The interaction between dislocations and intergranular cracks

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The interaction between dislocations and intergranular cracks

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The elastic interactions of dislocations and intergranular cracks in isotropic materials have been studied. In the first part of the paper, a model based on the Rice-Thomson theory is established under which the conditions for dislocation emission and crack propagation can be described in terms of an emission surface, cleavage surface, and loading line in the local k-space associated with a mixed mode intergranular crack. For a given crack, the local k-field changes with the emission of dislocations from the crack tip, which alters the balance of cleavage and emission. In the second part, we present experimental results of in situ TEM observations of intergranular cracks in molybdenum. Alternating brittle crack propagation and dislocation emission is observed. The number of emitted dislocations corresponding to each crack propagation is in good agreement with the calculated values.

I. INTRODUCTION

Intergranular fracture has been studied for many years. It is well known that grain boundaries act as fracture paths and as special sites for the accumulation of impurities which are believed to be the major cause of intergranular embrittlement. Over the years, research on intergranular fracture has concentrated on various types of segregation-induced intergranular embrittlement, such as temper-embrittlement (P, Pb, Sn, etc. in steels, etc.), hydrogen-embrittlement (H in Ni), and embrittlement of some alloys (Bi in Cu). It is believed that the Griffith criterion can be applied to intergranular brittle fracture after simple modifications, which can be expressed in terms of the critical strain energy release rate, $J_c$.

$$J_c = 2\gamma = 2\gamma_s - \gamma_b$$

where $\gamma$ is the fracture energy, $\gamma_s$ the surface energy, and $\gamma_b$ is the energy of the pre-existing grain boundary. Since both $\gamma_s$ and $\gamma_b$ are affected by concentration of impurities, one can expect that fracture energy may change greatly with impurity segregation.

However, for most engineering materials, it is rare to have pure brittle intergranular fracture unless extremely high impurity levels occur. Therefore, brittle propagation of intergranular cracks combined with plastic deformation is the general finding. McMahon and Vitek\textsuperscript{1} suggested that by extending the Orowan equation to intergranular fracture, the fracture energy, as well as the critical strain energy release rate, can be rewritten as

$$J_c = 2\gamma = 2\gamma_s - \gamma_b + \gamma_p = 2\gamma' + \gamma_p$$

where $\gamma' = \gamma_s - \frac{1}{2}\gamma_b$ represents the cohesive energy of the grain boundary and $\gamma_p$ is the plastic work associated with dislocation motion during the propagation of the intergranular crack. In Eq. (2), it is implied that $\gamma_p$ is a material parameter in the same sense as $\gamma_s$ and $\gamma_b$, and is independent of crack geometry, loading condition, etc. As a macroscopic and qualitative criterion, Eq. (2) is accepted by many investigators. However, it is clear that $\gamma_p$, which depends on dislocation mobility, has no direct relation with segregation but that the cohesive strength, $\gamma'$, can be expected to be strongly affected by segregation of elements which cause large changes in the bonding across the interface. The problem is that $\gamma_p$ may be orders of magnitude larger than $\gamma'$\textsuperscript{2}, so $\gamma'$ is only a negligible amount of the entire fracture energy. How this small fraction of the energy can influence the behavior of materials so much, and actually dominate the properties of materials, is a fundamental question that has been a paradox since the early papers of Orowan and Irwin, but its qualitative answer was suggested many years ago by Rice\textsuperscript{3}.

More recently, McMahon and Vitek\textsuperscript{1} and Jokl et al.\textsuperscript{4} proposed that $\gamma_p$ can be regarded as a function of $\gamma'$ instead of as an independent material parameter. Based on the assumption that during fracture the processes of bond breaking and dislocation emission at the crack tip are concomitant processes, they derived an exponential dependence of $\gamma_p$ on $\gamma'$ so that a relatively small change in $\gamma'$ may lead to a large change in $\gamma_p$. A similar semi-quantitative reasoning was put forward by Thomson\textsuperscript{5} and Weertman\textsuperscript{6,7} for homogeneous materials. However, our recent in situ TEM studies on intergranular cracks have shown that the process is more complex, and that
alternate processes of dislocation emission and brittle crack propagation occur (Zhang and King, unpublished results). This indicates that bond breaking and dislocation emission at the crack tip are competitive processes, which is consistent with the initial assumption of the theory of dislocation and crack interaction proposed by Rice and Thomson.6

