# Ductile versus brittle behaviour of crystals $\dagger$ 

By $J_{\text {ames }}$ R. Rice<br>Brown University, Providence, Rhode Island 02912, U.S.A.<br>and Rone Thomson<br>National Bureau of Standards, Washington, D.C. 20234, U.S.A.

[Received 21 May 1973, and after revision 13 September 1973]


#### Abstract

A necaseary criterion for britile freoture in oryatale ja esteblighed in terme of tho sponteneous ernission of dislocations from an atomicelly sharp elabvage orac. We hevo caleulatect the atability of a sharp orack against emiasion of a blunting dialocation for a numher of oryatale ench ceystal typos in two dimensions and the energy to form a stable loop of dialocgtian. from thegreok tip in three dimensions. We find that eoritray to previous expeotations, an atomically sharp cleavage crack ig ateble in a wide ronge of eryatal types, but that in the face centred cubic motale inveatigated, blunting reations oceur spontaneously. Of the body centred matals investigated, iron is an intermecliete case botween tho brittle and duetile coses, and the ionic and covalent arystals investigateal are all stable ageingt dislocation emisgion. Qunlitatively, we find that eryatals whose dialocations have wide cores, and amall values of the parametel $\mu b / \gamma(\mu b / \gamma \leqslant 7.5$ to 10$)$ ace ductile while erystals with narrow coros and largo valuos of $\mu \mathrm{j} / \mathrm{y}$ ere brittle.


## § 1. Inthoduotion

This paper is concerned with the problem of the ductile versus brittle response of crystals. There is in the literature of this subject a conventional understanding that a solid will either be ductile or truly brittle depending upon the ratio of theoretical shear berength to theoretioal tensile strength (Kelly 1966). We believe that a correct description of this competition should include actual dislocation processes at cracks, since the ductile response of the solid must produce dislocations in order to yield.

A truly ductile material like pure copper apparently oannot ausiain a cleavage crack, but may fail by plastic instability and necking on a gross scale. Stronger materials apparently also exhibit the same essentiaily plastic necking phenomenon on a more microscopic acale through the process of hole growth, although the maoroscopic appcurence of the failure

[^0]is orack-like. On the opposite end of the scale, some materials like diamond and mioa apparently can undergo pure brittle cleavage with no disooverable plasticity associated with the process. In between these two extremes, there apparently exists a class of materials where a cleavage crack in tbe true atomically sharp sense existh, but is surrounded and associated with an atmosphere of dislocations. (Burns and Webb 1970, Burns 1970). This intermediate case exhibits many complexities, such as high effective surface energies, plastic zones surrounding the creack tip, etc., but there is no reason to suppose that, provided hole growth is not occurring, the crack tip is not sharp on the atomic level. Of course, experimental proof of this statement in any given case will be indirect at beat, but the theoretical desoriptions of cleavage and of hole growth are sufficiently different as to make one wish to distinguish as clearly as possible between the separate physioal onses.

Kelly, Tyson and Cottrell (1967) were the first to pose this problem of brittle versus ductile fracture in an essentially proper way when they attempted to test the self-consistency of the proposition that a cleavage oraok can exist in a particular type of cryatal. They, in effeot, asked: " If a cleavage crack were oreated by some process in a crystal, would the tip spontaneously blunt as the result of shear by the atoms of the tip region?" They then postulated that such would be the cuse if the highest shear stress in the vicinity of the crack exceeded the theoretical shear strength of the material. However, this criterion cannot be sufficient for the crack to blunt, because the shear stress near a orack is not everywhere constant on the shear plane as it would have to be to cause the atoms to shear past one another uniformly. Instead, the stress is highly localized in the vicinity of the crack tip. By geometrical neceseity, localized shear on a plane intersecting the crack tip caused by the high shear stresses there, matohed to a non-sheared region at greater distances on the same plane, Where the stress is below the theoretical strength simply defines a dislocation. Hence, a blunting reaction at the crack tip requires the production (or annihilation) of dislocations.

Of course it is recognized that a complete resolution of thit problem must rely on a discrete lattice calculation involving realistic non-linear force fields. Calculations of this sort are extremely complex, and vequire acculate knowledge of atomic force fields over their entire range, but have been attempted for iron by Markworth, Kanninen and Gehlen (1973). These considerations enter the present work only indirectly insofar as they determine parameters such as clislocation core cut-off, surface energy, etc. With our method, however, it is possible to gain an overview of a wide clase of materials.

Kelly, Tyson, and Cottrell indeed alisoussed one kind of dishocation renction for NaCl . They calcnlated the approximate energy to form a full metastable loop of clislocation near the crack in NaCl , and found the energy to be prohibitivoly high. Others have also discussed dislocation formation near the crack tip (Armatrong 1960, Kitajima 1960).

Armstrong has, in particular, estimated the formation energy of a dislocation dipole loop completely surrounding $a$ cirouler orack in a eryatal. However, this type of dislocation interaction does not correspond to a blunting reaction and does not directly address the question we pose.

In this paper, we shall propose models for the production of a dislocation from the tip of the erack in such a way that after the dislocation expands under the external atreas field as concentrated by the presence of the crack, an atomioally sharp crack will have been blunted by one atomic plane (fig. 1). This blanted crack will then be trapped at the original lattice position until the extermal stress is increased substantially (when


An atomically sharp eraek is blunted when a dislosation is emitterl from the tip when the Burgers vector has a normal component to the fracture plane.
probably further dislocation blunting may be possible). Crystals for which dislocation emission is spontaneous can be expected to be good candidates for essentially plastic opening of the craok, Crystals for which there exists a large energy barrier for this emission can be expected to be good candidates for brittle cleavage (but perhaps where the crack has associated with it clouds of dislocations which are formed or captured through other processes in the nearby lattice). In order for a dislocation to blunt a crack, it is necessary for the Burgers vector to have a component normal to the crack plane, and for the slip plane to intersect the crack line (or crack front) along its whole length, i.e. the crack line must be contained within the slip plane.

It is, of course, possible to conceive of a process by which the crack may be blunted by dislocations which are formed from nearby sources and which are emitted on precisely the right plane to blunt the crack tip. In view of the fact that the stress field in a region surrounding a cleavage crack will be above the macroscopic plastic flow atress for the material, one might suppose this could be an effective blunting meahanism. However, macroscopic yield is a property associated only with regions of the size of many microns, even for fairly ductile materials. Hence, for a random position of the crack tip, the probability of finding a source on the correct plane at a distance from the crack for which the source can operate is small.

The plan of the paper is as follows. In the next section, we shall consider the various forces operating between a creok and a dislocation in two dimensions. These forces are (1) the force on a dislocation due to the stress field surrounding the crack, (2) the surfaco tension force caused by creating more surface at the blunted crack, and (3) the image force of the dislocation in the free aurface of the oraok. The first term repels the dislocation, and the lattor two attract it toward the crack tip, giving rise to the possibility of a position of unstable equilibrium. In § 3 we eatimate the activation energy for formation of a dislocation half loop out of the crack under the action of these forces when an energy barrier exiats. Finally, in § 4 we discuss the physical consequences of our calculations.

