Nucleation of dislocations from crack tips under mixed modes of loading: implications for brittle against ductile behaviour of crystals

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ABSTRACT

The variational boundary integral method of Xu and Ortiz is taken as a basis for studying dislocation nucleation from atomically sharp cracks under combined mode I–mode II loading. The tension–shear potential of Rice et al. is extended to allow for skewness in the shear resistance curve and to account for the surface production resistance which accompanies ledge formation. The calculated unstable equilibrium configurations of the incipient dislocations and the dependence of the associated activation energies on crack tip energy release rate are found to differ from the Rice–Beltz perturbation solution and the Schöck–Püschl more approximate solution. Simulations of dislocation nucleation on inclined slip planes reveal that, while tension softening facilitates nucleation, surface production resistance impedes it. The extent to which these two effects influence critical conditions for dislocation nucleation is quantified. The calculations suggest that homogeneous dislocation nucleation on inclined planes is not favoured for materials with all but the lowest of unstable stacking-energy-to-surface-energy ratios. This emphasizes the importance of heterogeneous dislocation nucleation and nucleation on oblique slip planes on which free surface production should play a much weaker role. The implications of these findings on the nucleation-controlled brittle–ductile transition in cleavage fracture are discussed.

NOMENCLATURE

- \( b \) magnitude of Burgers vector
- \( c \) uniaxial strain elastic modulus
- \( G_{cd} \) critical driving force to nucleate a dislocation
- \( G_I \) crack driving force under mode I loading
- \( G_{II} \) crack driving force under mode II loading
- \( G_{Rc} \) critical cleavage crack driving force under mode I loading
- \( h \) interatomic layer spacing
- \( K_{Ild} \) critical stress intensity factor \( K_{II} \) to nucleate a dislocation
- \( T_{BD} \) brittle-to-ductile transition temperature
- \( \Delta U^{2D}_{act} \) activation energy per unit length for nucleating a straight dislocation in two dimensions

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\( \Delta U^{3D}_{\text{act}} \) activation energy for nucleating a dislocation loop in three dimensions
\( \hat{\beta} \) skewness parameter for the shear resistance
\( \gamma_s \) surface energy
\( \gamma_s^{(u)} \) unrelaxed unstable stacking energy
\( \gamma_s^{(r)} \) relaxed unstable stacking energy
\( \delta_r \) inelastic shear displacement between adjacent atomic layers
\( \delta_{r\parallel} \) interlayer inelastic displacement at the crack tip
\( \delta_{r\perp} \) inelastic opening displacement between adjacent atomic layers
\( \Delta_s \) shear displacement between adjacent atomic layers
\( \theta \) opening displacement between adjacent atomic layers
\( \lambda \) angle of inclination between slip plane and the crack surface
\( \mu \) decay parameter for the shear resistance to surface production
\( \nu \) Poisson's ratio
\( \sigma \) tensile stress between adjacent atomic layers
\( \tau \) shear stress between adjacent atomic layers
\( \tau_s \) periodic shear resistance between adjacent atomic layers
\( \tau_s \) shear resistance to surface production
\( \phi \) oblique angle between the Burgers vector and the crack front
\( \Phi \) inelastic potential between adjacent atomic layers
\( \Psi \) potential between adjacent atomic layers

§ 1. INTRODUCTION

The transition in the behaviour of materials from brittle to ductile continues to be of major scientific and technological interest. It was recognized early that cleavable materials are distinguished by having substantial energy barriers to dislocation nucleation from atomically sharp cracks on the verge of propagation (Armstrong 1966, Kelly, Tyson and Cottrell 1967, Rice and Thompson 1974). Moreover, pioneering experiments carried out on initially dislocation-free Si (St John 1975, Brede and Haasen 1988, Hirsch, Samuels and Roberts 1989) have demonstrated that, at least in this material, the brittle-to-ductile transition is not controlled solely by dislocation nucleation but also by the mobility of trains of dislocations nucleation from crack tips (Chiao and Clarke 1989, Samuels and Roberts 1989, George and Michot 1993) have established that dislocation nucleation is heterogeneous, singling out geometrical crack-tip imperfections.

Evidently, a full understanding of these processes necessitates some degree of atomistic modelling (for example Bulatov, Yip and Argon 1995). Despite being deficient in this respect, continuum approaches of the Peierls type have revealed useful insights (Rice 1992, Rice Beltz and Sun 1992, Sun Beltz and Rice 1993, Schöck 1991). For instance, continuum theories have in their own way confirmed that the saddle-point configuration of a nucleating dislocation consists entirely of dislocation core material, and that the accurate modelling of the atomic-level decohesion and shear response is of vital importance for the theory to be predictive. Within this framework, Rice and Beltz (1994) have computed saddle-point energies of three-dimensional dislocation nuclei by a first-order perturbation analysis. The activation energies obtained by this means differ somewhat from those determined by Schöck and Püschl (1991) by a different approach.

The analyses of Schöck and Püschl (1991) and Rice and Beltz (1994), while three dimensional, severely limit the range of possible geometries available to the incipient dislocation loop: the form by considering the dislocat

Here we present an analysis of interacting distribution of cracks and introduces no artificial interplanar separation. A potential in the manner of modifications to account for the analysis is restricted to isotropic generalizations to anisotropy.

In this paper we further nucleation occurs on a slit.

Following a brief desc of the modified interplanar nucleation of a straight disloca mode II loading, with par sinusoidal shear resistance provide a direct test of the scope of the analysis by all are compared with the app Püschl (1991). In § 6 we tu II loading. Our results reve

\( K_{\text{th}} \) for dislocation emiss compute the dependence of the phase angle of the appl proposed by Sun et al. (1999) for the shear resistance due a free surface. The result dislocation emission into particular cases of \( \alpha \)-Fe an remarks are added, evalu
dislocation loop: the former by prescribing its shape to be rectangular, and the latter by considering the dislocation to be nearly straight, in the spirit of perturbation theory. Here we present an analysis of dislocation nucleation from a crack tip which is free of a priori restrictions on the shape of the dislocation. Our calculations are based on a numerical method developed by Xu and Ortiz (1993) for the analysis of three-dimensional cracks in linear elastic solids. Because the method regards the crack as a continuous distribution of dislocation loops, it is readily extended to account for systems of interacting cracks and discrete dislocations such as envisaged here. This approach introduces no artificial discontinuity between elastic crack opening and inelastic interplanar separation. Additionally, we introduce a non-sinusoidal interplanar potential in the manner of Foreman, Jaswon and Wood (1951), as well as additional modifications to account for the resistance due to surface production. While the present analysis is restricted to isotropic elasticity in dealing with dislocation line properties, generalizations to anisotropic elasticity are straightforward but will not be pursued here. In this paper we further restrict our attention to geometries in which dislocation nucleation occurs on a slip plane containing the crack front.