According to Rice and Thomson, the stability of an 'atomistically' sharp crack against dislocation nucleation is a necessary condition for brittle cleavage to be possible. This criterion involves the concept of an activation energy, $U_{act}$, for generating a metastable dislocation loop from the crack tip. $U_{act}$ is presumed to be a function of the orientation factors of the slip system with respect to the crack front, the elastic constants of the material, and cohesive energy, $2\gamma$. If $U_{act}$ is positive, the work for dislocation nucleation is greater than that for crack propagation and unstable brittle crack growth is expected. If $U_{act}$ is negative, dislocations will be generated from the crack tip spontaneously before the critical Griffith condition can be reached. They introduced a critical stress intensity factor $k_e$ for the generation of dislocations and $k_c$ which is the critical stress intensity factor for brittle crack propagation. As the crack is loaded, the local $k$ is increased. The manner in which the crack grows will depend on whether $k$ reaches $k_e$ or $k_c$ first.

Anderson and Rice9 extended the Rice–Thomson model to interfacial cracks by taking into account elastic anisotropy. The effect of including elastic anisotropy in the competitive process enters largely through a set of parameters $S_i$, such that $K_S S_i \rho^{-1/2}$ (summation over loading $i = 1, 2, 3$) is the shear stress exerted on the slip plane in the slip direction, at distance $\rho$ from the crack tip. For Cu and Cu alloys [anisotropic factor, $2C_{44}/(C_{11} - C_{12})$ is 3.21], the difference in $K_i$ between the isotropic and anisotropic elastic analyses is about 20%.

One of the difficulties associated with this model is that, for materials for which $k_e < k_c$, once $k$ reaches $k_e$, since the emitted dislocation will interact with the crack and reduce the local stress intensity factor $k$, through the so-called 'dislocation shielding', and the next dislocation cannot be emitted until $k$ reaches $k_e$ again. Hence local $k$ cannot exceed $k_e$ and reach $k_c$. This model was extended by Lin and Thomson,10 where general relations are derived for the elastic interactions between a cleavage crack and a dislocation and between pairs of dislocations in the presence of the crack under mixed loading. Using these results for mixed loading, it is possible to account fully for the interactions between cracks and associated dislocation distributions in terms of the local $k$-field.

In this paper, we will first extend the theory of dislocation-crack interactions to intergranular fracture. The basic concepts, such as local stress intensity factor $k$, critical stress intensity factor for dislocation emission $k_e$, dislocation shielding, etc. can all be extended to encompass studies of intergranular cracks. By adding a loading line in the local $k$-space we can actually describe the change of the local $k$ with the emission of dislocations from the crack tip and explain the alternation of brittle crack propagation and dislocation emission. Secondly, we will present some experimental results from in situ TEM observations, which show in detail how the dislocations interact with an intergranular crack. Finally, a quantitative description of fracture process based on the theoretical model will be given.

II. THEORETICAL MODEL

A. The condition for dislocation emission

We consider a crack situated on a grain boundary plane, Fig. 1. The slip planes are inclined at an angle $\theta$ to the grain boundary plane and $b$ is the Burgers vector of the emitted dislocation and $b_i$ are those of the shielding ones. We will work in the isotropic approximation, so that no crack tip displacement oscillations occur.11,12 Therefore, an intergranular crack is similar to a transgranular one, except that the crack path follows grain boundary instead of a crystallographic plane and that for a given slip system it is rare to have an equivalent slip plane mirrored in the crack plane. According to Thomson13 and Lin and Thomson,10 the force on an emitted dislocation form crack tip is composed of three terms, i.e.,

$$F = F_i(Kb) + F_2(b^2) + \sum_j F_3(bb_j)$$

where $K$ is the applied stress intensity factor. The first term is the crack force on the dislocation, the second term is the image force, and the third term is the interaction force between the emitted dislocation and other dislocations present. This is a very complicated equation which was given in detail by Thomson13 and Lin