## § 2. Forces on a dislocation near a crack tre

Let us suppose that the loads on the body considered aet symmetricalky about the plane of a straight crack, so that before emission of the dislocation, only the tensile opening mode of relative crack surface displacemont is present. If $K_{\mathrm{I}}$ is the 'elastic stress intensity factor' (see, for example, Rice 1008) due to the loads, then in two dimensions the in-plane shenr stress acting at distance $\rho$ on the slip plane of fig. 2 is

$$
\begin{equation*}
\sigma_{p \phi}=K_{[ }(8 \pi \rho)^{-1 / 2} \sin \phi \cos \phi / 2 . \tag{1}
\end{equation*}
$$

For this equation to be valid, $\rho$ must be a small fraction of overall crack length. The anti-plane shear stress component (i.e. in the direction of
$b_{8}$ ) in zero. 'lhe release of potential energy of the body and load system per unit of new crack area is

$$
\begin{equation*}
G=\frac{1-v^{2}}{\bar{B}} K_{\mathrm{I}}^{2} \tag{2}
\end{equation*}
$$

( $E=$ Young's modulus, $\nu=$ Poisson's ratio.) At the fracture load predicted on the Griffith theory, $G=2 \gamma$ where $\gamma$ is the true aurface energy of the craek plane. Thus, if the applied load on the body is chosen as that which would cause frocture if no disloeations were emitted, then the force (shear stress times Burgers vector) on the dislocation segment shown in fig. 2 dne to the applied lond is

$$
\begin{equation*}
f_{o}=\sigma_{p \phi} b_{c}=\left[\frac{E \gamma b}{4 \pi\left(1-\nu^{2}\right) \xi}\right]^{1 / 2} \sin \phi \cos \phi / 2 \cos \psi \tag{3}
\end{equation*}
$$

Here $\xi=\rho / b$ and $b_{\mathrm{e}}=b \cos \psi$ is the edge component. The sorew component $b_{\mathrm{s}}$ does not appeas since the applied load induces no shear stress in this direction.

Fig. 2


Geometry of the dislocation, crack configuration in two dimensions. $b_{e}$ and $b_{3}$ are perpendicular and parallel components of the Burgers vector relative to the crack.

There will be an 'image ' force which tends to pnll the dialocation back into the crack. This may be inferred from direct solution of the eorresponding elasticity problem, as presented in most general form by Atininson (1066) for anisotropio materials. A rather different derivation is presented in the Appendix, for a straight dislocation parallel to the crack tip in an isotropic material. (The procedure of the Appendix is based on energy eonsiderations and properties of point functions, rather than on direct solution of the elastic field equations for a dialocntion near a crack. The
approach is readily generalized to other elastic interaction problems, and may be of some interest in itself.) The resulting image force (eqn. A14) is

$$
\begin{equation*}
f_{\mathrm{i}}=-\frac{E b_{\mathrm{c}}{ }^{2}}{8 \pi\left(1-\nu^{2}\right) \rho}-\frac{E b_{\mathrm{B}}^{2}}{8 \pi(1+\nu) \rho} . \tag{4}
\end{equation*}
$$

This is a remarkable result, because precisely the same expression for the image force is obtained in the case of a dislocation in a half space with its core lying parallel to, and at perpendicular distance $\rho$ from, the free surface (see, for example, Hirth and Lothe 1968). Both of the above forces are calculated on the assumptions of 'infinitesimal ' elasticity, and actual geometry changes at the crack tip due to emission of the dislocation have been neglected. The image force term may be rewritten from fig. 2 as

$$
\begin{align*}
f_{i} & =-\frac{E b\left(1-\nu \sin ^{2} \psi\right)}{8 \pi\left(1-\nu^{2}\right) \xi},  \tag{5}\\
\xi & =\rho / b .
\end{align*}
$$

In fig. 1 , as the dislocation is formed, a ledge is left behind, and as the core comes through the surface, forces due to the formation of the ledge must be included. As a function of the position, $\xi=\rho / b$, of the dislocation, the ledge energy is given by

$$
\begin{equation*}
V_{l=}=\frac{2}{\pi} \gamma b \cos \psi \sin \phi \tan ^{-1} \frac{2 \xi}{e^{3 / 2 \xi} \xi_{0}} . \tag{6}
\end{equation*}
$$

In deriving (6), we have used the misfit function for a Peierls model of the dislocation with a width or core cut off $\xi_{0}$, which is consistent with the quantity $r_{0} / b$ where $r_{0}$ is defined by Hirth and Lothe (1968), p. 212. The $\sin \phi$ dependence is taken to approximately represent the modification of ledge energy from $\gamma b_{\mathrm{o}}$ due to slip plane inclination. The force is consequently

$$
f_{l}=-\frac{2}{\pi} \frac{\gamma \alpha \cos \psi \sin \phi}{\xi^{2}+\alpha^{2}} \quad \text { where } \quad \alpha=e^{3 / 2} \xi_{8} / 2 .
$$

Note that the $\xi^{-1}$ and $\xi^{-2}$ attraction back toward crack, due to the image and ledge forees, outweighs the $\xi^{-1 / 2}$ force resulting from the applied load when $\xi$ is small, whereas just the opposite happens when $\xi$ is large. Hence, the equilibrium position of the dislocation is unstable, and the dislocation will be driven away indefinitely, until it reaches some obstacle, if it ever attains a distance from the crack tip greater than the equilibrium distance.

The critical distance, $\xi_{\mathrm{c}}$ at which a straight dislocation is in unstable equilibrium under these three forces is, from (3), (5), and $\langle 6\rangle$, given by the solution of

$$
\begin{equation*}
f_{\mathrm{tot}}=\mu b\left[-\frac{1}{4 \pi \xi} \frac{1-\nu \sin ^{2} \psi}{1-\nu}-\frac{2}{\pi \eta^{2} \beta^{\prime}} \frac{\alpha}{\xi^{2}+\alpha^{2}}+\frac{1}{\eta \beta}\left(\frac{1}{2 \pi(1-\nu) \xi}\right)^{1 / 2}\right]=0 . \tag{7}
\end{equation*}
$$

We have used the following abbreviations,

$$
\begin{align*}
& \frac{1}{\beta}=\cos \psi \sin \phi \cos \phi / 2 \\
& \frac{1}{\beta^{\prime}}=\cos \psi \sin \phi  \tag{B}\\
& \eta^{2}=\mu b / \gamma
\end{align*}
$$

where $\mu$ is the shear modulus, If the value of $\xi_{c}$ is leas then the core out-off, we presumably have a case where the method does not apply, and apontaneous generation is a good possibility. Equations (3) and (5) diverge for $\xi \rightarrow 0$, but, of course, the forces they represent must actually in toto approach zero as $\xi \rightarrow 0$ because of non-linear core effects.

We digplay in table 1 the relevant physical data with the values we have chosen. The values of $\gamma$ contain the greatest degree of uncertainty, and we discuss the problems associated with surface energy for our calculation in § 4. Table 2 displays the results of the solution of eqn (7) for the various solids, together with auggested values from Hirth and Lothe (1968) for the elastic cut-off for comparison. We alao list some cruder ertimates of the critical distance, $\xi_{\mathrm{c}}{ }^{\prime}$ and $\xi_{\mathrm{c}}{ }^{\prime \prime}$. In $\xi_{c}{ }^{\prime}$, we neglect the effect of the ledge in eqn. (7), and then the condition is given by

$$
\begin{equation*}
\xi_{\mathrm{o}}^{\prime}=\frac{\left(1-\nu \sin ^{2} \psi\right)^{2}}{8 \pi(1-\nu)} \beta^{2} \frac{\mu b}{\gamma} \tag{9}
\end{equation*}
$$

In the second estimate, we average over the geometrical and orystallographic effects still present in $\langle 9)_{\text {, giving an even cruder estimate, }}$

$$
\begin{equation*}
\xi_{0}{ }^{\prime \prime} \simeq \frac{\mu b}{10_{\gamma}} \tag{10}
\end{equation*}
$$

