Critical configurations for dislocation nucleation from crack tips

By G. Xu†, A. S. Argon‡
Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
and M. Ortiz
California Institute of Technology, Pasadena, California 91125, USA

[Received 25 January 1996 and accepted in revised form 16 June 1996]

Abstract
In the present paper, we analyse several activation configurations of embryonic dislocations nucleated from the tip of a cleavage crack. The activation configurations include nucleation on inclined planes, on oblique planes and on cleavage ledges and are treated within the classical framework of Peierls. A variational boundary integral method with an interplanar tension–shear potential developed earlier is used to solve for the saddle-point configurations of embryonic dislocation loops and their associated energies. Based on the assumption that the brittle-to-ductile transition in cleavage fracture is a nucleation-controlled process (as is expected to be the case in bcc transition metals such as α-Fe) the results of the calculations are used to estimate the brittle-to-ductile transition temperatures. It is concluded that only dislocation nucleation on cleavage ledges furnishes realistic values of the transition temperature. The homogeneous nucleation of dislocations on either inclined or oblique planes requires transition temperatures well above the melting point. This implies that nucleation of dislocations from a crack tip in intrinsically brittle crystals is only possible at local crack front heterogeneities such as cleavage ledges, and that the homogeneous nucleation of dislocations from a straight crack front is not possible. This conclusion is supported by the experimental observation that dislocation nucleation from a crack tip is a rare event which occurs preferentially on heterogeneities.

§ 1. Introduction
The abrupt transition in the fracture behaviour of some materials from ductile to brittle (or brittle to ductile) with small changes in temperatures remains a key concern in many structural applications. This phenomenon has been viewed from two different perspectives. In applications where the ductility of a material is relied upon, the transition is viewed as the sudden onset of brittleness. The complex phenomena associated with a ductile-to-brittle (D–B) transition in polycrystalline steels, involving as a key step the deformation-induced production of propagating cleavage microcracks, have been studied experimentally in detail (Hahn, Averbach, Owen and Cohen 1959) and have been modelled theoretically to some degree (Stroh 1954, 1955, 1957, Lin, Evans and Ritchie 1986, 1987).

†Present address: TerraTek, Inc., 420 Wakara Way, Salt Lake City, Utah 84108, USA.
‡Author for correspondence.
By contrast, in the brittle-to-ductile (B–D) transition a competition is believed to take place between cleavage fracture and plastic shielding, with eventual blunting of the propagating cleavage crack either by dislocation emission from the crack tip or by background plastic relaxation. The crack arrest and eventual blunting mechanism depends upon temperature, loading rate and the ability of the vicinity of the crack tip to undergo plastic deformation. This B–D transition has been explained either in the static framework of a stationary crack (St John 1975, Brede and Haasen 1988, Hirsch, Roberts, Samuels and Warner 1989a, Hirsch, Samuels and Roberts 1989b, George and Michot 1993), or in the dynamical framework of the arrest of a propagating cleavage crack with increasing temperature and decreasing loading rate (Gilman, Knudsen and Walsh 1958, Brede, Hsia and Argon 1991, Hsia and Argon 1994).

Models of the B–D transition just described (Kelly, Tyson and Cottrell 1967, Rice and Thomson 1974) have led to the notion of intrinsically ductile materials (most fcc metals, some hcp metals and bcc tantalum), which do not cleave and do not undergo a fracture transition. The remaining solids, including most bcc transition metals, are intrinsically brittle, that is cleavable, and are therefore susceptible to a B–D transition. The fundamental supposition is that, while background plastic relaxations can suppress the transition temperature, the ultimate arbiter of the transition is the ability, or the lack of it, of the crack tip to emit dislocations that can shield the crack and trigger widespread plastic deformation before the crack can propagate by cleavage.

The accumulating experimental evidence on Si (St John 1975, Brede and Haasen 1988, Hirsch et al. 1989a, b, George and Michot 1993) and the insight provided by the most recent modelling studies (Schöck and Püschi 1991, Rice and Beltz 1994, Xu, Argon and Ortiz 1995a) suggest that the activation configuration of a dislocation embryo is in the form of a double kink. This observation permits the identification of two distinct types of B–D transition. In the bcc transition metals where barriers to kink mobility are low, the B–D transition is likely to be governed directly by the formation of dislocation embryos at the crack tip, resulting in a nucleation-controlled transition. By contrast, in semiconductors and compounds the observational evidence suggests (Yonenaga, Onose and Sumino 1987, Maeda and Yamashita 1989, Sumino 1989, Yonenaga et al. 1989, Yonenaga and Sumino 1989), and modelling verifies (Bulatov, Yip and Argon 1995), that kink mobility is hindered by substantial energy barriers, rendering the B–D transition controlled by dislocation mobility away from the crack tip.

Ultimately, a full understanding of the nucleation-controlled or the mobility-controlled B–D transitions must come from atomistic models of the formation and outward propagation of the dislocation embryo at the crack tip. Before such modelling can be meaningfully attempted, much progress can be made by recourse to hybrid continuum-atomistic approaches (Schöck and Püschi 1991, Rice, Beltz and Sun 1992, Rice and Beltz 1994, Xu et al. 1995a) based on the use of a Peierls interplanar potential (Peierls 1940, Nabarro 1947, Foreman, Jaswon and Wood 1951). In a recent development of this technique by Xu et al. (1995a), an additional surface production resistance was introduced into the interplanar potential, and the appropriate saddle-point configurations of the dislocation embryo were determined by recourse to a variational boundary integral method advanced by Xu and Ortiz (1993). Xu et al. (1995a) concluded that the energetics of dislocation embryo formation on inclined slip planes containing the crack tip, against an additional surface
production resistance, is quite unfavourable and does not explain the known B–D transition temperatures. On this basis, it was conjectured that nucleation may be more favourable on oblique slip planes or, as numerous experimental observations have suggested, may occur heterogeneously at the crack front (Chiao and Clarke 1989, Samuels and Roberts 1989, George and Michot 1993). These dislocation nucleation mechanisms are investigated in this communication.

In §2 we begin by describing the three alternative mechanisms to be appraised, namely nucleation on inclined planes, on oblique planes and on cleavage ledges on the crack front. Following a brief description in §3 of the fundamental methodology employed in calculations, the three nucleation mechanisms are analysed in turn in §4. In particular, the B–D transition temperature is estimated from the calculated activation energies. We find that only nucleation on cleavage ledges leads to realistic estimates of the transition temperature. In §5 we endeavour to put our findings in general perspective.

§ 2. DISLOCATION NUCLEATION MODES

Several alternative modes of dislocation nucleation from crack tips have been contemplated in the past. The modes differ mainly in the relative geometry of the slip plane, the crack surface and the crack front. The configurations considered include nucleation of dislocations on the extension of the crack surface (fig. 1(a)), nucleation on an inclined plane containing the crack front (fig. 1(b)), nucleation on an oblique plane (fig. 1(c)) and nucleation on a cleavage ledge (fig. 1(d)).