![FIG. 1. Coordinate system for intergranular crack and emitted dislocation.](image)
The expression is simplified in slip plane coordinates and the first two terms of Eq. (3) on the slip plane take the form

\[ F_s = \frac{b_x}{\sqrt{2\pi r}} \left[ K_{sI} f_1(\theta) + K_{sII} f_2(\theta) \right] + \frac{K_{sII} b_x}{\sqrt{2\pi r}} f_3(\theta) \]

\[ f_1(\theta) = \frac{1}{2} \sin \theta \cos(\theta/2) \]

\[ f_2(\theta) = \cos(3\theta/2) + \frac{1}{2} \sin \theta \sin(\theta/2) \]

\[ f_3(\theta) = \cos(\theta/2) \]

where \( K_{sI}, K_{sII}, \) and \( K_{sIII} \) are the components of the stress intensity factor, \( b_s \) and \( b_s \) are the edge and screw components of the Burgers vectors, respectively, \( \mu \) is the shear modulus, \( v \) is Poisson's ratio, and \( r \) and \( \theta \) are the polar coordinates of the dislocation. For an emerging dislocation, the elastic crack force, as given by the first two terms of Eq. (4), exerts a repulsive force on the dislocation and hence will tend to drive the dislocation away from the crack tip. The imaging force, the third term of Eq. (4), is always attractive and thus will attract the dislocation to the crack surface. Very close to the crack tip, the force on the dislocation is negative, and an emerging dislocation will experience a barrier to emission. The distance, \( r \), at which the force on the dislocation becomes positive is inversely proportional to the square of \( K \) and hence decreases with increasing \( K \), i.e., with the applied stress. Rice and Thomson proposed that if the applied stress is sufficiently high so that the range of attractive interaction is less than or equal to \( r_0 \), where \( r_0 \) is a measure of the collective core size of dislocation plus crack, emission will occur spontaneously. The emission condition will be \( k > k_e \) where \( k_e \) is defined as that \( k \) for which \( F_s = 0 \) with \( r = r_0 \) in Eq. (4). Thus

\[ b_s[k_{sI} f_1(\theta) + k_{sII} f_2(\theta)] + b_b k_{sIII} f_3(\theta) \geq \frac{\mu}{\sqrt{8\pi r_0}} \left( \frac{b_s^2}{1} \right) \]

where \( b_s, b_s, \) and \( \theta \) are fixed by knowing slip system, dislocation line direction, and crack plane, i.e., the grain boundary plane in our case, and \( r_0 \) is assumed here to be a material constant, approximately equal to the Burger's vector of the given material. This equation defines a plane in \( (k_{sI}, k_{sII}, k_{sIII}) \) space called the emission surface, as shown in Fig. 2. The intercepts at each axis of \( (k_{sI}, k_{sII}, k_{sIII}) \) space define the critical stress intensity factor for emission in pure loading modes and denoted by \( k^p_e \), etc. as given by

\[ k^p_e = \frac{\mu b_x}{(1 - \nu) \sqrt{8\pi r}} [3 \sin \theta \cos(\theta/2)] \]

\[ k^p_{II} = \frac{\mu b_x}{(1 - \nu) \sqrt{8\pi r}} [2 \cos \theta \cos(\theta/2) - \sin \theta \sin(\theta/2)] \]

\[ k^p_{III} = \frac{\mu b_x}{\sqrt{2\pi r}} [\cos(\theta/2)]. \]
B. Brittle cleavage

As mentioned before, brittle crack propagation occurs if the local $k$ somehow reaches $k_c$, the critical stress intensity factor for brittle fracture. For a mode I intergranular crack, $k_I$ is given by the modified Griffith criterion

$$\frac{(1 - \nu)}{2\mu}k_I^2 = 2\gamma = 2\gamma_t - \gamma_h$$  \hspace{1cm} (9)

if a mixed-mode loading is applied. Knott$^{14}$ and Sinclair and Finnis$^{15}$ have suggested that Eq. (9) should be replaced by

$$\frac{1}{2\mu}(k_{II}^2 + (1 - \nu)(k_{I}^2 + k_{II}^2)) = 2\gamma$$  \hspace{1cm} (10)