It is interesting to enquire how splitting the dislocation will affect the calculations, since certainly in the face centred metals, splitting does occur. In this case, the Burgera vector will be lowered in magnitude, and the angle, $\psi$, will be changed. So far as the size of the Burgera vector is concorned, eqn. (7) is dimensionless, and is not affected. The size of the cutoff is sensitive to $b$, however, and in fact the value we have chosen is just that appropriate to the split dialocation in the face centred metale. Equation (7) does contain the crystallography of the Burgers vector through the angle, $\psi$, however, in arather complicated manner. For the whole dislocation, $\psi=30^{\circ}$, and there are two possibilities for the two partials, $\psi=0^{\circ}$ and $\psi=60^{\circ}$. For the firgt value, the ratio of the various terms in eqn. (7) is only changed about $5 \%$ from their values for the whole dislocation, thus leaving the results of table 2 unchanged. For the second case, where $\psi=60^{\circ}$, the first term in egn. (7) becomes about $50 \%$ larger than for the whole dislocation, thereby increasing the value of $\xi_{\mathrm{c}}$. We show a few values for this partial in table 2.
Table l．Physical parameters of crystals

| $\stackrel{i n}{2 \mid}$ |  <br>  |  $\dot{-1} \dot{\text { ले }}$ | 的的会的辛 | 苓会会淢 | 枵㖪 |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  <br>  |  के क्षारां तो |  <br>  |  | 号荌 |
| ： |  000000 | 高雨品慗 －ío |  |  |  |
|  |  －© 的和 |  |  | 或简守 | － |
|  |  |  |  |  |  |
| 悉薄 | E | 㤩焉 票 |  | E |  |
|  | 家弟 | 家兑 高 |  | E气 | 镸呂 |
|  |  |  |  |  |  |

Table 2. Two-dimensional results

| Cryatal | Core cut-off $\xi$ | Critical diatance $\xi$ 。 | Approximate values |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  | w/oledge | $\begin{aligned} & \xi_{\mathrm{c}}{ }^{n}= \\ & \mu b / 10_{\gamma} \end{aligned}$ |
| Pb | 2 | $1 \cdot 1$ | 0.88 | 0.58 |
| Au | 2 | $0 \cdot 85$ | 0.65 | $0 \cdot 48$ |
| Cu | 2 | 1.00 | $0 \cdot 77$ | 0.61 |
| Ag | 2 | 1.09 | 0.85 | $0 \cdot 65$ |
| Al | 2 | $1 \cdot 4$ | $1 \cdot 1$ | 0.85 |
| Ni | 2 | 1.7 | 1.3 | 1.08 |
| Na | 2/3 | 1.2 | 0.54 | $0 \cdot 375$ |
| Fe | $2 / 3$ | 1.9 | 1.3 | 0.87 |
| W | 2/3 | $4 \cdot 0$ | 3.9 | $2 \cdot 6$ |
| Fe* | 2/3 | $2 \cdot 7$ | I. 9 | 0.87 |
| LiF | $0 \cdot 25$ | $3 \cdot 2$ | 2.9 | $2 \cdot 6$ |
| NaCl | $\left\{\begin{array}{c}0.25 \\ (0.25)\end{array}\right\}$ | $\left\{\begin{array}{c}3 \cdot 4 \\ 7 \cdot 0)\end{array}\right\}$ | $\left\{\begin{array}{c}3.2 \\ 160.9\end{array}\right\}$ | $\{2.6$ |
|  | $\{(0.25)\}$ | $\{(7 \cdot 0)\}$ | $\{(7 \cdot 0)\}$ | $\{(5.6)\}$ |
| MgO | $0 \cdot 25$ | $3 \cdot 4$ | $3 \cdot 2$ | $2 \cdot 9$ |
| $\mathrm{Al}_{2} \mathrm{O}_{3}$ | 0-25 | $2 \cdot 3$ | 2.1 | 1.8 |
| Si | $0 \cdot 25$ | $2 \cdot 2$ | 2.0 | 1.9 |
| Ge | $0 \cdot 25$ | 3.7 | $3 \cdot 3$ | $3 \cdot 3$ |
| C | $0 \cdot 25$ | $2 \cdot 4$ | 2.2 | $2 \cdot 4$ |
| Be | 2/3 | $4 \cdot 5$ | $4 \cdot 1$ | $3 \cdot 4$ |
| Zn | 2/3 | 43 | 3.9 | 33 |
| Partia] dislocations $b=\frac{1}{\sqrt{(12)}}[2 \Pi], \psi=80^{\circ}$ |  |  |  |  |
| Cu | 2 | 1.4 | 0.91 | 0.35 |
| Ni | 2 | $2 \cdot 3$ | 1.6 | $0 \cdot 62$ |

## §3. Energy congiderations

If the equilibrium point, $\xi_{c}$, is larger than the core cut-off, then there is an energy hump for the dielocation to jump in order to be emitted from the crack. Clearly, in this case, it will be impossible for a uniform straight line to be emitted from the crack, because for an infinite length of dislocation, the energy diverges. Instead, a local fuctuation in the form of an irregular loop will be formed which, beyond the saddle point configuration, will expand under the external stress. The factors determining the anddle point configuration are the same as before. Imnge and ledge forces will predominate for small loop sizes, while for larger ones the external stress is dominant.

In the elastic three-dimensional problem, even in the isotropic regime, the problem of determining the saddle point configuration and consequently its energy is intractable in part because the force fields are variable, and in part beoause rigorous treatments of three-dimensional dislocation problems are not possible when the shape is complicated. In fact, although we know the image force for a straight dislocation parallel to the crack, image terms are known to be complex when the shape is more complicated, even without the additional complexity of the crack half surface. We shall thus proceed by developing some qualitative insights into the problem, and then make some simplifying assumptions about the saddle point configuration which allow us to make meaningfal calculations.

First, the stress field due to the applied lond isstraightforward, and yields a normal force, $f_{\sigma}$, on a dislocation element, $d l$, given by the local value of the stress, $\sigma$. This force is

$$
\begin{equation*}
f_{0}=(o \cdot b) \times d l \tag{11}
\end{equation*}
$$

The ledge force is always a minor term, except possibly very near the crack surface. It will have the primary effect of drawing together the two ends of the loop where they touch the crack surface. It will act just like a pure aurface tension on these ends because of the surface energy required to expose the ledge as the loop expands.

The image force, as mentioned above, is more complex. In problems of dislocations interacting with normal surfaces, it is a useful first approximation to simply replace the image terms by the action of an image dislocation refleoted in the surface. This replacement is not normally rigorous, but yields a fair approximation. Since in our case of the crack, the straight dialocation yields the same reault as for a normal gurface, we shall adopt this simple stratagem for the crack. This means that in order to calculate the energy of a dialocation half loop configuration which ends at the crack surface, we need do no more than calculate the energy of a full loop including the reflected image, and take half of the reanlt. This energy will then include the image terms.

One further very important result follows from the presence of the image term. The image term requires that when a dislocation approaches an open surface, it must out the surface at normal incidence. The predominance of the image term in the immediate vicinity of the crack surface will require the same boundary condition on the dislocation at the crack surface. This condition, in conjunction with the magnitude of the stress in the region beyond $\xi_{c}$ are the crucial determinants of the total aetivation energy.

We note one final qualitative characteristie of the two dimensional force field which is very suggestive for our three-dimensional treatment. Except for the ledge term in eqn. (7), which is important only very near the crack tip, the net foree is the difference between $1 / \xi$ and $1 / \sqrt{ } \xi$, a very broad function which we have plotted in fig. 3. The point at which this fuution reaches one half its maximum value is about $1.5 \xi_{\mathrm{c}}$, and it

7ig. 3


The function $f=-A / \xi+B / \sqrt{ } \xi$ plotted to show ith broad maximum.
dwas not fall below this value again till $\xi$ becomes approximately $50 \xi_{\mathrm{c}}$. Thus, throughout this very broad range, the balance between these two major forces is nearly constant. Under a constant normal force, of course the equilibrium shape of the dislocation has constant curvature, and is circular. For values of $\xi$ less than $\xi_{c}$, the force becomes negative, and including the effect of the ledge, the curvature will also reverse. Hence the general shape of the saddle point configuration will be as sketched in fig. 4.