Alternative modes of dislocation nucleation from a crack tip.
Using the Peierls model of interplanar slip, Rice (1992) and Rice et al. (1992) analysed the athermal nucleation of straight dislocations on the extension of the crack surface under pure mode II and mixed mode loading (fig. 1(a)). From this pioneering analysis, Rice et al. concluded that nucleation occurs when the crack tip energy release rate attains the unstable stacking energy of the slip plane, at which point half a dislocation core has been formed at the crack tip. Rice and Beltz (1994) have performed a three-dimensional perturbation analysis of dislocation nucleation on the extension of the crack surface which gives the saddle-point configurations and their dependence on the applied energy release rate. Rice and Beltz (1994) also compared their analysis with an earlier approximate calculation of Schöck and Püschl (1991). Xu et al. (1995a) have applied a variational boundary integral method to the same problem. In the Xu et al. (1995a) approach, the tension–shear potential is modified so as to account for surface production resistance. The results of these calculations indicate that, with the incorporation of surface production, homogeneous nucleation of dislocations on inclined planes is unlikely. This observation notwithstanding, in the interest of completeness we revisit this mode of nucleation in § 4.2 for a particular configuration pertaining to α-Fe.

Experimental observations (Burns and Webb 1970a, b), and the consideration of peak stress levels at the crack tip (Argon 1987), point to dislocation nucleation on oblique planes, such as shown in fig. 1(c), as a likely dislocation nucleation mechanism. This mechanism has the additional advantage of involving nearly no free surface production. Moreover, as observed by Burns and Webb (1970a, b) and pointed out by Argon (1987), the nucleated dislocation can extent self-similarly as a loop attached to the crack tip, which results in steadily increasing shielding. These favourable features notwithstanding, approximate analyses carried out by Argon (1987) and A. S. Argon and D. Deng (1987, unpublished research available on request) suggest that this mode of nucleation also fails to furnish realistic values of the transition temperature. This conclusion is reinforced by the more accurate analysis of § 4.3.

The nucleation modes just described are examples of homogeneous nucleation, inasmuch as all points along the crack front are accorded an equal probability of being a nucleation site. However, numerous experiments (Chiao and Clarke 1989, Samuels and Roberts 1989, George and Michot 1993) have shown that actual dislocation nucleation events are rare and occur only at special sites along the crack front, namely at heterogeneities. Extensive documentation of these special sites by George and Michot (1993) has shown them to be mostly cleavage ledges. These ledges form frequently in response to local deviations of the crack driving force away from the crack plane. In cases in which the local stress intensity factor on the cleavage ledge has a substantial $K_{III}$ component, a dislocation of screw type can be nucleated at the ledge without surface production. Moreover, a usually present substantial $K_I$ component acting across the plane of the ledge should further promote this mode of nucleation. The analysis presented in § 4.4 reveals that, of all the modes considered, dislocation nucleation on ledges is the most energetically favourable and that which leads to the most realistic estimates of the B–D transition temperature. For definiteness, we restrict our attention to α-Fe and the geometries displayed in fig. 2.

The preferred growth direction of a {100} cleavage crack in α-Fe can be ascertained by computing the dependence of the energy release rate on the crack front direction within the framework of anisotropic linear elasticity. For pure mode I
Alternative modes of dislocation nucleation from crack tips in α-Fe: (a) inclined plane; (b) oblique plane; (c) cleavage ledge.

loading, the analysis consigned to the Appendix reveals that the energy release rate is minimum for a crack front in the (110) direction, which is therefore taken to define the most likely crack front direction. Figure 2 displays the crystallography of the nucleation modes: a \( \frac{1}{2}[111] \) dislocation nucleating in an inclined (112) plane in fig. 2(a), a \( \frac{1}{2}[\bar{1}11] \) dislocation nucleating in an oblique (112) plane in fig. 2(b) and a \( \frac{1}{2}[\bar{1}11] \) dislocation nucleating in a cleavage ledge on the (112) plane in fig. 2(c). In our estimation, these cases represent the most likely configurations for each nucleation mode.

§ 3. METHOD OF ANALYSIS

The analysis builds on the recent developments of Xu et al. (1995a), who have extended the scope of the variational boundary integral method of Xu and Ortiz (1993) to encompass problems of dislocation nucleation from atomically sharp cracks. In this model, a slip plane connected to the crack is viewed as an extension of the crack surfaces with a nonlinear interlayer potential acting across it. Thus the crack and the slip plane on which the dislocation nucleates are jointly regarded as a three-dimensional crack system embedded in the linear elastic solid. The interlayer potential acting across the slip plane is modelled by combining the universal binding energy relation of Rose, Ferrante and Smith (1981) with a skewed shear resistance profile (Foreman et al. 1951). The interplanar displacements and the crack-opening displacements are represented by a continuous distribution of curved dislocations. This approach introduces no artificial discontinuity between the elastic crack opening and inelastic interplanar slip and separation. The technique has been described in complete detail by Xu and Ortiz (1993) and Xu et al. (1995a). In this section, we
briefly outline those aspects of the method which are pertinent to the treatment of the special activation configurations described in §2.

We consider a semi-infinite cleavage crack and a slip plane intersecting the crack front. The crack–slip plane system is loaded remotely by a \( K \) field. The crystallographic slip plane is chosen to be the most advantageous for slip. As the driving force increases, an embryonic dislocation forms progressively until it reaches an unstable equilibrium configuration. The load corresponding to this unstable configuration is defined as the critical driving force for nucleation. The embryonic dislocation profile is characterized as a distribution of interplanar inelastic displacements, defined by Rice (1992) as

\[
\delta = A - A^c,
\]

where \( A \) and \( A^c \) denote the total and elastic interplanar displacements respectively. The opening displacement \( u \) of the crack surface, including the inelastic displacements along the slip plane, can be written as

\[
u = \bar{u} + \delta,
\]

where \( \bar{u} \) represents the standard \( K \) displacement field for a reference semi-infinite crack. The term \( \bar{u} \) matches the behaviour of the crack-opening displacements far away from the tip. Consequently, the additional term \( \delta \) modifying \( \bar{u} \), which is the primary unknown in the analysis, is expected to decay rapidly to zero with distance away from the crack tip. In this manner, \( \delta \) can be restricted to a finite domain \( \hat{S}_c \cup \hat{S}_s \), where \( \hat{S}_c \) lies on the crack surface and \( \hat{S}_s \) on the slip plane, connected to the crack front.