This equation represents a curved surface in $k$-space. The implication of this equation is that $k_I$ and $k_{II}$ contribute to the elastic force on an equal footing with $k_{III}$. But Lin and Thomson$^{10}$ have shown that this equation is not physically correct, because when $k_I = 0$, no surface is created. By examining the theoretical strength of the solid in tension and shear, they have shown that the shear contribution even for brittle materials is of the order of 10% or less for cleavage to begin. So the major contribution for brittle crack propagation is from the mode I tensile loading. Thus, as a first approximation, we will use Eq. (9) as the cleavage criterion. This criterion actually gives a cleavage surface in the $k$-space, as shown in Fig. 3. All points in the region above the cleavage surface will cause brittle crack propagation, while values between emission surface and cleavage surface will generate dislocation emission. The intersection of the cleavage surface and emission surface is a transition line. Ductile to brittle transition occurs if the local $k$ passes this line.

C. Loading condition

In order to complete this model, we need to establish the loading condition in $k$-space. For uniaxial tensile loading, the geometry of crack tip deformation and the crack coordinate system is shown in Fig. 4, which corresponds to our TEM tensile specimens. According to Park and Ohr,$^{16}$ the applied stress intensity factor $K_i$ ($i = I, II, III$) due to applied stress, $\sigma_a$, for each mode of loading may be written as

$$K_I = \nu^2\sqrt{\pi c} \sigma_a$$
$$K_{II} = \nu\sqrt{\pi c} \sigma_a$$
$$K_{III} = \nu\sqrt{\pi c} \sigma_a$$  \hspace{1cm} (11)

where $u$, $v$, and $w$ are the direction cosines of tensile axis with respect to the crack coordinate system and can be described as

\[ u, v, w \]

\[ \sigma_a \]

\[ CD \]

\[ \beta \]

\[ \theta \]

\[ \alpha \]

\[ FN \]

\[ CF \]

\[ \sigma_a \]

FIG. 3. The emission surface and the cleavage surface in the $k$-space.

FIG. 4. Geometry of crack tip deformation and crack coordinate system for a TEM specimen.
$$u = \cos \beta$$

$$v = \cos \alpha \sin \beta$$

$$w = -\sin \alpha \sin \beta$$

(12)

where $\alpha$ is the angle between the crack front (CF) and the foil normal (FN) and $\beta$ is the angle between the crack direction (CD) and the tensile axis (TA). Experimentally, it is usually difficult to define the crack plane but for an intergranular crack, it becomes easy since the crack plane is the grain boundary plane itself. By doing this, we have added a loading line in $k$-space, Fig. 5. The line direction is given by $(K_i:K_{II}:K_{III})$. This approach is important because we can describe the loading condition and discuss crack behaviors without knowing the magnitude of the applied stress, which is very difficult to measure in TEM experiments.

For a certain material, the emission surface and cleavage surface are fixed if crack geometry and slip system are chosen. As the loading increases, the stress intensity factors, both applied $K_i$ and local $k_l$, keep increasing along the loading line until emission surface is reached, and then dislocation emission occurs. The dislocation emitted will shield the crack tip. Thus, the local $k$ decreases and emission ceases. As the applied $K$ is increased further, the local $k$ may reach the emission surface again and more dislocations are emitted. Because the three components of shielding, $k_{III}$, and that of applied, $K_i$, are not in the same ratio, the drop of local $k$ is not along the initial loading line. Therefore the second emission point on the emission surface may not coincide with the first one. Thus the local $k$ separates from the applied $K$ and moves along the emission surface. Lin and Thomson have shown that mode III shielding does not affect $k_i$. For a certain crack geometry and loading condition, if

$$\frac{k_{II}^P}{K_{III}} > \frac{k_{II}^P}{K_i}$$

(13)

we can expect that the $k_l$ component will increase as the number of emitted dislocations increases. Therefore the local $k$ will move toward the $k_{III}$ axis and meet the transition line somewhere on the emission surface, thus causing brittle crack propagation. The local $k$ reduces immediately during crack growth and the emission condition is re-established, as the effect of the shielding dislocations decreases when the crack tip moves into undeformed material. Therefore, as the applied $k$ increases, brittle crack propagation and dislocation emission will alternate.