17ig. 4


Schematic representations of saddle point dislooation configurations. At distances greater from the crack than $\xi_{c}$, the curvature is positive, while at less than $\xi_{\mathrm{c}}$, the curvature is negative. The dialocation always has normal incidence at the surface because of the preponderance of the image term near the surfnce. (a) $\xi_{c}$ is small and the region of negntive curvaturc is negligible. (b) Intermediato $\xi_{c}$ (c) Large $\xi_{\text {c }}$

In view of these qualitative background comments, we feel justified in proceeding with the assumption that the approximate equilibrium shape is the simple half circle depicted in fig. $4(a)$. In view of the broad maximum in the effective force field, we believe the energy of the activated state this computed is a reasonable estimate of the trie energy, and our use of the circular shape probably introduces no major errors in the calculation.

We thus calculate the total energy of the activated atate of the system, which consists of three parts. (1) The self energy of the dislocation half loop. As mentioned before, this energy will antomatioally include the image term contribution. (2) The energy of the ledge. (3) The energy gained by the dislocation loop as it expands under the influence of the stress surrounding the crack. In order to determine the size of the loop of the activated state, we locate the maximum energy of the loop as a function of the loop radius.

The self energy of a dislocation half loop as given by Hirth and Lothe (1988) is

$$
\begin{equation*}
U_{\text {self }}=\mu b^{3} r \frac{2-\nu}{8(1-\nu)} \ln \frac{5 r}{e^{2} \xi_{0}} . \tag{12}
\end{equation*}
$$

In this equation, $r$ and $\xi_{0}$ are respectively the radii of the half circle and radii of the core cut-off in units of the Burgers vector, $b$. $\quad \xi_{0}$ is the same quantity as used for the core cut-off in § 2 .

To the self energy must be added the energy of the ledge formed ns the loop expands. We write this in the form

$$
\begin{equation*}
U_{\text {ledge }}=2 \gamma b^{2} \cos \phi \sin \phi\left(r-\xi_{0}\right) . \tag{13}
\end{equation*}
$$

Equation (13) simplifies the expression for a ledge as we used it in $\% 2$. Here we assume that when the radius $r$ is greater than the cut-off radins, the ledge is fully formed, and that the energy is linear in the radius of the loop.

Finally, we compute the energy gained by the half loop in the stress field of the crack tip. In terms of eqn. (3) and fig. 5 , the energy to expand the loop from the initial radius, $\xi_{0}$, to $r$ is

$$
\begin{equation*}
U_{a}=-\left[\frac{E \gamma b}{4 \pi\left(1-v^{2}\right)}\right]^{1 / 2} b^{2} \cos \psi \sin \phi \cos \phi / 2 \int_{\xi_{0}}^{r} d r \int_{0}^{\pi} d \theta \frac{r}{\sqrt{(r \sin \theta)}} . \tag{14}
\end{equation*}
$$

Noting that

$$
\begin{equation*}
\int_{0}^{\pi} \frac{d \theta}{\sqrt{ }(\sin \theta)}=\pi^{1 / 2} \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{d}{4}\right)} \tag{15}
\end{equation*}
$$

we then have

$$
\begin{equation*}
U_{\mathrm{n}}=-0.9862 \sqrt{\left(\frac{2}{1-v}\right) \mu b^{3}} \sqrt{\left(\frac{\gamma}{\mu}\right)} \sin \phi \cos \psi \cos \phi / 2\left(r^{3 / 2}-\xi_{0}^{3 / 22}\right) . \tag{16}
\end{equation*}
$$

Fig. 5


Configuration for adculating the work done under the crack stress by the expanding dislocation. The work integration has the lower limit shown when $t=\xi_{0}$.

The total energy ehange for a crack which has emitted a dislocation loop is thon

$$
\begin{align*}
U_{\mathrm{act}} & =\mu b^{3}\left[r U_{0} \ln \frac{r}{\xi_{0}}+U_{l}\left(r-\xi_{0}\right)-\frac{3}{3} U_{\mathrm{s}}\left(r^{3 / 2}-\xi_{0}^{3 / 2}\right)\right], \\
U_{0} & =\frac{2-\nu}{8(1-\nu)}, \\
U_{l} & =2 \frac{\gamma}{\mu b} \cos \psi \sin \phi, \\
U_{\mathrm{s}} & =\frac{2 \cdot 092}{\sqrt{(1-\nu)}} \sqrt{\left(\frac{\gamma}{\mu b}\right) \sin \phi \cos \psi \cos \phi / 2} \tag{17}
\end{align*}
$$

$\left(8 / e^{2} \approx 1\right)$. From (17), the condition for the activated state is

$$
\begin{equation*}
\frac{d U_{\text {nct. }}}{d r}=0=U_{0} \ln e r / \xi_{0}+U_{l}+U_{3} r^{1 / 2} . \tag{18}
\end{equation*}
$$

Schematically, the three terms in (17) are sketched in fig. 6. The stress term eventually always dominates the other two for large $r$, but depending upon the parameters, the self energy plus the ledge term may be dominant for values near $\xi_{0}$. That is to say, depending upon the parameters, there may be a spontaneous emission of a dislocation loop with no activation energy, or there may be a finite activation energy to form the loop whose radius is determined by eqn. (18).

We have solved eqn. (18) for the critical loop size, and calculated the aetivation energy for the list of materials given in table 1. The results are listed in table 3. Further, the functional varintion of the activation energy with $\gamma / \mu b, \xi_{0}$, and orientation parameters is shown in fig. 7. In

Fig. 6


Sehematic variation of the three terms in eqn. (17) as a function of the radius.

Table 3. Three-dimensional results

| Crystal | Activation energy <br> (electron voltes) | Radius of activated loop (in units of b) |
| :---: | :---: | :---: |
| Pb |  |  |
| Au |  |  |
| Gu |  |  |
| Ag | Spontaneous emission-No activated state for $r>\xi_{0}$. |  |
| Al |  |  |
| Ni |  |  |
| N ${ }^{\text {d }}$ | $0 \cdot 02$ | $1 \cdot 5$ |
| Fe | $2 \cdot 2$ | $5 \cdot 1$ |
| W | 329 | $50 \cdot 7$ |
| Fe* | 19 | 17 |
| LiF | 58 | 32 |
| NaCl | $\left\{\begin{array}{c}62 \\ (240)\end{array}\right\}$ | $\left\{\begin{array}{c}39 \\ (95)\end{array}\right\}$ |
| MgO | $(240)$ 205 | $\left\{\begin{array}{c}(95) \\ 37\end{array}\right\}$ |
| $\mathrm{A}_{2} \mathrm{O}_{3}$ | 852 | 20 |
| Si | 111 | 20 |
| Ge | 260 | 42 |
| C | 351 | 27 |
| Be | 180 | 23 |
| Zn | 107 | 21.2 |

this plot, the activation energy (eqn. (17)) is plotted after $r$ is eliminated through eqn. (18). Here it is convenient to plot the dimensionless energy

$$
\begin{equation*}
u_{\text {aect. }}=\frac{U_{\text {nst }}}{\frac{(2-\nu)^{2}}{8(1-\nu)}} \frac{\beta^{2}}{\beta^{\prime}} \mu b^{3} \tag{19}
\end{equation*}
$$

in terms of

$$
\begin{equation*}
S=\frac{16(1-v)}{5 \beta^{\prime}(2-v)} \frac{\gamma}{\mu b} \quad \text { and } \quad R_{0}=\frac{16 \beta^{\prime}}{5(2-v) \beta^{2}} \xi_{0} \tag{20}
\end{equation*}
$$

Indeed, these forms have been chosen because, for typical values of $v$ and the orientation parameters, they reduce to

$$
\begin{equation*}
u_{\mathrm{act}} \approx \frac{U_{\mathrm{act}}}{\mu b^{3}}, S \approx \frac{\gamma}{\mu b}, R_{0} \approx \xi_{0} \tag{21}
\end{equation*}
$$

Fig. 7


Dependence of retivation energy for disloontion mucleation on $S(\approx \gamma / \mu b$ ), and $R_{0}\left(\approx \xi_{0}\right)$; exact definitions of 5 and $R_{0}$, and normalization of energy are given in text.