Following the procedure introduced by Xu et al. (1995a) and Xu and Ortiz (1993), the potential energy of the whole system can be written in the form

\[
\Pi[\bar{u} + \delta] = W[\bar{u} + \delta] + V[\delta] = W_1[\bar{u}] + W_1[\delta] + W_2[\bar{u}, \delta] + V[\delta],
\]

where we identify \( W_1[\bar{u}] \) as the elastic strain energy of the system, free of inelastic modifications, \( W_1[\delta] + V[\delta] \) as the self-energy of the system of inelastic modifications consisting of the distributed dislocations and the interplanar interaction energy on the slip plane, and \( W_2[\bar{u}, \delta] \) is the interaction energy of the initial unmodified system with the second system of modifications. Of these energies those of relevance in the variational approach are those that depend on the unknown inelastic modification \( \delta \). They have the forms given below. The self-energy of the inelastic modification is given as

\[
W_1[\delta] = \frac{\mu}{4\pi} \int_{\hat{S}_c + \hat{S}_s} \int_{\hat{S}_s + \hat{S}_c} \left[ \frac{\mathbf{e}_i \cdot (\mathbf{n} \times \nabla \delta_j)_2}{R} \right] \mathbf{e}_j \cdot (\mathbf{n} \times \nabla \delta_i)_1 \ dS_1 \ dS_2
\]

\[
- \frac{\mu}{8\pi} \int_{\hat{S}_s + \hat{S}_c} \int_{\hat{S}_c + \hat{S}_s} \left[ \frac{\mathbf{e}_i \cdot (\mathbf{n} \times \nabla \delta_j)_1}{R} \right] \mathbf{e}_j \cdot (\mathbf{n} \times \nabla \delta_i)_2 \ dS_1 \ dS_2
\]

\[
+ \frac{\mu}{8\pi(1 - \nu)} \int_{\hat{S}_s + \hat{S}_c} \int_{\hat{S}_c + \hat{S}_s} \left[ \mathbf{e}_i \cdot (\mathbf{n} \times \nabla \delta_j)_1 \right] \cdot \mathbf{T} \cdot \left[ \mathbf{e}_j \cdot (\mathbf{n} \times \nabla \delta_j)_2 \right] \ dS_1 \ dS_2,
\]

where \((.)_1\) and \((.)_2\) denote two different points on the domain \( \hat{S}_c \cup \hat{S}_s \), \( R \) is the distance between these two points, \( \mathbf{e}_i, i = 1, 2, 3 \), are Cartesian basis vectors, \( \mathbf{n} \) is the normal vector to the crack surface or the slip plane and \( \mathbf{T} \) is a tensor with components
The interaction energy between the elastic crack field and the inelastic modifications is

\[ W_2[\mathbf{u}, \delta] = K_1 Q_1[\delta] + K_{II} Q_{II}[\delta] + K_{III} Q_{III}[\delta], \]

where

\[ Q_1[\delta] = \int_{S_c+S_A} \mathbf{n} \cdot \mathbf{\sigma}_1 \cdot \delta \, dS, \]

\[ Q_{II}[\delta] = \int_{S_c+S_A} \mathbf{n} \cdot \mathbf{\sigma}_{II} \cdot \delta \, dS, \]

\[ Q_{III}[\delta] = \int_{S_c+S_A} \mathbf{n} \cdot \mathbf{\sigma}_{III} \cdot \delta \, dS, \]

and \( \mathbf{\sigma}_1, \mathbf{\sigma}_{II} \) and \( \mathbf{\sigma}_{III} \) are stresses of the standard \( K \) fields in modes I, II and III respectively, for unit stress intensity factor. The integration is partly extended over the real crack surface since the front of the reference semi-infinite crack is actually located some distance away from the physical crack front. This treatment permits the use of a non-singular Dugdale–Barenblatt crack as a reference crack to improve systematically the quality of the numerical solution (Xu and Ortiz 1993). Finally, the potential energy of the interplanar inelastic deformation on the slip plane is

\[ V[\delta] = \int_{S_t} \Phi[\delta] \, dS, \]

where \( \Phi[\delta] \) is an interplanar potential defined per unit area of the slip plane. It is possible to model the general potential \( \Phi[\delta] \) with shear displacements allowed in all directions on the slip plane. However, atomistic simulations have shown that displacements and the attendant shear resistance take place predominantly in the direction of the dominant Burgers vector (Yamaguchi, Vitk and Pope 1981, Sun et al. 1991, Juan and Kaxiras 1996). Therefore we adopt the constrained displacement hypothesis of Rice (1992) and Sun et al. (1994), whereby the interplanar shear displacement \( \Delta_r \) is constrained to be aligned with the Burgers vector direction. The shear separation resistance \( \tau \) and tension separation resistance \( \sigma \) follow from the inelastic shear displacements \( \delta_r \) and tensile separation displacement \( \delta_\theta \) through the relations (Beltz and Rice 1991, Xu et al. 1995a)

\[ \delta_r = \Delta_r - \frac{h}{\mu} \tau(\Delta_r, \Delta_\theta), \]  \hspace{1cm} (9a)

\[ \delta_\theta = \Delta_\theta - \frac{h}{c} \sigma(\Delta_r, \Delta_\theta), \]  \hspace{1cm} (9b)

and

\[ \tau(\Delta_r, \Delta_\theta) = A(\Delta_\theta) \left[ \sin \left( \frac{2\pi \Delta_r}{b} \right) + \frac{\beta - 1}{2} \sin \left( \frac{4\pi \Delta_r}{b} \right) \right], \]  \hspace{1cm} (10a)

\[ \sigma(\Delta_r, \Delta_\theta) = B(\Delta_r) \left( \frac{\Delta_\theta}{L} - C(\Delta_r) \right) \exp \left( - \frac{\Delta_\theta}{L} \right), \]  \hspace{1cm} (10b)

with
\[
A(\Delta \theta) = \frac{\pi \gamma^{(u)}_{\text{us}}}{b} \left[ 1 + \frac{1}{q} \frac{\Delta \theta}{L} \right] \exp \left( -\frac{\Delta \theta}{L} \right), \\
B(\Delta_r) = \frac{2\gamma_s}{L} \left\{ 1 - \frac{q}{1-p} \left[ \sin^2 \left( \frac{\pi \Delta_r}{b} \right) + \frac{\beta-1}{4} \sin^2 \left( \frac{2\pi \Delta_r}{b} \right) \right] \right\}, \\
C(\Delta_r) = \frac{2\gamma_s}{L} \frac{p(1-q)}{1-p} \left[ \sin^2 \left( \frac{\pi \Delta_r}{b} \right) + \frac{\beta-1}{4} \sin^2 \left( \frac{2\pi \Delta_r}{b} \right) \right],
\]

\[
q = \frac{\gamma^{(u)}_{\text{us}}}{2\gamma_s}, \\
p = \frac{\Delta \theta^*}{L},
\]

where:

- \( \mu \) is the shear modulus,
- \( c \) is the uniaxial strain elastic modulus,
- \( b \) is the magnitude of Burgers vector,
- \( h \) is the interatomic layer spacing,
- \( L \) is the interplanar tensile displacement at \( \sigma = \sigma_{\text{max}} \),
- \( \gamma^{(u)}_{\text{us}} \) is the unrelaxed unstable stacking energy,
- \( \gamma_s \) is the surface energy,
- \( \Delta_r \) is the total interplanar shear displacement,
- \( \Delta_{\theta} \) is the total interplanar normal displacement, and
- \( \Delta_{\theta}^* \) is the relaxed interplanar tensile displacement at \( \sigma = 0 \) in the saddle-point configuration and
- \( \beta \) is the skewness parameter in the interplanar shear resistance.