The influence of grain boundary segregation is understandable in this model because the segregation will change the position of the cleavage plane in $k$-space (Fig. 5). The smaller the $k_{III}$ is, the fewer the emitted dislocations are needed in order for $k_{III} = k_i$. If the $k_{III}$ is so small that for certain loading conditions $k_i$ will reach the cleavage plane before it reaches the emission plane, the crack will propagate without any dislocation emission. In many cases, this complicated model can be simplified by ignoring a component of $k$ which has a small contribution to the local $k$-field. Therefore, the three-dimensional $k$-space degenerates into a two-dimensional plane, which leads to a simple picture and is easy to understand.

### III. EXPERIMENT AND RESULTS

In order to examine the theoretical model, in situ TEM experiments have been performed. Polycrystalline samples of molybdenum (99.8% with 36 ppm C, 24 ppm O, and 600 ppm W) have been chosen, since it has been shown that Mo polycrystals have intrinsic intergranular brittleness and it is relatively easy to get intergranular cracks. The specimens are in the form of a sheet approximately 3 mm x 6.6 mm in size and 0.2 mm thick with two pinholes. The specimens are annealed at 2000 °C for 2 h in order to get a uniform and dislocation-free structure with grain size about 50 µm, and the specimens then are electropolished in a tenu-pol unit in a solution of 14% H₂SO₄ + 86% C₂H₄OH at −10 °C.

In situ fracture experiments are carried out in an electron microscope in order to observe the behavior of the intergranular cracks directly. Kikuchi patterns are taken from both sides of intergranular cracks to determine the crystallographic details of the grain boundaries. An analytical procedure based on the methods developed by Chen and King has been established, by which misorientation, crack plane, crack direction, tensile axis, dislocation line direction, Burgers vector, and
slip plane can be characterized with high accuracy from Kikuchi patterns.

When stress was applied to a specimen, cracks were usually initiated at the edge of the polishing hole and propagated rapidly into the specimen. Many of the cracks were transgranular, because the orientation of the tensile axis was not favorable to grain boundary fracture. However, by careful loading, several intergranular cracks were obtained.

Figure 6 is a crack along a grain boundary which was near the \( \Sigma 19 \) misorientation. A dislocation array was observed on a slip plane which is inclined to the crack plane. The slip system was identified as \([101]-[111]\). The dislocation density was higher near the crack tip and decreased away from the crack tip. The dislocations were, therefore, in the form of an inverse pileup. Dislocations moved quickly away from the crack tip to join the dislocation array in the plastic zone, and the next dislocation started to initiate at the crack tip. Between them was a dislocation free zone (DFZ). The length of DFZ at this point was about 0.6 \( \mu \)m. This distribution could be expected according to the theory of crack-dislocation interaction.\(^{18}\) As the applied force increased, more dislocations were generated (Fig. 7). When they joined the pileup, the dislocations then moved very slowly as a group. The emission stopped after a certain number of dislocations were generated. The cessation of dislocation emission was followed immediately by brittle crack propagation, which is shown in Fig. 8. It was noted that when the crack moved away, some dislocations nearer to crack returned to the crack and annihilated there (Fig. 8). This crack finally stopped at a triple point (Fig. 9). The fracture surface was not flat. The height of steps on the crack surface corresponded accurately to the total Burgers vectors of the dislocations emitted and still remaining in the grain. The spacing of the steps gave the distance for each propagation.

According to the analysis of Kikuchi patterns, the crack and the loading geometry are given in Table I, where \( \alpha, \beta, \theta \) are as defined in Fig. 4, and \( \phi \) is the angle between the dislocation line and the Burgers vector. By knowing these data, the positions of the emission plane and the loading line in \( k \)-space, as well as the shielding effect by each dislocation in terms of shielding \( k Q \) can be calculated. In Table II, we have listed the values of the \( k \)'s for the components of all three modes.