It is reen that the behaviour divides mainly into two kinds: If the orien -tation-dependent core parameter, $R_{0}$, is small, there is a substantial energy barrier to dislocation nucleation for all values of $\gamma / \mu b$ (i.e., $\left.U_{\text {act }} \geqslant 0^{1}\right] \mu b^{3}$ ). On the other hand, if $R_{0}$ is large there will be an energy barrier only if the surface energy parnmeter, $S$, is smaller than that at which the curves cross the $S$ axis; otherwise there is spontaneous nucleation. The curves for the larger values of $R_{0}$ rise so ateeply that there is essentially a critical value of $\$$ below which the energy barrier is substantial, and above which there is spontaneous nucleation, although finer examination shows that there is a narrow range of $R_{0}$ and $S$ values for which $U_{\text {nct. }}$ is low enough that thermal activation could blunt the crack for sufficiently long time scales of load application.

## § 4. Phybioal resulirs and interpretation

### 4.1. Surface energy

Among the experimentally determined values listed in table 1 , the values of $\gamma$ are the onee for which the only important uncertainties exist.

For tungsten, Cordwell and Hull (1969) find that the surface energy varies from a low value of 1700 cgs at low temperature to 0000 cgs at higher temperature. The higher vaiue apparently is due to plasticity induced in the vicinity of the moving crack. Other values have been measured by other workers intermediate to these extremes, but we believe the low value listed represents the baje crack.

NaCl is claimed by Class (1904) in his thesis to have a surfuce energy of 115 cgs , and this value is adopted by Kelly ( 1966 ). On the other hand, we believe the value 250 is more likely. It is in the range of the experiments of Gilman (1960), Wiederhorn, Voses and Bean (1970), and Benson and Benson (1955), Benson, Schreiber and Van Zeggeren (1956) and Benson and Balk (1959), and is in reasonable agreement with the theoretionl ealculations, which for this crystal should not have a large error (Tosi (1964), MaoMillan and Kelly (1972)). We list both valnes, and results for both, however.

For $\mathrm{Al}_{2} \mathrm{O}_{3}$, we have a range of values in the literature all the way from 1000 cgs as given by Kingery (1954) for the basal plane to 6000 cgs as determined in cleavage exporiments on the rhombohedrol planes by Wiederhorn (1969). Wiederhorn also reports that oleavage is not possible on the basal planes, and in a private communication has noted that the cleavage surface energy for these planes must in consequence be in excess of 40000 cgs ! One wonders if the value reported by Kingery (not measured in cleavage) is not actually either that for a restruotured surface or a composite value for a dimpled surface whose average orientation is [0001], but not the true basal plane. Consequently, we use $\gamma=6000 \mathrm{cgs}$ in our work.

In Zn, Naitland and Chadwick (1069) have measured a range of values from 100 egs (confirmed by other previous author's), to 575 cgs , depending
upon the technique used for making the messurement. Because of weaknesses in the anelysis as applied to the experiments yielding the lower value, thay believe the value of 575 cgs is to be preferrcd.

But experimental difficulties do not exhaust our problems with the surface energy. One muat also be certain that the surface energy as measured experimentally and the surface energy as we use it are synonymous. In our work, the correct $\gamma$ is derived as the energy necessary to break bonds at a crack tip. Even in a pure elenvage event where no dislocations are produced, this process may not correspond to the thermodynamic surface energy beoange of relaxation effects which are possible on some crystal surfaces, such as Si , where the surface is entirely restructured. For this raseon, the value chosen for Si is derived in a cleavage experiment, and for diamond is calculated from the value of the carbon-carbon bond, Unfortunately no cleavage surface energies are available for Ge. We also note a further point of rigor. In crystals with high Peients barriers where the discrete lattice force fields can trap a crack (Hsieh and Thomson 1973) the $\gamma$ measured to grow a crack is different from the $\gamma$ measured to heal a orack.

### 4.2. Two-dimenaional results

The results in table 3 suggest that the face-centred orystals, with the possible exception of Ni which has a borderline $\xi_{\text {c }}$, are unstable to dislocation formation, since the critical distance, $\xi_{\mathrm{c}}$, is less than the core radius, $\xi_{0}$. Since all the elastic forces become impossible to define inside the core radius, and since the repulsive forces are dominant for all distances larger than the core, we believe a crack in these crystals cannot sustain the large shear forces at its tip without forming the dislocation spontaneously. Na, of the body-centred cryatals, probably also spontaneously emits the dislocation because of the small size of $\xi_{c}$, and also because we believe that in this case $\xi_{0}$ is not so small as $2 / 3$, as is nssumed for the other body-centred cubics. In all other cases, $\xi_{\mathrm{a}}$ is sensibly larger than the core size, and we believe this gives rise to an energy hump which the dislocation must negotiate as it is formed.

We have listed in table 2 two other cruder estimates of $\xi_{\mathrm{a}}$. In the first, we neglect the ledge term and in the second average over the geometry. Both are fair approximations to the more accurate values for the brittle materials in the lower half of the table. The ledge term is seen to be important for the softer crystale, as one would expect.

The dimensionless ratio, $\mu b / \gamma$, related to our $\xi_{\mathrm{c}}{ }^{\prime \prime}$ has already entered into Armstrong's (1969) discussion of the brittle versus ductile competition, and we see that it is indeed explicit in our own worls. However, in our theory, as one progresses down the list of crystals in tahle 2, it is the opposite tendency of the growing value of $\mu b / \gamma$ and the decrensing valuc of the core cut-off which makes the difference between the ductile facecentred cubics and the more brittle body-centred cubics.

We note in table 2 the positions of iron and nickel between the obviously ductile and obviously brittle solids. We give two calculations for iron, In one, the erack line runs along a cube direction, [100], and in the second, the crack line runs along [110]. The second is actually that observed by Tetelman and Robertson (1963) in silicon iron, but it is the former which hes the interesting low value of $\xi_{\mathrm{c}}$.

We have listed the results for a split dislocation for a noble metal and for niokel. (Aluminium has small or no splitting.) The results shown are for only one of the partials. In the case shown, the partial has unfavourable geometrical factors, since it is not oriented to cause the crack to open effectively. In this unfavorable case, the critioal radii are slightly increased, but not enough to change our general results.

### 4.3. Three-dimensional results

The three-dimensional results for the estimated activation energy as given in table 3 confirm the two-dimensional findings. We find a negative activation energy for the face-centred cubics, which ogain means that since all energies are cut off at the core radius, by the time any dislocation is well formed, it is under the primary infuence of the repulsive forces. Again, Na would seem to have an essentially spontaneous emission, not only because of the small value of the calculated activation energy, but also because we have probably tnderestimated the true dislocation core size of this very soft orysten.