A traction–displacement relation including the effect of surface production on an inclined slip plane at the crack tip has been proposed by Xu et al. (1995a). The material constants for \( \alpha \)-Fe used in calculations are taken from table 1 of Xu et al. (1995a) and are reproduced here for convenience in table 1.

The unknown displacements \( \delta \) follow by rendering the potential energy \( \Pi[\mathbf{u} + \delta] \) stationary. This is achieved by discretizing the integral equation with six noded elements distributed on the crack surface. The nonlinear equations are solved by a Newton–Raphson iteration. The saddle-point configurations are activated by introducing a small perturbation into the system at the bifurcation point, based on the solution of a first-order eigenvalue problem if necessary. Solutions are obtained by

<table>
<thead>
<tr>
<th>Slip system</th>
<th>( T ) (K)</th>
<th>( \mu ) (10^2 MPa)</th>
<th>( c )</th>
<th>( \gamma^{(u)}_{\text{us}} ) (J m(^{-2}))</th>
<th>( 2\gamma_s ) (J m(^{-2}))</th>
<th>( \beta )</th>
<th>( p )</th>
<th>( q )</th>
<th>( L/b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{1}{2}<a href="110">111</a> )</td>
<td>4.2</td>
<td>0.756</td>
<td>3.125</td>
<td>0.517</td>
<td>3.33</td>
<td>2.25</td>
<td>0.217</td>
<td>0.155</td>
<td>0.187</td>
</tr>
<tr>
<td>( \frac{1}{2}<a href="112">111</a> )</td>
<td>4.2</td>
<td>0.756</td>
<td>3.125</td>
<td>0.581</td>
<td>3.80</td>
<td>1.74</td>
<td>0.210</td>
<td>0.153</td>
<td>0.215</td>
</tr>
</tbody>
</table>
recourse to interplanar displacement control achieved through the introduction of Lagrange multipliers.

§ 4. DISLOCATION NUCLEATION ANALYSIS

4.1. Three modes of nucleation

In this section we analyse the nucleation of dislocations from a cleavage crack in α-Fe as processes typical of bcc metals in which kink mobility is high. We consider the three competing mechanisms discussed in § 2, namely nucleation on an inclined plane, on an oblique plane, and on a cleavage ledge. The principal objective of the calculations is the determination of the saddle-point configurations and the dependence of the corresponding activation energies on the crack driving force. These results are subsequently used to estimate the B–D transition temperatures for each geometry. The geometry furnishing the most realistic value of the B–D transition temperature may be reasonably identified with the preferred nucleation configuration in α-Fe.

4.2. Nucleation of dislocations on the inclined plane

The previous analysis of Xu et al. (1995a) showed that nucleation of dislocations on the inclined planes is quite unlikely for most crystals. Nevertheless, for comparison with the other modes of nucleation, we shall re-examine the nucleation of dislocations on the inclined plane (112) in α-Fe as depicted in fig. 2(a).

We begin by solving the saddle-point configuration of a dislocation under a pure mode II type of loading. The crack surface on the (001) plane probes the (112) slip plane with the crack front being parallel to the [110] direction. Two representative saddle-point configurations of the dislocation embryo under normalized loading levels $G_{II}/G_{Hed}$ of 0.75 and 0.50 are illustrated in fig. 3 and fig. 4 respectively. The dependence of the activation energy on the crack front driving force from a series of such solutions is plotted in fig. 5.

![Fig. 3](image)

$G_{II}/G_{Hed} = 0.75$

The saddle-point configuration at $G_{II}/G_{Hed} = 0.75$ under mode II loading.
The saddle-point configuration at $G_{II}/G_{IIed} = 0.50$ under mode II loading.

The activation energy for dislocation emission under pure mode II loading.

To obtain remote mode I loading, we assume that the nucleation process is essentially equivalent to the mode II crack case under a loading equal to the effective stress intensity factors on the inclined plane, which are,

$$K_1^{eff} = K_1 \cos^3 \left(\frac{\theta}{2}\right),$$  \hspace{1cm} (13a)

$$K_{II}^{eff} = K_1 \cos^2 \left(\frac{\theta}{2}\right) \sin \left(\frac{\theta}{2}\right).$$  \hspace{1cm} (13b)
More precisely, these stress intensity factors are those at the tip of a small crack emanating from the crack tip in the direction of the slip plane ( Cotterell and Rice 1980). The critical mode I loading for nucleation of a straight dislocation in two dimensions on the inclined plane can then be estimated from the analysis of Rice using eqn. (13b) and is given by
\[
\frac{G_{\text{Ikd}}}{G_{\text{IC}}} = \frac{8}{(1 + \cos \theta) \sin^2 \theta \, 2\gamma_\text{s}}.
\] (14)

However, this estimate which considers neither tension softening nor surface production resistance underestimates the energetics of the configuration for most transition metals and intermetallics (Xu et al. 1995a) because, while the tension softening does make nucleation somewhat easier, the surface production resistance makes it comparatively much more difficult. The dependence of the activation energy of the actual three-dimensional saddle-point configuration analysis on the remote mode I loading is shown in fig. 6, as rescaled from fig. 5 through eqn. (13b).

4.3. Nucleation of dislocations on the oblique plane

As remarked in §2, dislocation nucleation on oblique planes has been put forth as a likely mode of nucleation. However, the capability required for the analysis of this mechanism had been heretofore unavailable. Approximate analyses based on the consideration of perfect dislocations and the introduction of a core cut-off radius have led to estimates of the B–D transition temperatures several orders of magnitude higher than what is experimentally observed, prompting suggestions that nucleation should involve fractional dislocations (Argon 1987).