As we can see, this is a mixed mode crack. However, mode II loading has little effect on dislocation emission since \( k Q \) is too large. The emission plane is nearly parallel to the \( k Q \) axis in the \( k \)-space. Therefore, the problem degenerates to a two-dimensional \((k_{1} - k_{11})\) plane (Fig. 10). In order to locate the cleavage line, Eq. (9) has been used with \( \gamma s = 3 \) J/m² and \( \gamma b = 1 \) J/m² as representative values.\(^{19,20}\) As the stress is applied, the applied \( K \) and the local \( k \) increase gradually along the loading line until the emission line is reached and dislocation emission occurs. The emission point, i.e., \((k_{1}, k_{11})\), can be obtained by solving the simultaneous equations of the loading line and the emission line.

\[
\begin{align*}
K_{11} &= \left( \frac{K_{11}}{K_{1}} \right) k_{1} \quad \text{(loading line)} \\
K_{11} &= -\left( \frac{k_{11}^{x}}{k_{11}^{y}} \right) k_{1} + k_{11}^{x} \quad \text{(emission line)}
\end{align*}
\]

The emitted dislocation will shield the crack after it leaves the crack tip, and the local \( k \) (plotted on the load line of Fig. 10) will drop to a new, shielded value,

\[
\begin{align*}
K_{1} &= K_{1} - k_{1}^{D} \\
K_{11} &= K_{11} - k_{11}^{D}.
\end{align*}
\]

In the experiment, when an emission event occurs, the external load, \( K_{s} \), continues to rise along a new load line, as shown in Fig. 10, until the emission condition is satisfied again, and the process repeats. As additional
The emission point for a given total $k_I^p$ and $k_{III}^p$ is obtained by combining (18) and (16). Eliminating $k_{III}$ from these two equations yields

$$k_I = \frac{K_{III}}{k_{III}^P} \left( \frac{\eta}{K_I} \right) k_I^P$$

(19)

where $\eta = k_{III}^P/k_I^P$. This equation determines the amount of shielding required before the system can cleave, that is, when $k_I = k_k$.

The direction of the drift of the emission point on successive emissions is crucial to this argument. This direction is given by the sign of the derivative, $dk_I/dk_I^P$, and for cleavage to occur the derivative must be positive.

$$\frac{dk_I}{dk_I^P} = \frac{\eta - K_{III}}{K_I} \frac{k_{III}^P}{K_I + k_{III}^P}$$

(20)

For the derivative to be positive, $\eta > K_{III}/K_I$. This condition is valid for the particular configuration studied, as shown in Table II, so our results are self-consistent.

From these equations, we have also calculated the total number of dislocations required in order to achieve cleavage, and found that 240 are needed, assuming that the spacing between the emitted dislocations is uniform. As we see from Fig. 6, the shielding comes mainly from two dislocation arrays which are near the crack tip. The number of dislocations counted in these arrays is 150, which is excellent agreement.

IV. DISCUSSION

The present study provides direct evidence for excellent agreement between the theory of dislocations and cracks and experiments on intergranular fracture. Furthermore, these results can be extended to explain embrittlement by grain boundary segregation. As we mentioned before, the main dilemma of the Orowan postulate is how the fracture work, $\gamma$, but not the plastic work, $\gamma_p$, which is much larger than $\gamma$, controls the properties of materials.