Following a brief description of the numerical procedure in §2, and a derivation of the modified interplanar potential in §3, in §4 we consider the problem of the nucleation of a straight dislocation within the plane of the crack under the action of pure mode II loading, with particular emphasis on the effect of departures from Frenkel’s sinusoidal shear resistance relation. The analytical results of Rice and Beltz (1994) provide a direct test of the accuracy of the numerical procedure. In §5 we broaden the scope of the analysis by allowing for arbitrary dislocation configurations, and the results are compared with the approximate analyses of Rice and Beltz (1994) and Schöck and Püschl (1991). In §6 we turn to the tension-softenning effect under mixed mode I–mode II loading. Our results reveal the dependence of the critical mode II stress intensity factor $K_{II}$ for dislocation emission on the applied mode I stress intensity factor $K_{I}$. We also compute the dependence of the critical energy release rate for dislocation emission on the phase angle of the applied loads, and compare the results with the analytical relation proposed by Sun et al. (1993). In §7, we generalize the interplanar potential to account for the shear resistance due to surface production in cases where the slip plane intersects a free surface. The resulting interplanar potential is taken as a basis for the analysis of dislocation emission into inclined slip planes emanating from the crack front. The particular cases of α-Fe and Si are considered in some detail. Finally, in §8 some general remarks are added, evaluating the present findings.

§2. Method of Analysis

Our analysis builds on recent theoretical developments in the modelling of dislocation nucleation at a stressed crack tip (Beltz and Rice 1991, Rice 1992, Rice et al. 1992, Sun et al. 1993, Rice and Beltz 1994). In consonance with these developments, we consider a semi-infinite crack with a straight crack front lying on a slip plane in an elastically isotropic solid. We additionally assume that the crack surfaces do not interact and that, beyond the crack front, the shear separation resistance $\tau$ and tension separation resistance $\sigma$ follow as functions of the inelastic displacements $\delta_\tau$ and $\delta_\sigma$ on the slip plane. A precise definition of $\delta_\tau$ and $\delta_\sigma$ has been given by Rice (1992) and Sun et al. (1993). As the crack is subjected to combined mode I–mode II loading, an incipient dislocation can form progressively and reach a nucleation configuration, where it is emitted into the slip plane as the load reaches a critical value. Consideration
of a mode I loading component enables a systematic study of the tension-softening effect, as modelled by the modified interplanar potential to be introduced subsequently.

The geometry of the problem is illustrated in fig. 1. A semi-infinite atomically sharp crack and an inclined slip plane containing the crack front are subjected to a remote load, resulting in dislocation nucleation along the slip plane. The crystal is idealized as an isotropic linear elastic solid with shear modulus $\mu$ and Poisson’s ratio $v$. This describes applies everywhere in the crystal except for the relative displacement of the atomic layers bounding the slip plane, which is governed by a Peierls interlayer potential. The remote loading, characterized by stress intensity factors $K_1$, $K_2$ and $K_3$, induces a standard $K$ field in the absence of a dislocation.

The profile of the nucleated dislocation and the crack opening displacement $u$ follow by minimization of the potential energy

$$II[u] = W[u] + V[u] - P[u], \quad (1)$$

where $W$ is the elastic strain energy, $V$ the interlayer energy and $P$ the potential energy of the applied forces. By representing the inelastic displacement along the slip plane and opening displacement of the crack as a continuous distribution of dislocation loops, and using known expressions for the interaction energy between dislocation loops (Hirth and Lothe, 1982), Xu and Ortiz (1993) derived the general form of the strain energy

$$W[u] = \frac{\mu}{4\pi} \int_{S_c + S_s} \left[ \frac{[\mathbf{e}_r \cdot (\mathbf{n} \times \nabla u_1)] [\mathbf{e}_r \cdot (\mathbf{n} \times \nabla u_2)]}{R} \right] dS_1 dS_2$$

$$- \frac{\mu}{8\pi} \int_{S_c + S_s} \left[ \frac{[\mathbf{e}_r \cdot (\mathbf{n} \times \nabla u_2)] [\mathbf{e}_r \cdot (\mathbf{n} \times \nabla u_2)]}{R} \right] dS_1 dS_2$$

$$+ \frac{\mu}{8\pi(1 - v)} \int_{S_c + S_s} \left[ \frac{[\mathbf{e}_r \times (\mathbf{n} \times \nabla u_1)] \cdot \mathbf{T} [\mathbf{e}_r \times (\mathbf{n} \times \nabla u_2)]}{dS_1 dS_2} \right], \quad (2)$$

where $S_c$ and $S_s$ represent the crack surface and slip plane respectively, $(.)_1$ and $(.)_2$ denote two different points on the surfaces $S_c$ and $S_s$, $R$ is the distance between these two points, $\mathbf{e}_r$, $i = 1, 2, 3$, 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

$$T_{ij} = \frac{\partial^2 R}{\partial x_i \partial x_j}. \quad (3)$$

The interlayer energy is $\lambda$

where $\Phi[u]$ is the interplanar expressions for $\Phi$ are derived on the crack surfaces is

In subsequent analyses, the and, consequently, $t = 0$.

To solve for the displacement $u$, choose Cartesian axes $\bar{u} = 0$ for $x_1 < 0$ and $x_1 = 0$. The term $\bar{u}$ in $x_1$, that is far from the crack plane, and becomes negligibly small where $S_c$ lies on the crack plane and the interlayer potential of the crack-slip plane system is

$$II[\bar{u} + \delta] = W[\bar{u}]$$

where we identify $W_1(\bar{u}) = W_1(\delta) + V(\delta)$ as the self-distributed dislocation field $W_2(\bar{u}, \delta)$ is the inter-system of modifications.
The interlayer energy is expressible as

$$V[u] = \int_{S_c} \Phi[u] \, dS,$$

(4)

where $\Phi[u]$ is the interplanar potential defined per unit area of the slip plane. Suitable expressions for $\Phi$ are derived in § 3. Finally the potential energy of tractions $t$ applied on the crack surfaces is

$$P[u] = \int_{S_c} t \cdot u \, dS.$$

(5)

In subsequent analyses, the crack surfaces are presumed to be free of applied tractions, and, consequently, $t = 0$.