In this section, we provide a direct analysis of the formation of dislocation embryos on oblique planes in α-Fe. A comparison of resolved shear stresses on all

![Fig. 6](image)

Dependence of the activation energy for dislocation nucleation on the inclined \{112\} planes on the remote mode I loading.
potentially active slip systems points to the configuration in fig. 2(b) as the most favourable for nucleation. In calculations, we artificially constrain the cleavage plane from propagating to enable the computation of the critical driving force for dislocation nucleation. If the resulting athermal critical driving force is less than $G_{lc}$ for cleavage, the crystal is intrinsically ductile. Contrariwise, if the critical driving force is greater than that for cleavage, the crystal is cleavable or intrinsically brittle. However, on the verge of crack propagation by cleavage, a dislocation can still be nucleated through thermal activation. The calculation of the activation energy for such thermally assisted dislocation nucleation is therefore of primary interest.

Figure 7 shows the geometry of the problem and the mesh used in the analysis. A close-up view of a typical saddle-point configuration of an embryonic dislocation loop emanating from the crack tip is shown in fig. 8 for the geometry of fig. 2(b). The calculated dependence of the activation energy on the crack driving force near the athermal threshold is shown in fig. 9. The critical driving force at the athermal threshold and the attendant activation energies are so high that they render the nucleation mechanism highly improbable. The calculation was discontinued at $G_1/G_{lc} = 1.6$ when the improbability of the mechanism had become amply clear. The activation energy at $G_1/G_{lc} = 1.0$ can be estimated by extrapolation, which provides an adequate basis for reaching a firm negative conclusion vis-à-vis the likelihood of the mechanism. One factor which contributes to rendering the mechanism ineffective is the fact that the resolved shear stress decays away from the crack tip in all directions, making the area-averaged shear stress smaller than that on the inclined plane.

It should be noted that in the above analysis the inelastic displacements across the slip plane were treated as total displacements for computational convenience. This tends to underestimate slightly the activation energy as will be demonstrated subsequently. Moreover, we have only considered two-sided activation configura-

Fig. 7

Mesh used in the analysis of dislocation nucleation on an oblique plane in α-Fe for the geometry shown in fig. 2(b).
Dislocation nucleation from crack tips

Fig. 8

The saddle-point configuration of a dislocation embryo emitted from the crack tip on an oblique plane in the interior.

Fig. 9

Activation energy for dislocation nucleation on an oblique plane in the interior (---, ---) and near a free surface (- - -).

Tions in our analysis. One-sided configurations, in which dislocation embryos expand primarily on one side of the oblique plane, might conceivably require lower activation energies. However, in view of the results just described, it seems unlikely that this reduction in the activation energy should be sufficient to justify a detailed analysis of one-sided configurations.
The above analysis establishes convincingly that nucleation of dislocations on oblique planes in the interior of the cracked solid is most unlikely. A very different conclusion can be reached, however, for this mechanism where the crack front reaches a free surface where no plane strain stress is present, and the resolved shear stresses on the oblique planes become much higher. An estimate of this enhanced nucleation probability on the oblique plane near the surface is easily obtained by rescaling the driving forces in fig. 9, in proportion to the resolved shear stresses on the oblique slip planes near the free surface against those in the interior as (for the geometry of fig. 2(b))

\[
\frac{G_{ls}}{G_{li}} = \left( \frac{3 - 4\nu}{3} \right)^2,
\]

where \(G_{ls}\) and \(G_{li}\) are respective energy release rates required for initiation of a dislocation near the free surface and in the interior. The result for \(\sigma-Fe\) with \(\nu = 0.291\) is shown as the chain curve in fig. 9, which now suggests almost spontaneous embryo formation near the free surface. This, however, is not true, since in this case at least a partial surface ledge must be produced, which will make the nucleation more difficult, but presumably still much easier than in the interior. An abundance of such nucleation events has been observed by George and Michot (1993).

4.4. Nucleation of dislocations on a cleavage ledge

Cleavage surfaces in metallic crystals invariably contain ledges parallel to the direction of crack propagation. These are likely to form when the principal tension driving the crack deviates slightly on a local scale, requiring the crack to make small adjustments along its front. This microroughness of the cleavage surface depends also on the crystallography of the cleavage planes and crack propagation direction as well as on temperature. The height of the observed ledges can range from several atomic spacings to microns. Numerous observations (Chiao and Clarke 1989, Hirsch et al. 1989a, b, George and Michot 1993) have revealed that dislocation nucleation at a crack front is a relatively rare phenomenon associated with crack front heterogeneities. This strongly suggests that ledges are likely sites for heterogeneous nucleation of dislocations (Zhou and Thomson 1991). In what follows we analyse this mechanism as it is likely to operate in \(\sigma-Fe\).

Consider a cleavage crack propagating under mode I loading. The crack contains ledges of a width of roughly a hundred atomic spacings distributed along its front, as depicted later in fig. 11. The presence of a considerable local mode III stress intensity factor acting on the ledge is expected to promote nucleation. Moreover, the direction of the Burgers vector of the dislocation embryo, which is parallel to the local crack front on the ledge, requires no fresh surface production. In view of the mesh size requirements to resolve adequately the dislocation embryo, a direct simulation of the complete system does not appear possible at present. This difficulty can be sidestepped by the approximate two-scale approach sketched in fig. 10. The distribution of stress intensity factors along the front of the crack, including the ledge, is first calculated by recourse to a linear elastic analysis. The small stretch of ledge on which the dislocation embryo nucleates is then idealized as a semi-infinite crack subjected to the local stress intensity factors determined in the first analysis. Because of the vastly disparate scales of the ledge and the activation configuration, the results
Dislocation nucleation from crack tips

Dislocation nucleation on a cleavage ledge.

obtained in the manner just outlined should be ostensibly identical with those obtained from a direct simulation.

The distribution of stress intensity factors on the crack front can be readily calculated by the boundary element method of Xu and Ortiz (1993). The mesh used in the analysis is shown in Fig. 11. As is evident from the figure, two symmetric ledges are included in the mesh. This permits the enforcement of periodic boundary conditions.

Mesh used in the computation of the stress intensity factors along a crack front containing cleavage ledges.
conditions, which greatly facilitates the calculations (Xu and Ortiz 1993). For small width-to-separation ratios, the interaction between the ledges may be expected to be negligible. The calculated stress intensity factors are shown in fig. 12. On the ledge, the dominant stress intensity factors are $K^\text{ledge}_I \approx 0.81K_I$ and $K^\text{ledge}_\text{III} \approx 0.35K_I$. On the verge of brittle fracture, it therefore follows that $K^\text{ledge}_\text{III} \approx 0.35K_{ic}$. For mode III loading, Rice (1992) has determined the athermal critical condition for nucleation of a screw dislocation to be

$$G_{\text{IIIcd}} = \frac{1}{2\mu} K^2_{\text{IIIcd}}.$$  

(16)

Using the relation

$$G_{ic} = 2\gamma_s = \frac{1 - \nu}{2\mu} K^2_{ic},$$  

(17)

we obtain

$$K_{\text{IIIcd}} = \left( \frac{(1 - \nu)\gamma_{us}}{2\gamma_s} \right)^{1/2} K_{ic} = 0.357K_{ic} > 0.350K_{ic}. \quad \text{(18)}$$

This calculation suggests that screw dislocations cannot be nucleated spontaneously below the critical condition for cleavage, which is consistent with the expectation that $\alpha$-Fe single crystals be intrinsically brittle. However, the small difference between the numerical factors is most likely to be below the accuracy of the calculation, which viciates the argument to a considerable extent. Indeed, consideration of tension softening, the effect of anisotropy and uncertainties in the material parameters can all change eqn. (18) to some degree. The calculation does nevertheless provide a first indication that screw dislocation nucleation from a ledge may indeed be much easier than nucleation on inclined and oblique planes.