The main surprise wben comparing the two-with the three-dimensional reaults is the very large values obtained for the activation energy of the brittle crystals, even though $\xi_{\mathrm{c}}$ is usually a small number. One might suppose that it would take only a small energy to pusha a local segment of dislocation past $\xi_{0}$, say in NaCl , over a small front of the crack tip, and that the repulsive force would then be able to dominate the picture sufficiently to expand the fluctuation indefinitely. However, the reason this is not so is that the dislocation mast meet the crack surface at normal incidence. Otherwise, the forces there will collapse the fluctuation no matter what happens to that portion lying over the homp beyond $\xi_{\mathrm{c}}$. In order for the dislocation to meet the surface perpendicularly, a full half loop of dislocation must be formed in the region of repulsive forces, which is costly in clislocation line energy.

### 4.4. Gonclusions

We find a very strong tendency for crystale to be aither completely ductile, or completely brittle, so far as dislocation emiseion is concerned. Iron and nickel are the only interesting cuses wherc our calculatione suggest that the activation energy may be sufficiently low that thermal fuctuations could play a role. With the various uncertainties in our calculations,
we are unfortunately not able to pin down the values in these cases sufficiently to make a definite prediction.
Except for iron, sodium, and the face-centred oubics we feel confident in predicting that no spontaneous or thermally assisted blunting of a crack tip can occur in the other crystale investigated. Even with the uncertainties in the $\gamma$ and the other approximations made, orystals like LiF and NaCl (to say nothing of the hexagonal metels) seem immune enough to this process. This conclusion means that if bhnting does ocent it must be because of cislocations prodnced outside the tip region, and which are then attracted toward, and collide with it.
Our conclusions are at variance with the often quoted claim that cracks cunnot remain sharp (and the crystals thus be brittle) if the shear stress at the crack tip is larger than the theoretical shear stress of the homogeneous crystal. As we stated in the introduction, a shear stress at the value of the theoretical shear strength will cause the crystal to break down only if the stress is homogeneously applied across an entire plane running through the crystal. If the stress is only appled locally on that plane, then atoms where the atress has dropped below the maximum value will not be displaced from their lattice positions, and atoms where the force is maximum will not necessarily be displaced even though the stress is above the theoretical shear strength because of the resistance offercd by atoms in the undeformed region of the plane.
Our conclusions suggest that so far as spontaneous emission is concerned, atomically sharp cleavage cracks are by no means a minority occurrence in materials. When the condition $\mu b / \gamma>7.5-10$ is approximately satisfied, we have reason to expect the crack to remain sharp, though geometrical factors and variations in core size make this condition only approximate. This condition, in the cases investigated, is satisfied for all but the facecentred cubio metals, and certain borderline body-centred metals.

Our conclusions leave the precise morphology of cleavage cacks ultimately undetermined, however, because they do not address blunting reactions due to dislocations which might be attracted to the crack tip from the surrounding erystal. Processes which lower the cleavability by increasing the effeotive cleavage aurface energy through the action of dislocation atmospheres trapped by the stress field of the crack are also not addressed here. On the other hand, our work does allow an evaluation of environmental effects which can be undergtood in terms of a lowering of $\gamma$. By increasing the ratio $\mu b / \gamma$, these could presumatly make possible atomically sharp cracking, even in solids such as f.e.c. crystals which normally show ductile response. Then the 'cleavage' is not necessarily fast-running, but ean proceed only as fast as reactions take place to bring about the requisite lowering of $\gamma$ at the tip. It is possible that some environinentally assisted crack growth ean be underatood in this way.

## APPENDIX

Image force on dislocation near a crack tip
To compute the image force, consider fig. 8 in which a straight dislocation line lies parallel to a crack front, with the slip plane intersecting the fincture plane at distance $a$ ahead of the tip. We are ultimately interested in the case $\alpha=0$, but by considering $\alpha$ as variable we can ase energy methods to compute the force.

Fig. 8


Configuration of orack and dislocation for computation of the imago force.

Suppose that the body containing the crack is subjected to three generalized boundary forces $Q_{\mathrm{I}}, Q_{\mathrm{II}}$, and $Q_{\text {III }}$, each of which if exerted singly upon a dislocation free body would aanse only a Mode I, II, or III crack tip singularity, respeotively. Let $q_{I}, q_{I I}$, and $q_{\text {III }}$ be the associated generalized displacements. These are defined so that

$$
\sum_{J} Q_{J} d q_{J}
$$

is the work of boundary loadings per unit thickness into the plane of the figure. The sum on $J$ extends from I to III. Hence, if we let $U$ be the strain energy of the body per the same unit thickness,

$$
\begin{equation*}
d U=\sum_{J} Q_{J} d q_{J}+G d \alpha-f d_{p} \tag{Al}
\end{equation*}
$$

where the respective contributions to energy changes come from lood-point displacements $d q_{J}$, crack advance $-d \alpha$, and dislocation glide $d \rho ; G$ is the orack extension force (or energy release rate) and $f$ is the force on the dislocation.

The last equation may be rewritten as

$$
d\left(U-\sum_{J} Q_{J} q_{J}\right)=-\sum_{J} q_{J} d Q_{J}+G d \alpha-f d \rho
$$

Further, since the terms on the right constitute an exact differential, we may write the Maxwell relation

$$
\begin{equation*}
\left(\frac{\partial G}{\partial \rho}\right)_{a, Q}=-\left(\frac{\partial f}{\partial \alpha}\right)_{p, Q} \tag{A2}
\end{equation*}
$$

This is a fundamental relation for it allows us to compute the force on the dislocation solely from a knowledge of elastic fields induced by each of the forces $Q_{J}$. To see this, recall that the crack energy release rate is given by (e.g., Rice 1968)

$$
\begin{equation*}
G=\frac{1-\nu^{2}}{E}\left(K_{\mathrm{I}^{2}}+K_{\mathrm{II}}^{2}\right)+\frac{1+v}{E} K_{\mathrm{IIL}}^{2} \tag{AB}
\end{equation*}
$$

where the $K$ 's are stress intensity factors for the three modes. These are due both to the boundary forces $Q_{J}$ and to the interaation of the dislocation stress field with the crack, and take the forms

$$
\begin{equation*}
K_{J}=k_{J}(\alpha) Q_{J}+L_{J}(\alpha, \rho), \quad J=I, I I, I I I \tag{A4}
\end{equation*}
$$

Here each $k_{J}$ is the Mode $J$ stress intensity factor induced per unit of the corresponding boundary force. Euch is assumed to be known for all crack lengths and hence can be considered as given function of $\alpha$. The unknown functions $L_{J}$ are the stress intensity factors induced by the dislocation. The force on the dislocation is given by

$$
\begin{equation*}
f=b_{e}\left[t_{1}\left([,, \rho) Q_{\mathrm{I}}+t_{\mathrm{HI}}(\alpha, \rho) Q_{\mathrm{II}}\right]+b_{k} t_{\mathrm{IIL}}(\alpha, \rho) Q_{\mathrm{III}}+g(\alpha, \rho)\right. \tag{A5}
\end{equation*}
$$

Here $b_{c}$ is the edge and $b_{s}$ the screw Burgers vector component; $t_{\mathrm{I}}$ and ${ }^{\prime}{ }_{\text {II }}$ are the shear stresses induced on the glide plane, at the dislocation position, in the edge direction per unit boundary force $Q_{\mathrm{I}}$ and $Q_{\mathrm{II}}$, respectivaly; $t_{\text {III }}$ is the shear stress in the serew direction induced per unit force $Q_{\text {III }}$. These shear stresses are to be considered as known functions of crack length and dislocation position, and hence of $\alpha$ and $\rho$. The unknown force term $g$ is that due to the dislocation itself, i.e., the image force, and our object is to compute it.