To solve for the displacements $u$ numerically, the analysis has to be reduced to a bounded domain. Following the treatment of semi-infinite periodic cracks given by Xu and Ortiz (1993), this reduction can be achieved by writing

$$u = \bar{u} + \delta,$$

(6)

where $\bar{u}$ is the displacement of a standard $K$ field for a reference semi-infinite crack. Choose Cartesian axes such that the crack occupies the domain $x_3 = 0$, $x_1 > 0$. Then, $\bar{u} = 0$ for $x_1 < 0$ and

$$\bar{u}_1 = \frac{K_1 4(1-v)}{\mu (2\pi)^{1/2}} x_1^{1/2},$$

(7a)

$$\bar{u}_2 = \frac{K_\Pi 4(1-v)}{\mu (2\pi)^{1/2}} x_1^{1/2},$$

(7b)

$$\bar{u}_3 = \frac{K_{\Pi 3} 4}{\mu (2\pi)^{1/2}} x_1^{1/2},$$

(7c)

for $x_1 \geq 0$. The term $\bar{u}$ matches the behaviour of the opening displacements for large $x_1$, that is far from the crack front. Consequently, the remaining term $\delta$, which is the primary unknown in the calculations, may be expected to decay rapidly to zero with $x_1$. This situation is exploited by setting $\delta = 0$ for $x_1 > x_1^*$, that is beyond some distance $x_1^*$ from the crack front. Far from the crack front on the slip plane, $\delta$ may also be expected to become negligibly small. In this manner, $\delta$ can be restricted to a finite domain $\tilde{S}_c \cup \tilde{S}_s$, where $\tilde{S}_c$ lies on the crack surface and $\tilde{S}_s$ on the slip plane. Noting that $P[\bar{u}] = 0$ on $\tilde{S}_c$ and the interlayer potential only applies on the slip plane, the potential energy of the crack-slip plane system can then be written as

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

(8)

where we identify $W_1[\bar{u}]$ as the self-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 where $W_2[\bar{u}, \delta]$ is the interaction energy of the initial unmodified system with the second system of modifications.
Then,

$$W_1[\delta] = \frac{\mu}{4\pi} \int_{S_1} \int_{S_2} \left[ \mathbf{e}_i \cdot (\mathbf{n} \times \nabla \delta) \right]_2 \left[ \mathbf{e}_j \cdot (\mathbf{n} \times \nabla \delta) \right]_1 \frac{dS_1}{R} dS_2$$

$$- \frac{\mu}{8\pi} \int_{S_1} \int_{S_2} \left[ \mathbf{e}_i \cdot (\mathbf{n} \times \nabla \delta) \right]_1 \left[ \mathbf{e}_j \cdot (\mathbf{n} \times \nabla \delta) \right]_2 \frac{dS_1}{R} dS_2$$

$$+ \frac{\mu}{8\pi(1-v)} \int_{S_1} \int_{S_2} \left[ \mathbf{e}_i \times (\mathbf{n} \times \nabla \delta) \right]_1 \cdot \mathbf{T} \times \left[ \mathbf{e}_j \times (\mathbf{n} \times \nabla \delta) \right]_2 dS_1 dS_2,$$

(9)

and

$$V[\delta] = \int_{S_1} \Phi[\delta] dS.$$

(10)

Following the treatment of semi-infinite periodic cracks given by Xu and Ortiz (1993), the interaction energy $W_2$ of the displacement $\mathbf{u}$ of the standard $K$ field and the inelastic displacement correction $\delta$ can be written as

$$W_2[\mathbf{u}, \delta] = -K_I Q_1[\delta] - K_{II} Q_{II}[\delta] - K_{III} Q_{III}[\delta],$$

(11)

where

$$Q_1[\delta] = \int_{S_1} \mathbf{n} \cdot \mathbf{\sigma}_I \cdot \delta dS,$$

(12 a)

$$Q_{II}[\delta] = \int_{S_1} \mathbf{n} \cdot \mathbf{\sigma}_{II} \cdot \delta dS,$$

(12 b)

$$Q_{III}[\delta] = \int_{S_1} \mathbf{n} \cdot \mathbf{\sigma}_{III} \cdot \delta dS,$$

(12 c)

and $\mathbf{\sigma}_I, \mathbf{\sigma}_{II}$ and $\mathbf{\sigma}_{III}$ are stresses of $K$ 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 crack front of the reference semi-infinite crack is actually located some distance from the physical crack front. This treatment allows us to use a non-singular Dugdale–Barenblatt crack as a reference crack, so that the quality of the solution can be improved (Xu and Ortiz 1993).

The unknown displacements $\delta$ follow by rendering the potential energy $H[\mathbf{u} + \delta]$ stationary. Noting that the first term on the right-hand side of eqn. (8) is independent of $\delta$ and can therefore be disregarded, the variation leads to the Euler equation

$$\frac{\partial W_2[\delta]}{\partial \delta} + \frac{\partial V[\delta]}{\partial \delta} - K_I \frac{\partial Q_1[\delta]}{\partial \delta} - K_{II} \frac{\partial Q_{II}[\delta]}{\partial \delta} - K_{III} \frac{\partial Q_{III}[\delta]}{\partial \delta} = 0.$$

(13)

This equation is of integral type, by virtue of the first term, and nonlinear, by virtue of the second term. A finite-element method of spatial discretization of eqn. (13) has been given by Xu and Ortiz (1993) in the case $V = 0$. The extension to the case $V \neq 0$ is straightforward and leads to a system of nonlinear equations which can be solved by a Newton–Raphson iteration.

A non-trivial complication arises in applying this program, owing to the loss of stability of the equations beyond the critical load. This difficulty may be circumvented by recourse to displacement control. For purposes of illustration, consider the pure mode II case corresponding to $K_II = K_{III} = 0$. Under these conditions, the finite-

§ 3. AN ATOMIC LEVEL

A coupled tension–shear law and the Rose–Ferrari Beltz and Rice (1991) half-crystals sliding unit...
Block-like lattice sliding and opening displacement of atomic layers bounding a slip plane. Element discretization of the crack–slip plane system results in a system of equations of the form

$$\mathbf{F}(\delta) = K_{II} \mathbf{f},$$

(14)

where $\delta$ now denotes the array of nodal values of the field $\delta(x)$, $\mathbf{F}$ is the internal force array, and $\mathbf{f}$ is the external force array normalized to $K_{II} = 1$. Instead of enforcing the value of $K_{II}$, which is not possible beyond the critical point, we augment the system (14) by the addition of the kinematic constraint

$$\mathbf{f} \cdot \delta - \bar{\delta} = 0,$$

(15)

Here, $\mathbf{f} \cdot \delta$ is the displacement parameter conjugate to $K_{II}$ and $\bar{\delta}$ its prescribed value. The unknowns of the combined system of eqns (14) and (15) are $\delta$ and $K_{II}$. Thus $K_{II}$ is not prescribed but computed as a function of the effective displacement $\delta$, which can be increased monotonically from zero. Linearization of eqns (14) and (15) yields an incremental system of the form

$$\begin{bmatrix}
K & -\mathbf{f} \\
-f^T & 0
\end{bmatrix}
\begin{bmatrix}
\Delta\delta \\
\Delta K_{II}
\end{bmatrix}
= \begin{bmatrix}
0 \\
-\Delta\delta
\end{bmatrix},$$

(16)

where $K$ is a symmetric tangent stiffness matrix. The form of eqn. (16) is indeed characteristic of a system with equality constraints enforced by Lagrange multipliers.