Next we consider a semi-infinite crack under simple mode III loading. Tension softening has been shown to be of little consequence up to values of $K_I$ of the order of 0.9$K_{ic}$ (Xu et al. 1995a) and can therefore be safely neglected. Figures 13 and 14 show two saddle-point configurations of the embryonic screw dislocations for nor-

Fig. 12

Distribution of stress intensity factors on a cleavage ledge.
The saddle-point configuration for nucleation of a screw dislocation from a cleavage ledge, $G_{III}/G_{IIICd} = 0.75$.

The saddle-point configuration for nucleation of a screw dislocation from a cleavage ledge, $G_{III}/G_{IIICd} = 0.50$.

ormalized load levels $G_{III}/G_{IIICd} = 0.75$ and 0.50. Interestingly, these saddle-point configurations are flatter than those of edge dislocations, shown in figs. 3 and 4, as befits the lower line energies of screw dislocations. As the screw dislocation bows out, it tends to form double kinks with short edge components. By way of contrast, the screw double kinks of the edge dislocation embryo tend to be longer and the edge segment shorter (figs. 3 and 4). Computationally, this requires a larger periodic domain in the case of the screw embryo, which inevitably increases the size of the problem. The dependence of the activation energy on the crack driving force is
shown in fig. 15. The low values of the activation energy relative to those computed for nucleation on inclined and oblique planes is particularly noteworthy.

Finally, we endeavour to ascertain the magnitude of the errors incurred as a result of the various simplifications adopted in the calculations. In order to estimate the effect of tension softening, we consider the simple two-dimensional problem of a semi-infinite crack subjected to mixed mode I and III. We take the ratio $K_{III}/K_I$ to be $0.35/0.81 = 0.43$, which is the case of interest in the ledge problem. We also wish to estimate the effect of identifying the interlayer inelastic displacements with the total displacements, that is of setting $\Delta = \delta$, a simplification which has been adopted for computational convenience. Physically, this corresponds to taking the interplanar distance $h$ across the slip plane to be zero. In the ledge problem, we have additionally set the parameter $p = 0$ for want of a better estimate. Figure 16 shows the effect on the activation energy of variations in these parameters. As is evident from the figure, the $h = 0$ approximation accounts for modest errors of the order of 15% at most, over much of the range of $G_I/G_{IIc}$. The effect of tension softening in the range $0 \leq K_I \leq 0.43K_{III}$ is indeed seen to be negligible. The lowest curve for the activation energy has been calculated for $p = 0.217$ as a reasonable estimate. It shows that non-zero values of $p$ can reduce the activation energy significantly, which indicates the need for more reliable estimates of this parameter. The effect of the periodicity of the computational model on the activation energy was found by Xu et al. (1995a) to decay rapidly with increasing size of the period.

4.5. Estimates of the brittle-to-ductile transition temperature

As noted in the foregoing, the B-D transition in bcc transition metals, and particularly in $\alpha$-Fe, is most likely probably controlled solely by dislocation nucleation. Therefore, the preceding results can be used to estimate the B-D transition temperatures attendant to the three nucleation modes considered, namely nucleation on inclined planes, on oblique planes, or on cleavage ledges. No precise experimental

![Fig. 15](image)

The activation energy for dislocation emission in simple mode III loading, at the cleavage ledge.
measurements of the transition temperature of single-crystal α-Fe are available. The transition temperature for polycrystalline low-C steel is about 250 K, as determined from Charpy impact experiments (McClintock and Argon 1966). In the absence of more direct measurements, we shall suppose the transition temperature for pure α-Fe to be in the range 250–300 K. A B–D transition scenario achievable experimentally was proposed by Argon (1987) and consists of the arrest of a cleavage crack propagating against a temperature gradient.

The evaluation of the B–D transition temperature from the activation energy can be effected as suggested by Xu et al. (1995a), who give the relation

$$ T_{BD} = \left( \frac{\ln(c/v)}{\alpha} + \eta \frac{T_0}{T_m} \right)^{-1} T_0. \quad (19) $$

Here $T_0 \equiv \mu b^3/k(1-\nu) \approx 1.2 \times 10^3$ K; the melting temperature $T_m = 1809$ K for α-Fe; $\alpha = (1-\nu) \Delta U_{act}/\mu b^3$ is the normalized activation energy; $c$ is the speed of sound; $v \approx 1 \text{ cm s}^{-1}$ is a typical crack propagation velocity, giving $\ln(c/v) \approx 10$; $\eta \approx 0.5$ is a coefficient describing the temperature dependence of the shear modulus which, to a first approximation, is presumed of the form

$$ \mu = \mu_0 \left( 1 - \eta \frac{T}{T_m} \right). \quad (20) $$

The dependence of the activation energy for nucleation of dislocation embryos on the energy release rate $G_1$ is shown in fig. 17 for each of the three modes of nucleation considered in the foregoing. The activation energy at the critical driving force for cleavage, that is, at $G_1/G_{lc} = 1$, determines the transition temperature through eqn. (19). This relation is plotted in fig. 18, together with the activation energies for nucleation on inclined planes, oblique planes and ledges. Also shown in the figure is the value of the transition temperature for polycrystalline Fe. It is evident from this comparison that only nucleation on cleavage ledges results in transition temperatures which approach the expected value for α-Fe. The remaining two mechan-
The activation energies for dislocation nucleation at a crack tip in $\alpha$-Fe, for three different modes of nucleation.

The estimated B–D transition temperatures in $\alpha$-Fe.

isms grossly overestimate the transition temperature. These results strongly suggest that dislocation nucleation from a crack tip in $\alpha$-Fe is an inhomogeneous process. The dislocation loops which eventually shield the crack are emitted from ledges distributed along the crack front.