By substituting for $G$ and $f$ as above in the Maxwell relntion (A2), we obtain

$$
\begin{gathered}
\frac{2\left(1-\nu^{2}\right)}{W}\left[\left(k_{\mathrm{I}} Q_{\mathrm{I}}+L_{\mathrm{I}}\right) \frac{\partial L_{\mathrm{I}}}{\partial \rho}+\left(k_{\mathrm{II}} Q_{\mathrm{II}}+L_{\mathrm{II}}\right) \frac{\partial L_{\mathrm{II}}}{\partial \rho}+\frac{1}{1-\nu}\left(k_{\mathrm{III}} Q_{\mathrm{III}}+L_{\mathrm{III}}\right) \frac{\partial L_{\mathrm{III}}}{\partial \rho}\right] \\
=-b_{\mathrm{e}} \frac{\partial t_{\mathrm{I}}}{\partial \mathrm{I}} Q_{\mathrm{I}}-b_{\mathrm{e}} \frac{\partial t_{\mathrm{II}}}{\partial_{\alpha}} Q_{\mathrm{II}}-b_{\mathrm{s}} \frac{\partial t_{\mathrm{III}}}{\partial \alpha} Q_{\mathrm{III}}-\frac{\partial g}{\partial \alpha}
\end{gathered}
$$

This must hold for all volues of the $Q$ 's. Hence by equating coefficients of each $Q_{J}$,

$$
\begin{equation*}
\frac{\partial L_{J}}{\partial \rho}=\frac{-E b_{\mathrm{c}}}{2\left(1-\nu^{2}\right) k_{J}} \frac{\partial t_{J}}{\partial \alpha}, \text { fol } J=\mathrm{I}, \mathrm{II} ; \frac{\partial L_{11 \mathrm{I}}}{\partial \rho}=\frac{-E b_{s}}{2(I+\nu) h_{111}} \frac{\partial t_{\mathrm{III}}}{\partial \alpha} \tag{AG}
\end{equation*}
$$

And by equating sides when each $Q_{J}=0$,

$$
\begin{equation*}
\frac{\partial g}{\partial \alpha}=-\frac{1-\nu^{2}}{E} \frac{\partial}{\partial \rho}\left(L_{1}^{2}+L_{1 \mathrm{I}}^{2}+\frac{1}{1-\nu} L_{\mathrm{III}}^{2}\right) . \tag{A7}
\end{equation*}
$$

## J. R. Rice and R. Thomson on the

The calculation of the image force now involver simple integrations: (i) First, we note that the right sides in (AG) involve known functions of $\alpha$ and $\rho$; each $L_{J}$ is deternined by integrating these at fixed $\alpha$ from the $\rho$ of interest to a large value of $\rho$, say to $\infty$ or to the specimen boundary, at which the $L$ 's may be taken as zero. (ii) Thus the right side of (A7) is determined, and $g$ is obtained by integration from the $\alpha$ value of interest (zero in our case) to a large value of $a$ at which $g$ may be taken as zero.

Now, since we are interested in a dislocation rather near to the crack tip, it will suffice to consider a semi-infinite crack in an infinite body. Also, the solution for the $L$ 's and $g$ cannot depend on the particular nature of the lond systems denoted by the $Q^{\prime}$ s. Indeed, the right sides of (A0) are universal functions, the same for all load systems inducing a given crack tip mode (see Rice 1972). Heuce, for simplicity, we can choose loacl systems which act so far from the ornok tip that the characteristic inverse-square-root elastic stress distribution gives the entire stress field, and that the $k$ 's are virtually constant, for all crack distances $\alpha$ of interest. Let $\left(\sigma_{[j}\right)_{J}$ denote the stress field for in given loading mode, $J$; this will be of the form

$$
\begin{equation*}
\left(\sigma_{i j}\right)_{J}=\frac{k_{J} Q_{J}}{\sqrt{r}}\left[F_{t_{j}}(\theta)\right]_{J}, \quad i, j=x, y, z \tag{A8}
\end{equation*}
$$

Here the $P$ 's are functions of $\theta$, particular to each mode, that are tabulated e.g. by Rice 1968, pp. 216-217. From these the shear stresses on the dislocation, per unit boundary loads, are identified from

$$
Q_{J} l_{J}=\frac{\left(\sigma_{y, y}\right)_{J}-\left(\sigma_{x x}\right)_{J}}{2} \sin 2 \phi+\left(\sigma_{x y}\right)_{J} \cos 2 \phi_{y}
$$

for $J=I$, II, and

$$
Q_{\mathrm{III}} t_{\mathrm{III}}=\left(\sigma_{y s}\right)_{\mathrm{III}} \cos \phi-\left(\sigma_{x z}\right)_{\mathrm{III}} \sin \phi .
$$

Upon substitution from (A8), these give

$$
\begin{align*}
t_{\mathrm{I}} & =k_{\mathrm{I}}(8 \pi)^{-1 / 2} \sin \phi \operatorname{Re}\left[e^{1 \phi}\left(\xi^{-1 / 2}-\alpha \xi^{-3 / 2}\right)\right], \\
t_{\mathrm{II}} & =k_{\mathrm{II}}(8 \pi)^{-1 / 2} \operatorname{Re}\left[2 e^{2 \mathrm{idi} \phi} \xi^{-1 / 2}\right]+\sin \phi \operatorname{Im}\left[e^{1 \phi}\left(\xi^{-1 / 2}-\alpha \xi^{-3 / 2}\right)\right],  \tag{A9}\\
t_{\mathrm{III}} & =k_{\mathrm{III}}(2 \pi)^{-1 / 2} \operatorname{Re}\left[e^{i \phi} \xi^{-1 / 2}\right],
\end{align*}
$$

where $i$ is the unit imaginary number, Re and Im denote veal and imaginary parts, and where

$$
\xi=r e^{1 p}=\alpha+\rho e^{i \phi} .
$$

Hence the first of (A6) becomes

$$
\begin{aligned}
\frac{\partial L_{\mathrm{I}}}{\partial \rho} & =-\frac{E b_{c}}{2\left(1-\nu^{2}\right) k_{\mathrm{I}}}\left\{k_{\mathrm{I}}(8 \pi)^{-1 / 2} \sin \phi \frac{\partial}{\partial \alpha} \operatorname{Re}\left[e^{i \phi}\left(\xi^{-1 / 2}-\alpha \xi^{-3 / 2}\right)\right]\right\} \\
& =\frac{3 E b_{e} \sin \phi}{8\{2 \pi)^{1 / 2}\left(1-\nu^{2}\right)} \quad \operatorname{Re}\left[e^{1 \phi}\left(\xi^{-3 / 2}-\alpha \xi^{-5 / 2}\right)\right] .
\end{aligned}
$$

Multiplying by $d p$ and recognizing that $\boldsymbol{1}^{1} d p=d \xi$, so that integration on $\rho$ becomes integration on $\xi$ inside the brackets, we have

$$
\begin{align*}
L_{\mathrm{I}} & =\frac{3 E b_{\mathrm{e}} \sin \phi}{8(2 \pi)^{1 / 2}\left(1-\nu^{2}\right)} \operatorname{Re}\left[-2 \xi^{-1 / 2}+2 \alpha \xi^{-3 / 2}\right] \\
& =\frac{-E b_{e}}{4\left(1-v^{2}\right)(2 \pi r)^{1 / 2}}\left[3 \sin \phi \cos \frac{\theta}{2}-\sin (\phi-\theta) \cos \frac{3 \theta}{2}\right], \tag{A10}
\end{align*}
$$

where the constant of integration is chosen so that $L_{I}$ vanishes at $\rho=\infty$. In a similar way we find.

$$
\begin{align*}
& L_{\mathrm{fI}}=\frac{-E b_{\mathrm{E}}}{4\left(1-v^{2}\right)(2 \pi r)^{1 / 2}}\left[2 \cos \phi \cos \frac{\theta}{2}-\sin \phi \sin \frac{\theta}{2}+\sin (\phi-\theta) \sin \frac{3 \theta}{2}\right] \\
& L_{\mathrm{III}}=\frac{-E b_{s}}{2(1+v)(2 \pi r)^{1 / 2}} \cos \frac{\theta}{2} . \tag{A11}
\end{align*}
$$