§ 3. AN ATOMIC LEVEL INTERLAYER POTENTIAL FOR TENSION–SHEAR COUPLING

A coupled tension–shear interlayer potential which combines the Frenkel sinusoidal law and the Rose–Ferrante–Smith (1981) universal binding relation was derived by Beltz and Rice (1991). Following their development, we envisage two rigid half-crystals sliding uniformly across a slip plane of thickness $h$ (fig. 2). Let $A_x$ and $A_y$...
denote the shear and opening relative displacements respectively across the slip plane; \( \tau \) and \( \sigma \) are the shear and normal resistances respectively acting between the blocks. The inelastic relative displacements \( \delta_r \) and \( \delta_\theta \) are then defined as

\[
\delta_r = A_r - \frac{h\tau(A_r, A_\theta)}{\mu},
\]

\[
\delta_\theta = A_\theta - \frac{h\sigma(A_r, A_\theta)}{c},
\]

where \( c = \lambda + 2\mu \) is the uniaxial strain elastic modulus.

The point of departure in the Beltz–Rice theory is an interplanar traction–displacement relation of the general form

\[
\tau(A_r, A_\theta) = A(A_\theta) \sin \left( \frac{2\pi A_r}{b} \right),
\]

\[
\sigma(A_r, A_\theta) = \left( B(A_r) \frac{A_\theta}{L} - C(A_r) \right) \exp \left( - \frac{A_\theta}{L} \right),
\]

where \( A(A_\theta), B(A_r) \) and \( C(A_\theta) \) are functions to be determined. In eqns (18a) and (18b), \( b \) denotes the Burgers displacement and \( L \) the characteristic length of the decohesion process. This length is found to scale with the Thomas–Fermi screening distance in elemental metals (Rose et al. 1981). In simple tension, \( \sigma \) reaches its maximum level at \( A_\theta = L \).

Beltz and Rice (1991) determined the functions \( A(A_\theta), B(A_r) \) and \( C(A_\theta) \) by enforcing selected subsidiary constraints. Firstly, the traction–displacement relations are required to reduce to Frenkel’s sinusoidal form and the Rose–Ferrante–Smith universal binding relation in simple shear and tension respectively. This gives

\[
\tau(A_r,0) = \frac{\pi \gamma_{us}}{b} \sin \left( \frac{2\pi A_r}{b} \right),
\]

\[
\sigma(0,A_\theta) = \frac{2\gamma_{us} A_\theta}{L} \exp \left( - \frac{A_\theta}{L} \right),
\]

where \( \gamma_s \) is the surface energy and \( \gamma_{us}^{(u)} \) the unstable stacking energy parameter introduced by Rice (1992), defined as the (maximum) energy attained at the unstable equilibrium configuration in simple shear in the absence of opening displacement. If \( A_r = b^* \) in this configuration, then

\[
\gamma_{us}^{(u)} = \int_0^{b^*} \tau(A_r,0) \, dA_r.
\]

For slip along a translation vector of the lattice, such as attends a perfect dislocation, the symmetry of the lattice necessitates \( b^* = b/2 \). By contrast, the precise value of \( b^* \) for slip associated with a partial dislocation does not follow from symmetry considerations alone and requires an atomistic calculation for its determination.

Finally, the assumption of the existence of a joint potential \( \Psi(A_r, A_\theta) \) for the traction–displacement relations (18a) and (18b) requires that the Maxwell reciprocal relation

\[
\frac{\partial \tau}{\partial A_\theta} = \frac{\partial \sigma}{\partial A_r}
\]

be satisfied. In addition, displacement increases to \( A(d_1) \) and \( C(d) \) which satisfy

\[
A(d_1) = B(d)
\]

In these relations, \( A_\theta \) is the normal traction, \( \sigma = 0 \), at \( p \) is sometimes referred to characterize the tension–associated tension–shear

\[
\Psi(A_r, A_\theta) = \frac{A(A_\theta)}{B(A_r)}
\]

A similar potential in the context of interfacial debonding as the energy in the relaxation from the relation

\[
\frac{1}{\gamma_{us}^{(u)}}
\]

In Frenkel’s sinusoidal given by

\[
\gamma_{us}^{(u)} = \int_0^{b^*} \tau(A_r,0) \, dA_r.
\]

However, atomistic calculations and the density functional overestimates \( \gamma_{us}^{(u)} \). The values calculated from eqn. different temperatures are

The corresponding value

unstable stacking energy

Duesbery (1993) are also
be satisfied. In addition, the shear resistance must approach zero as the normal displacement increases to infinity, that is \( \tau \to 0 \), as \( \Delta_0 \to \infty \). The functions \( A(\Delta_0) \), \( B(\Delta_0) \) and \( C(\Delta_0) \) which satisfy these constraints are

\[
A(\Delta_0) = \frac{\pi \gamma_{us}^{(0)}}{b} \left( 1 + \frac{1 - q - p}{1 - p} \frac{\Delta_0}{L} \right) \exp \left( -\frac{\Delta_0}{L} \right), \tag{22a}
\]

\[
B(\Delta_0) = \frac{2 \gamma_{s}}{L} \left[ 1 - \frac{q - p}{1 - p} \sin^2 \left( \frac{\pi \Delta_0}{b} \right) \right], \tag{22b}
\]

\[
C(\Delta_0) = \frac{2 \gamma_{s} p (1 - q)}{1 - p} \sin^2 \left( \frac{\pi \Delta_0}{b} \right), \tag{22c}
\]

with

\[
q = \frac{\gamma_{us}^{(0)}}{2 \gamma_{s}}, \tag{23a}
\]

\[
p = \frac{\Delta_0}{L}. \tag{23b}
\]

In these relations, \( \Delta_0^s \) is the relaxed opening displacement corresponding to a vanishing normal traction, \( \sigma = 0 \), at the unstable equilibrium configuration in shear. The parameter \( p \) is sometimes referred to as the dilation parameter. The parameters \( p \) and \( q \) jointly characterize the tension–shear coupling in the traction–displacement relations. The associated tension–shear potential is

\[
\Psi(\Delta_r, \Delta_0) = 2 \gamma_{s} \left[ 1 - \left( 1 + \frac{\Delta_0}{L} \right) \exp \left( -\frac{\Delta_0}{L} \right) \right]
\]

\[
+ \sin^2 \left( \frac{\pi \Delta_0}{b} \right) \left( q + \frac{q - p}{1 - p} \frac{\Delta_0}{L} \right) \exp \left( -\frac{\Delta_0}{L} \right). \tag{24}
\]