§ 5. Discussion

We have viewed the transition in fracture behaviour from ductile to brittle or, more fundamentally, from brittle to ductile as a manifestation of crack-tip-initiated plasticity counteracting the tendency for brittle behaviour by cleavage cracking. In this regard, we have distinguished two different behaviours: that in which the transi-
Dislocation nucleation from crack tips

Dislocation nucleation from crack tips is controlled by nucleation of dislocation embryos from the crack tip, which is characteristic of bcc transition metals, and that in which the transition is controlled by the mobility of dislocations away from the crack tip, which is typical of semiconductors and compounds. The distinguishing characteristic between these two behaviours is the mobility of kinks on dislocations. Experiments indicate that in bcc transition metals (at anything but the lowest temperatures) there is little resistance to the motion of kinks along dislocation lines. By contrast, in semiconductors such as Si and other compounds for which good information on dislocation mobility exists (Yonenaga et al. 1987, 1989, Yonenaga and Sumino 1989) it is known that the stress dependence of the dislocation velocity is nearly linear, implying that a process of kink drift controls dislocation motion. Computer simulations (Bulatov et al. 1995) confirm that kink motion along dislocations is indeed hindered by very substantial energy barriers in Si. These observations suggest that the B–D transition is nucleation controlled in bcc transition metals and mobility controlled in semiconductors and semiconducting compounds.

An additional mechanism which can influence fracture behaviour is crack-tip shielding by general ‘background’ plasticity. A particularly elegant and compelling analysis of this mechanism was advanced by Freund and Hutchinson (1985). Based on the known rate dependence characteristics of steels, which exhibit a marked stress upturn at high strain rates, Freund and Hutchinson (1985) demonstrated that brittle fracture can take place at high crack propagation velocities. This results in progressively diminishing inelastic response but that the transition is smooth and spread out, and far from being abrupt. The importance of background plasticity effects has been demonstrated experimentally by Hirsch et al. (1989a), who have shown that the sharp B–D transition in dislocation-free Si becomes diffuse, and moves to somewhat lower temperatures, when the crystals are initially dislocated by a pre-deformation step. The effect of background plasticity can therefore be regarded as one of modulating the B–D transition, with the ultimate controlling mechanism residing in crack-tip-initiated processes.

It is observed that intrinsically brittle materials such as crack-free Fe (Allen 1959) and W (Argon and Maloof 1966a) single crystals can often be plastically deformed at cryogenic temperatures with low plastic resistance when they are in pure form but fracture in a brittle manner when they are less pure and exhibit a high plastic resistance. This observation has been used as an argument in support of the background plasticity model of the fracture transition. This is partly correct. An intrinsically brittle solid only demonstrates its brittle characteristics when a crack is present. In well prepared Fe and W crystals, cracks do not exist initially and need to be produced by plastic deformation, most prominently by the intersection of deformation twins (Argon and Maloof 1966b). This requires a relatively high stress to nucleate the twins. In pure metallic crystals, the plastic yield stress is usually below the critical stress required for twinning, and brittle microcracks are not produced until the flow stress is raised by strain hardening to a sufficient level for twinning.

In the present paper we have reported on the key process of dislocation nucleation from crack tips in bcc transition metals, and particularly in α-Fe, where nucleation is expected to be the controlling process. We have noted that, as is now well established (Schöck and Püschl 1991, Rice et al. 1992, Rice and Beltz 1994, Xu et al. 1995a), at the saddle point the critical activation configuration of the nucleated dislocation consists only of partially completed core matter. Consequently, we have termed these configurations dislocation embryos.
We note that a cursory examination of the shapes of the dislocation embryos shown in figs. 3 and 4, for the case of the inclined plane, and to a lesser extent, those in figs. 13 and 14, for the substantially screw-type embryos on cleavage ledges might give the counter-intuitive appearance of closed loops that are in the process of formation. This is an illusion since the level contours shown in these figures pertain to the total displacements at the crack tip where only the bulged portions of these, in the region of $x_1/b > 0$, could be associated with the inelastic displacements of the embryo. A reference line passed through $x_1/b = 0$ (the initial geometrical crack front) shows clearly that the embryo approximates to somewhat less than a half-ellipse but results in the partial penetration of the crack tip displacements into the embryo, giving an overall mushroom-type appearance.

The present study, as was our original work, as well as that of Rice et al. (1992), is based on the Peierls concept of describing the fundamental inelastic response by an interplanar tension–shear potential. The analysis of the shapes of the embryos and the dependence of the activation energies for their formation on the applied energy release rates were performed self-consistently, utilizing quantities such as $\mu$, $\gamma_{\text{us}}$, and $\gamma_{\text{s}}$ that had been determined by the best available atomistic approaches (Sun, Beltz and Rice 1993) and were presented also by us earlier (Xu et al. 1995a). Thus, while published information of these quantities based on experimental measurements may have a considerable latitude in certainty, our results should have greater accuracy in the relative placement of the modes of response that we have simulated. Clearly, however, on an absolute basis, such as in the determination of the transition temperatures of fig. 18, the results should be viewed with more caution. Nevertheless, the energetics of the embryos that we have analysed indicate that the very large uncertainties in the transition temperatures of previous considerations (discussed by Xu et al. (1995a)) have now been eliminated.

In our present study we have examined three plausible modes of nucleation: on inclined planes containing the crack front, on oblique planes intersecting the crack front, in the interior and near a free surface and, finally, on cleavage ledges along the crack front. Our analysis has confirmed our earlier finding (Xu et al. 1995a) that nucleation on inclined planes in $\alpha$-Fe entails energy barriers that are too high to be overcome, at impending crack advance, at temperatures below the melting point. Contrary to expectations, our analysis has also established that dislocation nucleation on oblique planes in $\alpha$-Fe requires even higher energies in the interior of the solid, which translates into transition temperatures well above the melting point. Since in this mode of nucleation no significant free surface is produced, the finding is surprising but can be explained by noting that, while the peak shear stress near the crack tip is higher on the oblique planes than on inclined planes, the area-averaged shear stress is significantly lower in the former case, owing to the rapid decay of stresses in all directions away from the tip. A rather different conclusion was reached, however, for oblique planes near a free surface where no plane-strain stress exists and shear stresses on oblique planes are much higher. Here, were it not for a need of some surface ledge production, emission of dislocations should be nearly spontaneous. Such preponderance of dislocation emission where the crack reaches free surfaces has been observed by George and Michot (1993).

Both the inclined plane modes and the oblique plane modes are instances of homogeneous nucleation, inasmuch as every segment of the crack front constitutes an equally likely nucleation site. However, numerous experiments (Chiao and Clarke 1989, Samuels and Roberts 1989, George and Michot 1993) have demonstrated that
Dislocation nucleation from crack tips

nucleation is a rare event and occurs only at particular sites along the crack front. These sites are nearly always associated with cleavage ledges. A preliminary analysis of heterogeneous nucleation at ledges had been carried out by Zhou and Thomson (1991), who found the mechanism to be quite favourable.