Considering that a crack propagates with dislocation emission in a thin film TEM specimen, the plastic work, $w_p$, associated can be estimated in three terms,

$$w_p = w_d + w_f + w_t$$

(21)

where $w_d$ represents the self energy of dislocations, $w_f$ is due to the lattice friction stress, and $w_t$ arises because of the step formation on the film surfaces as the dislocations move.23 In order, the three terms are
FIG. 9. Steps remain on the fracture surface. The height of steps corresponds to the total Burgers vectors of dislocations emitted and still remaining in the grain.

\[
wd = \left( \frac{\mu b^2 \ln \frac{R}{r_0}}{r_0} \right) \frac{tm}{l \cos \psi}
\]

\[
w_f = \sum_i \frac{\tau_i b t_i}{r_i}
\]

\[
w_i = \sum_i \frac{2 \gamma_i (b \cdot n)}{l} r_i
\]

Where \( t \) is the thickness of the specimen, \( \psi \) is the angle between foil normal and dislocation line, \( l \) is the spacing of dislocation arrays, \( m \) is the average number of dislocations in each array, \( \tau \) is the friction stress for single crystal, \( \gamma \) is the surface energy, \( n \) is the foil normal of specimen, and \( r_i \) is the glide distance of dislocation \( b_i \).

Thus, in terms of \( \gamma_p \), Eq. (22) becomes

\[
\gamma_p = \frac{w_p}{t} = \frac{\mu b^2}{l \cos \psi} \ln \frac{R}{r_0} m
\]

\[+ \left( \tau_b + \frac{2 \gamma (b \cdot n)}{t} \right) \frac{\sum_i r_i}{l} (23)
\]

The term in the parentheses of the equation represents the resistant force on a gliding dislocation in a thin film specimen. By introducing an average glide distance \( \bar{r} \) and the average spacing of emitted dislocations \( \Delta r \) (assuming that the distribution of the dislocations is uniform and \( \bar{r} = \Delta rm/2 \)), Eq. (23) can be rewritten approximately as

\[
\gamma_p = \frac{w_p}{t} = \frac{\mu b^2}{l \cos \psi} \ln \frac{R}{r_0} m
\]

\[+ \left( \tau_b + \frac{2 \gamma (b \cdot n)}{t} \right) \frac{\Delta r}{2l^2} (24)
\]

Therefore, the plastic work is proportional to the square of \( m \), the number of emitted dislocations. For molybdenum, we take \( \gamma = 3 \text{ J/m}^2 \) and \( b = 2.7 \times 10^{-10} \text{ m} \). We choose the specimen thickness as \( R \) and \( b \) as \( r_0 \). Since the friction stress, \( \tau_i \), is difficult to determine, Dewald et al.\(^2\) have suggested that the critical resolved shear stress, \( \tau_{CRSS} \), for a single crystal could be used. A reasonable value of \( \tau_{CRSS} \) for Mo is 50 MPa\(^2\) at room temperature. Experimentally, we measured \( l = 1 \mu \text{m}, \Delta r = 0.1 \mu \text{m}, t = 200 \text{ nm}, \) and \( m \approx 100 \). The plastic work, \( \gamma_p \), becomes 15.42 J/m\(^2\), which is larger than the surface energy.

As we can see from Fig. 10, if the crack geometry and the loading condition are given, the number of emitted dislocation depends on the position of \( k \) which is a function of fracture energy, \( \gamma \), Eq. (9). If segregation of impurities causes a decrease of \( k \), fewer shielding dislocations are needed in order that \( k \) reaches \( k_\text{n} \), and

<table>
<thead>
<tr>
<th>Mode</th>
<th>( K_a/(\sqrt{\pi \epsilon} \sigma_a) )</th>
<th>( k_a(\times 10^6 \text{ N m}^{-3/2}) )</th>
<th>( k_p(\times 10^6 \text{ N m}^{-3/2}) )</th>
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<tr>
<td>I</td>
<td>0.473</td>
<td>28.11</td>
<td>11.48/\sqrt{\gamma}</td>
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<tr>
<td>II</td>
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<td>-151.78</td>
<td>-0.71 \sqrt{\gamma}</td>
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<tr>
<td>III</td>
<td>0.272</td>
<td>8.19</td>
<td>9.13/\sqrt{\gamma}</td>
</tr>
</tbody>
</table>