A similar potential in which \( p = q \) was earlier introduced by Needleman (1990) in the context of interfacial debonding. The relaxed unstable stacking energy \( \gamma_{us}^{(r)} \) is defined as the energy in the relaxed unstable equilibrium configuration in shear, and it follows from the relation

\[
\frac{\gamma_{us}^{(r)} - \gamma_{us}^{(0)}}{\gamma_{us}^{(0)}} = \frac{1 - q}{q} \left( 1 - \frac{1}{1 - p} \exp(-p) \right). \tag{25}
\]

In Frenkel’s sinusoidal model, the unrelaxed unstable stacking energy \( \gamma_{us}^{(0)} \) is given by

\[
\gamma_{us}^{(0)} = \frac{\mu b^2}{2 \pi^2 \hbar}. \tag{26}
\]

However, atomistic calculations using the embedded-atom method (Sun et al. 1993) and the density functional theory (Kaxiras and Duesbery 1993) show that eqn. (26) often overestimates \( \gamma_{us}^{(0)} \). The values of the unstable stacking energy for Si, Ni, Al, Fe, Ni and Al calculated from eqn. (26) are given in the table, where the elastic constants at different temperatures are also collected (Simmons and Wang 1971, Curnich 1972). The corresponding values of the unrelaxed unstable stacking energy \( \gamma_{us}^{(r)} \) as calculated by Sun et al. (1993) and by Kaxiras and Duesbery (1993) are also displayed in the table for comparison. The discrepancies
Material properties.

| Material and slip system | $T$ (K) | $c_{11}$ ($10^5$ MN m$^{-2}$) | $c_{12}$ ($10^5$ MN m$^{-2}$) | $c_{44}$ ($10^5$ MN m$^{-2}$) | $\mu$ ($10^3$ MN m$^{-2}$) | $c$ ($\text{J m}^{-2}$) | $a_h$ (Å) | $\gamma_{\text{av}}$ ($\text{J m}^{-2}$) | $\gamma_{\text{av}}$ ($\text{J m}^{-2}$) | $\gamma_{\text{av}}$ ($\text{J m}^{-2}$) | $2\tau_s$ | $\beta$ | $p$ | $q$ | $L/b$ |
|-------------------------|---------|-------------------------------|-------------------------------|-------------------------------|---------------------------|------------------------|-----------|---------------------------|---------------------------|---------------------------|----------------|--------|-----|-----|
| Si(\{\}211)(111) (mi)  | 77.2    | 1.677                         | 0.650                         | 0.804                         | 0.610                      | 2.064                  | 5.41       | 1.932                     | 1.91                      | 2.02                      | 3.12           | 0.96   | 0.376| 0.647| 0.156|
| Si(\{\}011)(111) (m2) | 77.2    | 1.677                         | 0.650                         | 0.804                         | 0.610                      | 2.064                  | 5.41       | 1.932                     | 1.91                      | 2.02                      | 3.12           | 0.96   | 0.376| 0.647| 0.156|
| Ni$_2$Al(\{\}211)(111) (m3) | 4.2    | 2.431                         | 1.381                         | 1.219                         | 0.300                      | 3.125                  | 3.75       | 0.05                      | 0.08                      | 0.092                     | 1.13           | 0.147  | 0.081| 0.282|
| Ni$_2$Al(\{\}211)(111) (m5) | 4.2    | 2.431                         | 1.381                         | 1.219                         | 0.300                      | 3.125                  | 3.75       | 0.05                      | 0.08                      | 0.092                     | 1.13           | 0.147  | 0.081| 0.282|
| Ni$_2$Al(\{\}011)(111) (m6) | 0     | 2.642                         | 1.508                         | 1.317                         | 0.807                      | 3.632                  | 3.51       | 0.414                     | 0.226                     | 0.260                     | 2.87           | 1.59   | 0.152| 0.279|
| Al(\{\}211)(111) (m8) | 0       | 1.143                         | 0.619                         | 0.316                         | 0.280                      | 1.215                  | 4.05       | 0.166                     | 0.080                     | 0.092                     | 1.13           | 0.147  | 0.081| 0.282|
| Al(\{\}011)(111) (m9) | 0       | 1.143                         | 0.619                         | 0.316                         | 0.280                      | 1.215                  | 4.05       | 0.166                     | 0.080                     | 0.092                     | 1.13           | 0.147  | 0.081| 0.282|

Evidently, Frenkel's relation is still useful in the sense that $\lambda = 0$ for the spirit of Foreman et.

In order to reflect more accurately expansion, we shall require a wealth of experimental data. The parameters $\lambda$, $\mu$, and $c$ in the spirit of the shear modulus, we refer to the work of Argon (1982) and others.

This was recognized by many investigators to move a dislocation is not modeled by the spirit of a lattice model, and the results of Pearis (1940) and Nakasone (1955) have been of great practical use. The spirit of the interatomic potential such as a strong effect on the properties of the materials, the interatomic potential has provided a useful tool for the development of the shell model. The spirit of the investigation of the parameters $\lambda$ and $\mu$ in the spirit of the model is not modeled by the spirit of the lattice model, and the results of Pearis (1940) and Nakasone (1955) have been of great practical use.
between eqn. (26) and the atomistic calculations suggest that Frenkel's sinusoidal relation does not model the interlayer shear resistance accurately.

This was recognized by Foreman et al. (1951), who noted that the stress required to move a dislocation is usually far less than that which is predicted by the model of Peierls (1940) and Nabarro (1947), which is based on Frenkel's relation. Foreman et al. (1951) demonstrated that, when skewed shear resistance profiles are used in the Peierls-Nabarro model, wider dislocation cores are obtained which move at substantially reduced levels of stress. In the present context, modifications of the interlayer potential such as suggested by Foreman et al. (1951) will also be found to have a strong effect on activation energies for dislocation emission. We note, parenthetically, that in the well known bubble model of Bragg and Lomer (1949), which has provided a useful analogue for exploring crystal defects and structure in amorphous materials, the interbubble potential is very markedly skewed (Lomer 1949, Shi and Argon 1982).

In order to reflect more realistically the shear resistance properties of materials in the spirit of Foreman et al. (1951), and to decouple the unstable stacking energy from the shear modulus, we represent the shear resistance relation by the general Fourier expansion

\[ \tau(\Delta_r) = \sum_{n=1}^{\infty} \lambda_n \sin \left( \frac{2n\pi \Delta_r}{b} \right). \]  

Evidently, Frenkel's relation (19 a) is recovered by retaining only the first component in the expansion. The identification of the Fourier coefficients \( \lambda_n \) of all orders would require a wealth of experimental data or a full atomistic calculation. In all subsequent developments, we shall truncate eqn. (27) beyond the second term, that is we shall presume that \( \lambda_n = 0 \) for \( n > 2 \). The second term in the expansion furnishes the lowest order correction to the sinusoidal relation and this provides a basis for a systematic investigation of the effect of deviations from Frenkel's model.

