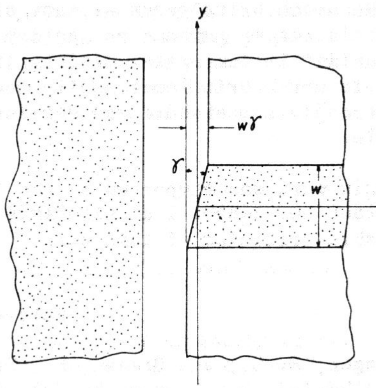

Fig. 1b

The crystal shown in Fig. 1a sectioned along the vertical plane and deformed freely as two separate bodies.

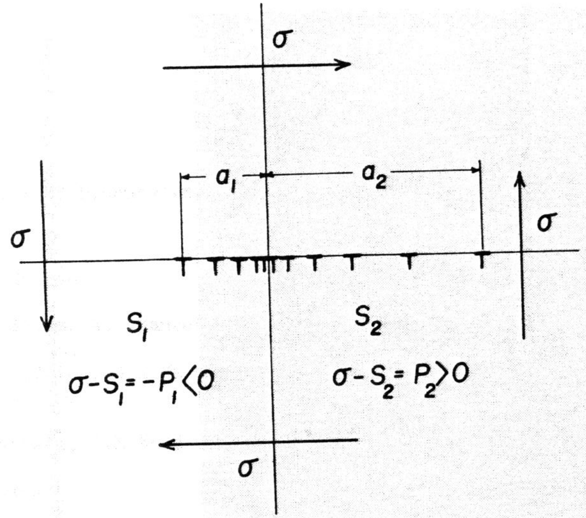

Fig. 2 The linear-array model for the plastically accommodated intersection.

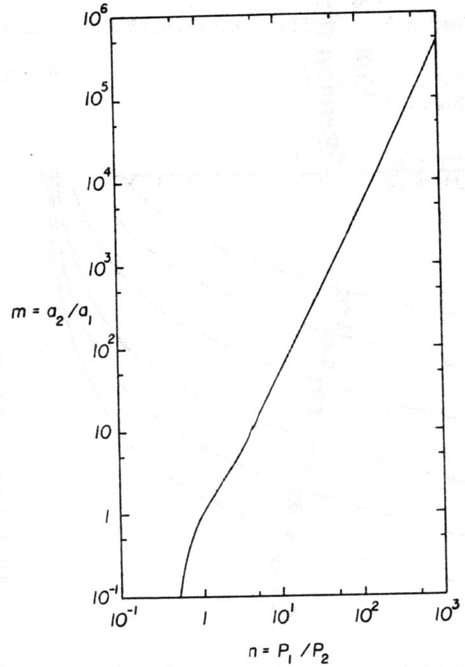

Fig. 3 Dependence of the ratio m on the net shear stress ratio n.

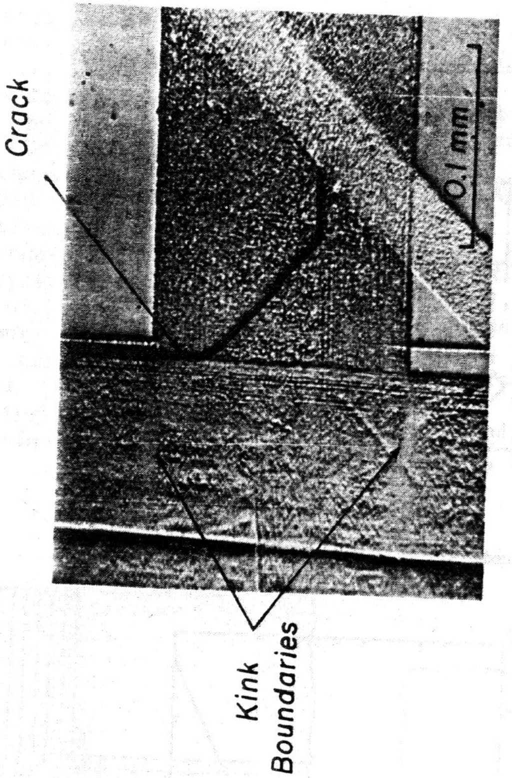

Fig. 5 A dislocation band intersection in MgO of the type studied.

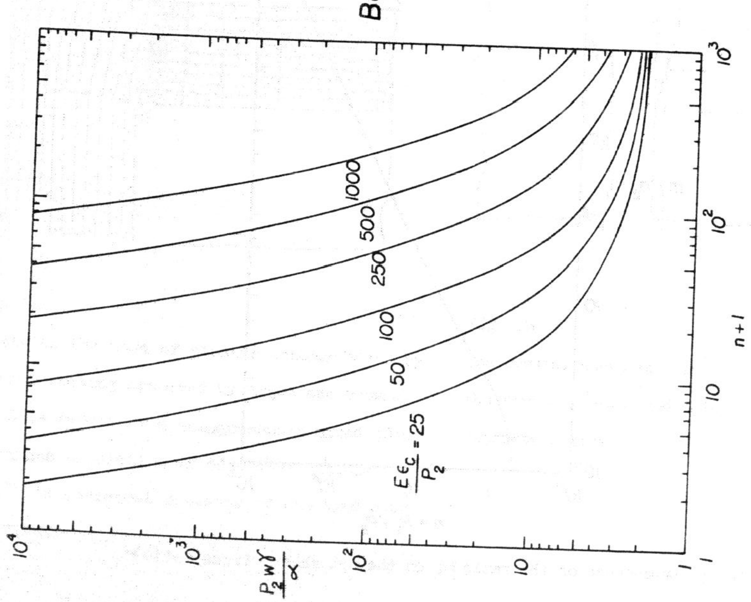

Fig. 4 Change of band width necessary for crack nucleation with change in the net shear stress ratio.

List of Discussors

Lecture Number	Name of Discussors	Lecture Number	Name Of Discussors
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DI-4	K.L.DeVries, S.S.Manson J.Weertman	DI-11	L.F.Coffin,Jr., K.U.Snowden
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