### Table I. Crack and loading geometry.

<table>
<thead>
<tr>
<th>Crack plane</th>
<th>Slip plane</th>
<th>Crack direction</th>
<th>Tensile axis</th>
<th>Foil normal</th>
<th>Crack front</th>
<th>Line direction</th>
<th>Burgers vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>(CP)</td>
<td>(SP)</td>
<td>(CD)</td>
<td>(TA)</td>
<td>(FN)</td>
<td>(CF)</td>
<td>(( \bar{b} ))</td>
<td>(b)</td>
</tr>
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<td>-0.827</td>
<td>-0.448</td>
<td>0.002</td>
<td>0.070</td>
<td>1.00</td>
</tr>
<tr>
<td>0.192</td>
<td>1.00</td>
<td>0.887</td>
<td>-0.529</td>
<td>-0.766</td>
<td>-0.707</td>
<td>-0.707</td>
<td>-1.00</td>
</tr>
<tr>
<td>( \theta = 74.1 )</td>
<td>( \beta = 52.5 )</td>
<td>( \alpha = -29.9 )</td>
<td>( \phi = 31.2 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIG. 10. Stability diagram for observed crack. As loading increases, local $k$ reaches emission line first and then oscillates along emission line until it meets cleavage line. The number of dislocations emitted can be given by calculating the number of oscillations.

the plastic work, $\gamma_p$, may drop significantly ($\gamma_p \propto m^2$). Figure 11 gives the relation of $\gamma_p$ and $\gamma$ for the observed crack.

As discussed by Dewald et al., the surface drag force is thickness dependent. As the thickness, $t$, increases, the surface drag force reduces and the friction force becomes more and more important. However, this variation does not change the physical configuration of present model, and also one may take any other resistant force in bulk systems into account. We believe similar mechanisms will also operate for bulk systems, as discussed by McMahon and Vitek. Thus, the plastic work should always be an increasing function of intrinsic surface energy. This point was made many years ago by Rice.

Comparing with the previous model proposed by Jokl, Vitek, and McMahon, the present model shows not only same tendency for $\gamma_p$ to change with $\gamma$ but also a minimum value of $\gamma$ for plastic deformation (Fig. 11).

This result is as one might intuit. When the reduction of $\gamma$ reaches a certain point, at which the local $k$ may meet the cleavage plane before the emission plane, the crack may propagate brittlely without any dislocation emission and the plastic work, $\gamma_p$, drops to zero. In addition, the sensitivity of $\gamma_p$ to $\gamma$ also depends on the loading condition. If more mode I component is applied, experimentally the crack plane tends to be perpendicular to the tensile axis and the loading line in Fig. 10 tends to $k_l$ axis, and the crack will show greater brittleness.

An important result following from the discussion relating to Eqs. (17)-(20) is that the transition from emission to cleavage depends on the generation of a mixed mode loading on the crack of the right amount. This, in turn, depends upon the differential (called $\eta$ in the paper), the loading conditions, and the relation between the cleavage plane and emission slip plane. Thus, we would expect to find boundary planes where cleavage will be favored from the outset, other planes where emission is initially favored, but where there is a cleavage transition for a critical number of emitted dislocations, and still other cases where the shielding will always favor emission. Also, in the case analyzed in the paper, we have only one active slip plane. Depending on the geometry of the boundary, it has been found that the emissions occur on both sides of the boundary (Zhang and King, unpublished results) simultaneously. Thus in a typical bulk situation, a very complicated situation will arise, governed by the boundary parameters, as well as by the considerations analyzed here. In general, then, intergranular brittleness will be enhanced by segregation of favorable impurities on the boundaries, but in detail, the process will be a very mixed bag of cleavage and deformation, where a quantitative prediction will be extremely difficult.

The effect of loading geometry is important. Even in highly embrittled materials, some grain boundaries may emit dislocations during crack propagation, and certain grain boundaries in otherwise ductile materials may undergo brittle fracture. Thus, observations of individual boundaries are of little value unless the loading geometry and slip geometry are specified. The effect of embrittling segregant is generally to move the cleavage surface so that the chance of a generating brittle fracture is increased for boundaries of random inclination to the stress axis. Brittle failure of a polycrystalline specimen will occur when a sufficient number of contiguous grain boundaries meet the conditions for brittle crack propagation.

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