The parameters \( \lambda_1 \) and \( \lambda_2 \) in eqn. (27) are readily determined by requiring that the
initial slope match the shear modulus, that is
\[ h \frac{d\tau}{d\Delta_r} \bigg|_{\Delta_r=0} = \mu, \]  
(28)

and that the unstable stacking energy (20) take a prescribed value. These requirements yield
\[ \lambda_1 = \frac{\pi y_{us}}{b}, \]  
(29a)
\[ \lambda_2 = \frac{\pi y_{us}}{b} \left( \frac{1}{2} \beta - 1 \right). \]  
(29b)

The new parameter
\[ \beta = \frac{\beta^\text{eq}}{y_{us}} = \frac{\mu b^2}{2\pi^2 h y_{us}^0}, \ 1 \leq \beta \leq 2, \]  
(30)
measures the skewness of the function \( \tau(\Delta_r) \) and effectively decouples the shear modulus from the unstable stacking energy. Using eqns (29a) and (29b), eqns (17a) and (27) become
\[ \tau = \frac{\pi y_{us}}{b} \left[ \sin \left( \frac{2\pi \Delta_r}{b} \right) + \frac{\beta - 1}{2} \sin \left( \frac{4\pi \Delta_r}{b} \right) \right], \]  
(31a)
\[ \delta_r = \Delta_r - \frac{b}{2\pi \beta} \left[ \sin \left( \frac{2\pi \Delta_r}{b} \right) + \frac{\beta - 1}{2} \sin \left( \frac{4\pi \Delta_r}{b} \right) \right]. \]  
(31b)

Evidently, Frenkel's model is recovered upon setting \( \beta = 1 \).

Complete traction–displacement relations can be derived following the Beltz–Rice approach as outlined above. The result is
\[ \tau(\Delta_r, \Delta_\theta) = A(\Delta_\theta) \left[ \sin \left( \frac{2\pi \Delta_r}{b} \right) + \frac{\beta - 1}{2} \sin \left( \frac{4\pi \Delta_r}{b} \right) \right], \]  
(32a)
\[ \sigma(\Delta_r, \Delta_\theta) = \left( B(\Delta_r) - C(\Delta_r) \right) \exp \left( -\frac{\Delta_\theta}{L} \right), \]  
(32b)
with
\[ A(\Delta_\theta) = \frac{\pi y_{us}}{b} \left( 1 + \frac{1}{2} \frac{q - p}{1 - p} \frac{\Delta_\theta}{L} \right) \exp \left( -\frac{\Delta_\theta}{L} \right), \]  
(33a)
\[ B(\Delta_r) = \frac{2\gamma_k}{L} \left[ 1 - \frac{q - p}{1 - p} \left[ \sin^2 \left( \frac{\pi \Delta_r}{b} \right) + \frac{\beta - 1}{4} \sin^2 \left( \frac{2\pi \Delta_r}{b} \right) \right] \right], \]  
(33b)
\[ C(\Delta_r) = \frac{2\gamma_k}{L} \left[ \frac{1 - p}{1 - p} \left[ \sin^2 \left( \frac{\pi \Delta_r}{b} \right) + \frac{\beta - 1}{4} \sin^2 \left( \frac{2\pi \Delta_r}{b} \right) \right] \right]. \]  
(33c)

The corresponding potentials are then
\[ \Psi(\Delta_r, \Delta_\theta) = 2\gamma_k \left[ 1 - \left( 1 + \frac{\Delta_\theta}{L} \right) \exp \left( -\frac{\Delta_\theta}{L} \right) \right] \]  
(34)
\[ + \left[ \sin^2 \left( \frac{\pi \Delta_r}{b} \right) + \frac{\beta - 1}{4} \sin^2 \left( \frac{2\pi \Delta_r}{b} \right) \right] \left[ q + \frac{q - p}{1 - p} \frac{\Delta_\theta}{L} \right] \exp \left( -\frac{\Delta_\theta}{L} \right) \]  
and
\[ \Phi(\delta_n, \delta_\theta) = \]  

The relation between \( y_{us}^{(i)} \) of \( p \) in the table are Al(311)(011), the valk \( y_{us}^{(i)}, y_{us}^{(0)} = 0.9 \), which is rox (Sun et al. 1993). For Fe(12), the largest possible depart Si in the glide system \( l \) \( (011) \) the table, \( L \) is determined relation

Figures 4 and 5 show the cases \( \Delta_\theta = 0 \) and \( \Delta_\theta \) apparent in fig. 5. It is re proportional to the value of energy. Similarly, figs 6 a and \( \Delta_r = b/2 \) respectively. displacement \( \Delta_r \). However The strong reciprocal soft traced to the existence of resistance in tension is cot resistance in shear is less i an interplanar potential an

In closing this section interplanar spacing \( h \) in eqr between the unstable stack communication has devis serves purposes similar to

§ 4. TWO-DIMENSION

We begin by consider of the plane of the crack. a stress intensity factor \( K_H \) assumed to hold on the sli \( \lambda_n = 0 \) for \( n > 2 \). This prob (1994) for \( \beta = 1 \). They det the crack tip, \( \delta_{tip} = \delta(0) \), a

As \( G_H \) increases from zero t dislocations form on the sli The parameter \( \delta_{tip} \) then me of the periodicity of the int point \( G_H = G_{cd} = y_{us}^{(i)}, \delta_{tip} \).
and
\[ \Phi(\delta_r, \delta_\theta) = \Psi(\Delta_r, \Delta_\theta) - \frac{h}{2\mu} \tau^2(\Delta_r, \Delta_\theta) - \frac{h}{2c} \sigma^2(\Delta_r, \Delta_\theta). \] (35)

The relation between \( \gamma_{us}^{(r)} \) and \( \gamma_{us}^{(n)} \) is given by eqn. (25) independently of \( \beta \). The values of \( p \) in the table are determined from eqn. (25). For Ni\([\frac{1}{2}][0\bar{1}1](111) \) and \( \text{Al}[\frac{1}{2}][0\bar{1}1](111) \), the value of \( \gamma_{us}^{(r)} \) is not available and \( p \) is determined by taking \( \gamma_{us}^{(r)}/\gamma_{us}^{(n)} = 0.9 \), which is roughly in keeping with ratios computed for other materials (Sun et al. 1993). For Fe\([\frac{1}{2}][111](1\bar{1}0) \) we obtain the limiting value \( \beta = 2 \), which signals the largest possible departure from Frenkel’s relation. By contrast, we obtain \( \beta = 1 \) for Si in the glide system \( [\frac{1}{2}][2\bar{1}1](111) \), in accordance with Frenkel’s model. To complete the table, \( L \) is determined by matching the uniaxial strain modulus \( c \), which yields the relation
\[ L = \left( \frac{2\gamma rh}{c} \right)^{1/2}. \] (36)