Now that the $L$ 's are known, we have determined the effect of the dislocation on the stress intensity factors $K_{J}$ (A4) and, further, we can substitute into (A7) to determine the image force. Since each of the $L^{\prime}$ 's is proportional to $r^{-1 / 2}$, (A7) is of the form

$$
\frac{\partial g}{\partial \alpha}=-\frac{\partial}{\partial \rho}\left[\frac{Q(\theta, \phi)}{r}\right],
$$

where

$$
\begin{equation*}
Q(\theta, \phi)=\frac{1-\nu^{2}}{E} v\left(L_{\mathrm{I}}^{2}+L_{\mathrm{II}}{ }^{2}+\frac{1}{1-\nu} L_{\mathrm{III}}{ }^{2}\right) . \tag{A12}
\end{equation*}
$$

But by using the relations

$$
\frac{\partial}{\partial \alpha}=\cos \theta \frac{\partial}{\partial r}-\frac{\sin \theta}{r} \frac{\partial}{\partial \theta}, \frac{\partial}{\partial \rho}=\cos (\phi-\theta) \frac{\partial}{\partial r}-\frac{\sin (\phi-\theta)}{r}-\frac{\partial}{\partial \theta}
$$

between pertial derivatives, one may rendily derive the identify

$$
-\frac{\partial}{\partial \rho}\left[\frac{Q(\theta, \phi)}{r}\right]=\frac{\partial}{\partial a}\left[\frac{\sin (\phi-\theta)}{\sin \theta} \frac{Q(\theta, \phi)}{r}\right] .
$$

This lets us integrate (A12) immediately. We must, however, append a 'constant' of integration, which may depend on $\rho(=r \sin \theta / \sin \phi)$, and which assures that $g \rightarrow 0$ as $\alpha \rightarrow \infty$. This means that $g \rightarrow 0$ as $r \rightarrow \infty, \theta \rightarrow 0$ in such a way that $v \sin \theta$ remains finite. Integration of (A12) subject to this condition gives the image force

$$
\begin{equation*}
g=\frac{\sin (\phi-\theta) Q(\theta, \phi)-\sin \phi Q(0, \phi)}{r \sin \theta}, \tag{A13}
\end{equation*}
$$

where $Q$ is defined from (A10, 11) via (A12).

In the text of the paper we were concerned with the case $\alpha=0$, so that $\theta=\phi$ and $r=\beta$. In that case

$$
\begin{equation*}
\theta=-\frac{Q(0, \phi)}{\rho}=-\frac{E b_{0}{ }^{2}}{8 \pi\left(1-\nu^{2}\right) p}-\frac{E b_{5}{ }^{2}}{8 \pi(1+\nu) p}, \tag{A14}
\end{equation*}
$$

where the latter form comes from identifying $Q(0, \phi)$, which is found to be independent of $\phi$. Remarkably, this is the same image force as for a dislocation line at distance $\rho$ along its slip plane from the boundary of $a$ half-space. In fact, the result for this latter case is also obtainable from (A13) by letting the crack tip pass far beyond the site of the dislocation, $\alpha \rightarrow-\infty$. This menns that we let $\theta \rightarrow \pi, r \rightarrow \infty$ while keeping $r \sin \theta$ finite (it equals $\rho \sin \phi$ ). By direct evaluation one finds that $Q(\pi, \phi)=0$, so that the image force from the half-space boundary is also given by (A14).

References
Armgtrona, R., 1966, Mater. Sci. Engng, 1, 251.
Atkinson, C., 1966, Int J. fracture Mech., 2, 567.
Benson, G., and BaLht, P., 1959, J. phys. Chem., 83, 1009.
Rerson, G. C., and Benson, G. W., 1955, Can. J. Chem., 33, 232.
Benson, G., Sofreiber, H., and Zeggeren, F. Van, 1956, Cah. J. Chem., 34, 1653.

Burns, S., 1970, Acta metall., 18, 969.
Burns, S., and Wrbe, W., 1970, J. appl. Phys., 41, 2078, 2086.
Clabs, W., 1964, Ph.D. Thesis, Columbia University,
Condwell, J., and Hull, D., 1969, Phil. Mag., 19, 951.
Gilman, J., 1960, J. appl. Phys., 31, 2208.
Hirth, J., and Lothi, J., 1968, Theory of Dislocations (New York: McGrawHill).
Hsedi, C., and Thomson, R., 1973, J. uppl. Phys., 44, 2051.
Kelly, A., 1066, Strong Solids (London: Oxford University Press).
Kelly, A., Tyson, W., and Cortrell, A., 1967, Phil. Mag., 15, 567.
Kingery, W., 1954, J. Am. Ceram. Soc., 37, 42.
Kitajima, K.,. 1906, Proceedings of the First International Gonference on Fracture, Vol. 2 (Sendai).
MacMillan, N., and Krlly, A., 1972, Proc. R. Soc., 330, 291.
Marisworth, A., Kanninezt, M., and Gehlen, P., 1973, Proceedings of the International Confercnce on Stress Corrosion, Cracking and Hydrogen Embrittlement of Iron Based Alloys (Natl. Assn. Corr. Eng., Houston, Texas).
Mattland, A., and Chadwiok, G., 1969, Plill. Mag., 10, 645.
Rice, J., 1968, Fracture, Vol. 2, edited by H. Liebowitz (New Yorls: Academic Press), p. 191; 1972, Int. J. Solidx Struct., 8, 751.
Tetelmak, A., and Robibrson, W., 1063, Acta metall., 11, 415.
Tosi, M., 1964, Solid Shate Physics, Vol. 16, edited by li. Seitz and D. Turnbull (New York: Academic Press).
Wiederhorn, S., 1969, J. Am. Cerain. Soc., 52, 485.
Wiederhorn, S., Voses, R., and Bean, B., 1970, J. Am. Ceram. Soc., $53,18$.

## Surtace energy refermeds

(1) Taydor, J. W., 1954, Metallurpia, 50, 161.
(2) Structure and Properties of Solid Surfaces, 1052, edited by R. Gomer and C. Smith (Chicago: University of Chicago Press); Grain Boundaries in Metals, 1957, by D. McLemm (London: Oxford University Press), p. 76.
(3) Imman, M., and Tifleet, H., 1063, Metall. Rev., B, 105.
(4) Prioe, A., Hall, M., and Greenovah, A,, 1964, Acta metall, 12, 49; Inman, M., and Tifler, H., 1963, Metall. Rev., 8, 105.
(b) Cordwall, J., and Holl, D., 1969, Phil. Mag., 19, 951.
(6) Borws, S., and WEBe, W., 1970, J. appl. Phys., 41, $2078,2086$.
(7) Tosr, M., 1064, Solid State Physics, Vol. 16, edited by F. Seitz and D. Turnbull (New York: Aoademic Press); gee also MaoMillian, N., and Kelly, A., 1972, Proc. R. Soc., 380, 291.
(8) Class, W., 1904, Ph.D. thesis, Columbia University.
(9) Maitland, A., end Chadwick, G., 1069, Phil. Mag., 19, 645.
(10) Wimderhorn, S., 1969, J. Am. Ceram. Soc., 52, 485.
(11) Kingery, W., 1954, J. Am. Ceram. Soc., $87,42$.
(12) Hawhes, W., 1941, J. chem. Phys., 10, 269.


[^0]:    $\dagger$ This paper has been prepured under initial support of tha ARPA. Materials Rescarch Conmeil, with subsequent support from AEC contrects at Brown Univeraity and SUNY/Stony Brook, and from the NBS.