We have analysed dislocation nucleation on cleavage ledges in α-Fe, where we have taken the crack front to coincide with the (110) direction and the ledges to be on {112} planes. This mode is favoured in two important ways. Firstly, the embryo is of a predominantly screw type and, hence, has a low line energy; it involves no surface production. Indeed, our results show that the energetics of this mode in α-Fe are so favourable that it borders on being a spontaneous process. The B–D transition temperatures that are estimated for this mode are well within the expected range for low-C steel, that is around 250–300 K. This mode of initiation of dislocation activity also furnishes a ready explanation for the observation of Michot (1988) and George and Michot (1993) that such activity often occurs on planes with low resolved shear stress.

Analyses based on Peierls potentials represent the best minimum-commitment approach to an atomistic analysis. Consequently, we view our results as less than a final answer. These limitations notwithstanding, it can be safely argued that the previously existing gap between experiment and theory pointed out by Argon (1987) has been substantially closed at present. Our finding that the key event is a process of heterogeneous nucleation is well in keeping with most other nucleation-controlled phenomena in nature (see Martin and Doherty (1976) for a discussion). Further refinements of the model can be derived from the direct atomistic simulation of the crack-tip processes. These, which have proven unwieldy in the past, can now be more readily attempted using our activation configurations as a first guess of the initial position of the crack-tip atoms. One outstanding problem that remains to be addressed concerns the mobility-controlled fracture transition. A perceptive model of Brede (1993) should be amenable to a more rigorous analysis by our variational boundary integral method. In particular, it should be possible to account for rate effects within the present theory by introducing a rate and temperature-dependent resistance law for dislocation motion.

In closing, we note that the ability of dislocation nucleation at the crack tip to account for the exceedingly sharp transitions observed in some materials has been questioned by Khanta, Pope and Vitak (1994a,b), who have advocated a critical phenomena approach akin to statistical mechanical theories of defect-mediated melting. However, the preponderance of the observational evidence appears to support the crack-tip dislocation nucleation mechanism. Indeed, the detailed and meticulous direct X-ray imaging experiments of George and Michot (1993) of the stages of evolution of the crack tip plastic response, starting from nucleation at crack tip heterogeneities and followed by the very rapid spread and multiplication of dislocation length from such sources, is a convincing direct demonstration of the vast number of degrees of freedom available to dislocations for populating the highly stressed crack tip zone. We know of no present experimental evidence for the large thermal equilibrium concentrations of stiffness-attenuating dislocation dipoles that are predicted by the model of Khanta et al. (1994a,b).

ACKNOWLEDGEMENTS

This research was supported by the Office of Naval Research (ONR) under Contract No. N00014-92-J-4022, with an additional supplement for the present
simulation for which we are grateful to Dr R. Barsoum of that agency. M.O. gratefully acknowledges support from the ONR under Contract No. N00014-90-J1758. We acknowledge fruitful discussions with Professor J. R. Rice and Professor E. Kaxiras of Harvard University and Dr R. Thomson of the National Institute of Standards and Technology. Moreover, we acknowledge support from the Army Research Office under a Supplementary Equipment Grant No. P-33768-MA-RIP for purchases of computer equipment used in this work. The computations were carried out in the facilities of the Mechanics of Materials group at Massachusetts Institute of Technology, and those of the Solid Mechanics group at Brown University.

APPENDIX

ASYMPTOTIC SOLUTIONS OF THE CRACK TIP IN THE ANISOTROPIC SOLID

Cracks and dislocations in anisotropic solids were investigated by Stroh (1958) in the manner most useful to our present study. A comprehensive review of the theory of dislocations in anisotropic solids has recently been given by Lothe (1992). The asymptotic solutions of the semi-infinite crack in anisotropic solids used here are obtained by taking the limit of the solution of a slit crack given by Barnett and Asaro (1972), who modelled the slit crack as the superposition of three sets of straight dislocations. The variational boundary integral method developed by Xu and Ortiz (1993) and Xu et al. (1995b) is an extension of this approach to three dimensions.

With reference to fig. A1, the three stress intensity factors \( K_i (i = 1, 2, 3) \) are defined as

\[
\sigma_{ij} x_i x_j x_i \rightarrow 0, x_2 = 0 = \frac{K_i}{(2\pi x)^{1/2}} + \text{non-singular terms.} \quad (A1)
\]

The opening displacements \( u_t \) are given by

Fig. A1

A semi-infinite crack in an anisotropic solid.
\[ u_i = 4B_{ii}^{-1}K_j \left( \frac{-x_1}{2\pi} \right)^{1/2}, \]  
\hspace{2cm} (A.2)

and the energy release rate \( G \) for crack extension is

\[ G = \frac{1}{2}K_iB_{ii}^{-1}K_j. \]  
\hspace{2cm} (A.3)

Here \( B \) is a positive-definite symmetric second-rank tensor that depends only on the direction of the crack front. For isotropic solids, \( B \) takes the diagonal form

\[ B_{11} = B_{22} = \frac{\mu}{1-\nu}, \quad B_{33} = \mu. \]  
\hspace{2cm} (A.4)

For anisotropic solids, \( B \) is given by the integral

\[ B = -\frac{1}{2\pi} \int_0^{2\pi} [(mn)(nm)^{-1}(nm) - (mn)] \, d\phi, \]  
\hspace{2cm} (A.5)

where \( m \) and \( n \) are mutually orthogonal unit vectors normal to the crack front; the matrix \( (mn) \) is, in components, \( (mn)_{jk} = m_i \epsilon_{ijk} n_l \), and \( \epsilon_{ijk} \) are elastic constants of the solid.

For \( \alpha \)-Fe, \( c_{11} = 2.431 \times 10^5 \) MPa, \( c_{12} = 1.381 \times 10^5 \) MPa and \( c_{44} = 1.219 \times 10^5 \) MPa. The resulting dependence of the energy release rate on crack front orientation is plotted in fig. A.2, where \( G_{\text{iso}} \) is the energy release rate computed from average elastic constants. Similar results are shown for Si on (111) and (110) planes, in which case \( c_{11} = 1.677 \times 10^5 \) MPa, \( c_{12} = 0.650 \times 10^5 \) MPa and \( c_{44} = 0.804 \times 10^5 \) MPa. It follows from this calculation that the preferred crack front orientation for cleavage fracture on the (001) plane in \( \alpha \)-Fe is parallel to the \{110\} direction. Likewise, the directions [110] and [111] are preferred for cleavage on (110) and (111) planes respectively in Si.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig_a2.png}
\caption{Variation in energy release rate with crack front orientation in Fe and Si.}
\end{figure}
REFERENCES


RICE, J. R., and THOMSON, R., 1974, Phil. Mag., 29, 73.


ST JOHN, C., 1975, Phil. Mag., 32, 1193.
Dislocation nucleation from crack tips