Figures 4 and 5 show the dependence of \( \tau \) on \( \Delta_r \) for the materials in the table and the cases \( \Delta_\theta = 0 \) and \( \Delta_\theta = L \) respectively. The tension-softening effect is clearly apparent in fig. 5. It is readily verified that the tension-softening effect is inversely proportional to the value of \( q \), the ratio of the unstable stacking energy to the surface energy. Similarly, figs 6 and 7 show the dependence of \( \sigma \) on \( \Delta_\theta \) for the cases \( \Delta_r = 0 \) and \( \Delta_r = b/2 \) respectively. Interestingly, the cohesive strength is also reduced by a shear displacement \( \Delta_r \). However, this effect is less pronounced than the reduction of \( \tau \) by \( \Delta_\theta \). The strong reciprocal softening effects between shear and tension can ultimately be traced to the existence of an interatomic potential. While the softening of the shear resistance in tension is consistent with intuition, the converse softening of the tensile resistance in shear is less intuitive. Nevertheless, we shall accept the consequences of an interplanar potential and shall not pursue other possible coupling relations.

In closing this section we remark that Rice and Beltz (1994) suggested taking the interplanar spacing \( h \) in eqn. (26) as an adjustable parameter in order to relax the relation between the unstable stacking energy and the shear modulus. J. R. Rice (1994 private communication) has devised a two-parameter tension–shear interlayer potential which serves purposes similar to our present modelling.

§ 4. TWO-DIMENSIONAL DISLOCATION NUCLEATION UNDER MODE II LOADING

We begin by considering the simple case of a slip plane which lies in the extension of the plane of the crack. The crack is subjected to pure mode II loading resulting in a stress intensity factor \( K_{II} \). The periodic shear resistance relation (31a) and (31b) is assumed to hold on the slip plane, with \( \lambda_1 \) and \( \lambda_2 \) given by eqns (29a) and (29b) and \( \lambda_n = 0 \) for \( n > 2 \). This problem has been investigated by Rice (1992) and Rice and Beltz (1994) for \( \beta = 1 \). They derived a relation between the inelastic shear displacement at the crack tip, \( \delta_{up} = \delta(0) \), and the applied energy release rate of the form
\[ G_{II} = \frac{1 - v}{2\mu} K_{II}^2 = \Phi(\delta_{up}) = \int_0^{\delta_{up}} \tau \, d\delta_r. \] (37)

As \( G_{II} \) increases from zero to its maximum value \( G_{cd} \), a stable cluster of distributed edge dislocations form on the slip plane and penetrate into the region ahead of the crack tip. The parameter \( \delta_{up} \) then measures the total Burgers vector of the dislocations. Because of the periodicity of the interplanar shear potential, an instability occurs at the critical point \( G_{II} = G_{cd} = \gamma_{us}^{(n)} \), \( \delta_{up} = b^* \), beyond which a fully formed straight dislocation is
Shear resistance $\tau$ against displacement $\Delta$, for tensile opening displacement $\Delta_0 = 0$. The nomenclature refers to the table.

Shear resistance $\tau$ against displacement $\Delta$, for tensile opening displacement $\Delta_0 = L$. The nomenclature refers to the table.
Tensile separation resistance $\sigma$ against tensile displacement $\Delta$ for a shear displacement $\Delta_s = L/2$.

The nomenclature refers to the table.

Nucleation of dislocations
The variation in the inelastic shear displacement $\delta_{\text{tip}}$ at the crack tip with the applied stress intensity factor $K_{\Pi}$.

Successive profiles of the emitted dislocation in pure mode II, $\beta = 1.0$.

emitted under decreasing $G_{\Pi}$. It therefore follows that, for any $G_{\Pi} < G_{\text{crb}}$, stable and unstable solutions exist corresponding to $\delta_{\text{tip}} < b^*$ and $\delta_{\text{tip}} > b^*$ respectively. These solutions are separated by an energy barrier

$$\Delta U_{\text{act}} = \Pi(\delta_{\text{sat}}(x)) - \Pi(\delta_{\text{sat}}(x)),$$

where $\Pi(\delta_{\text{sat}}(x))$ and $\Pi(\delta_{\text{sat}}(x))$ are the potential energies at the saddle point and stable equilibrium configurations respectively. $\Delta U_{\text{act}}$ may also be regarded as the activation energy required for bridging both configurations. In two dimensions, $\Delta U_{\text{act}}$ is defined necessarily as an energy per unit length.

In our calculations, the Burgers vector $b$ is taken as the normalizing length parameter and Poisson’s ratio $\nu$ is set to 0.3. Figure 8 shows the variation on $\delta_{\text{tip}}$ with the applied stress intensity factor $K_{\Pi}$. The corresponding profile of the dislocation being emitted is shown in fig. 9 for $\beta = 1$. In these figures represent configurations as $G_{\Pi}$ is in the displacement profiles. Various levels of the open stacking energy $\gamma_{\text{as}}$ is key according to eqn. (30). Int sensitively on $\beta$. For large is flatter, in agreement wi

The dependence of the $G_{\Pi}/G_{\text{crb}}$ is shown in figs 1 stacking energy $\gamma_{\text{as}}^0$, the increasing $\beta$. This implies
Nucleation of dislocations

Fig. 10

Successive profiles of the emitted dislocation in pure mode II, \( \beta = 1.5 \).

Fig. 11

Successive profiles of the emitted dislocation in pure mode II, \( \beta = 2 \).

is shown in fig. 9 for \( \beta = 1 \), in fig. 10 for \( \beta = 1.5 \) and in fig. 11 for \( \beta = 2 \). The solid curves in these figures represent the displacement profiles in the stable equilibrium configurations as \( G_H \) is increased from zero to \( G_{cd} \). The broken curves correspond to the displacement profiles in the unstable configurations as \( G_H \) decreases from \( G_{cd} \). The various levels of the opening front can be identified with reference to fig. 8. The unstable stacking energy \( \gamma^{(u)}_{st} \) is kept constant in all three cases, which requires \( \mu \) to be adjusted according to eqn. (30). Interestingly, the core width of the emitted dislocation depends sensitively on \( \beta \). For large \( \beta \) the displacement distribution at the centre of the dislocation is flatter, in agreement with the results of Foreman et al. (1951).

The dependence of the two-dimensional activation energy \( \Delta u_{\text{act}}^{(2d)} \) per unit length on \( G_H/G_{cd} \) is shown in figs 12 and 13. It is seen from fig 12 that, for the same unstable stacking energy \( \gamma^{(u)}_{st} \), the activation energy for dislocation emission increases with increasing \( \beta \). This implies that the activation energy for dislocation emission does not
The activation energy per unit length for two-dimensional dislocation emission in pure mode II scaled by unstable stacking energy.

The activation energy per unit length for two-dimensional dislocation emission in pure mode II scaled by line tension.

strictly scale with \( r_{\text{int}}^{(w)} \) but also depends on the skewness of the shear resistance curve. By contrast, when scaled with the line energy, the activation energy depends less strongly on \( \beta \) as shown in fig. 13. In comparison, the figures also display the analytical results of Rice (1992). The close agreement with our calculations attests to the accuracy of the numerical procedure.

§ 5. THREE-DIMENSIONAL DISLOCATION CONFIGURATIONS AND ACTIVATION ENERGIES

The preceding two-dimensional analysis artificially restricts the emitted dislocation to be straight. The three-dimensional problem has been investigated by Schöck and Püschl (1991) and Rice and Beltz (1994). However, these analyses also restrict the geometry of the emitted \( \epsilon \) (Schöck and Püschl 1991) configuration (Rice and Bel analysis which allows for a numerical procedure outline consider dislocation config. In this context, the activation While the assumption of pe can be minimized by adopting protruding dislocation loops quadratically with their sep.

We begin by considering in the three-dimensional analysis.

In order to trigger non-straight behavior is introduced, with \( \epsilon = 0.005 \) critical value \( G_{\text{cr}} \). This typ post-bifurcation analyses a (Koiter 1945, Hutchinson ar effective imperfection is for similar vein, the \( x_2 \)-dependence and Ortiz (1990) of unstable shows that the long-wavelength by the first-order perturbative trends. The longest wavelength the period \( T \) of the mesh, wh systematic method for determine Vineyard's (1957) theory of solution of a full eigenvalue which may be computationally considered in the manner of here appears effective, and

The unstable (saddle-potential) are depicted in figs 15–18 it is set to unity, which is representive of Fe. The displacement \( \delta \), in the \( x_1 \) diplace by the bulging out of: subsequently spreads out a The kinks spread out more: to the larger shear resistance where the drop of resistance.

The dependence of the Rice–Beltz (1994) solution: from it away from the critical analysis. By contrast, the SeC of the athermal critical point
geometry of the emitted dislocation, by prescribing its shape to be rectangular (Schöck and Püschl 1991), or by assuming small deviations from the straight configuration (Rice and Beltz 1994). In this section, we present a three-dimensional analysis which allows for arbitrary dislocation shapes. The analysis is based on the numerical procedure outlined in §2. In order to have a finite domain of analysis, we consider dislocation configurations which are periodic in the direction of the crack front. In this context, the activation energy is understood to be the activation energy per period. While the assumption of periodicity is in itself a geometrical restriction, its influence can be minimized by adopting a period $T$ much larger than the lateral dimension of the protruding dislocation loops, since the interaction energy between the loops dies off quadratically with their separation.

We begin by considering the pure mode II case. Figure 14 shows the mesh used in the three-dimensional analysis. The period of the mesh in the $x_2$ direction is $T = 24b$. In order to trigger non-straight unstable solutions, a small perturbation of the form

$$\Delta \delta(x_1, x_2) = \varepsilon \cos \left( \frac{2\pi x_2}{T} \right) \exp \left( -\frac{x_1^2}{b^2} \right)$$

is introduced, with $\varepsilon = 0.005b$, as the loading parameter $G_{II}$ begins to decrease from the critical value $G_{cd}$. This type of approach is commonly adopted in post-buckling or post-bifurcation analyses and has been developed by a number of investigators (Koiter 1945, Hutchinson and Koiter 1970, Budiansky 1974). In this context, the most effective imperfection is found to coincide with the most critical buckling mode. In a similar vein, the $x_2$ dependence of $\Delta \delta$ adopted here is suggested by the analysis of Bower and Ortiz (1990) of unstable crack growth into a region of diminishing toughness, which shows that the long-wavelength distortions of the crack front are the most critical, and by the first-order perturbation analysis of Rice and Beltz (1994), which reveals similar trends. The longest wavelength which is allowed by the present model coincides with the period $T$ of the mesh, which accounts for the term $\cos (2\pi x_2/T)$ in eqn. (39). A more systematic method for determining the dominant unstable modes is provided by Vineyard’s (1957) theory of rate processes. However, Vineyard’s theory requires the solution of a full eigenvalue problem obtained by linearization at the critical point, which may be computationally costly, even if a subspace iteration procedure is considered in the manner of Clough and Plumlee (1975). The simple approach adopted here appears effective, and therefore more rigorous alternatives will not be pursued.

The unstable (saddle-point) equilibrium configurations of the emitted dislocations are depicted in figs 15–18 for decreasing values of $G_{II}/G_{cd}$. The skewness parameter $\beta$ is set to unity, which is representative of Si. Figs 19–22 concern the case $\beta = 2$, which is representative of Fe. The curves represent level contours of the inelastic shear displacement $\delta$, in the $x_1$ direction. Remarkably, dislocation emission is seen to take place by the bulging out of a dislocation packet in the form of a ‘double kink’, which subsequently spreads out along the crack front at decreasing driving force $G_{II}/G_{cd}$. The kinks spread out more rapidly with increasing $\beta$. This effect may be attributable to the larger shear resistance in the direction of emission relative to the case of $\beta = 1$, where the drop of resistance is steeper in the forward direction.

The dependence of the activation energy on $G_{II}/G_{cd}$ is shown in figs 23 and 24. The Rice–Beltz (1994) solution is tangential to the curve $\beta = 1$ at $G_{II}/G_{cd} = 1$ but diverges from it away from the critical point, as expected from the perturbative character of their analysis. By contrast, the Schöck–Püschl (1991) solution is less accurate in the vicinity of the athermal critical point but closer to the curve $\beta = 1$ elsewhere.
The saddle-point configuration at $G_{W}/G_{cd} = 0.99$ in pure mode II loading, $\beta = 1$.

It should be carefully noted that the energy owing to the perimeter of neighboring kinks. This term is insensitive to $T$ for $G_{I}$ dislocation loops can be expressed as $T \rightarrow \infty$. The results of this estimation approximate closely the range of $G_{W}/G_{cd}$. 

Mesh used in the analysis of three-dimensional dislocation nucleation. The period of the domain is $24b$. 

Fig. 14

Fig. 15
Nucleation of dislocations

Fig. 16
\[ G_{II}/G_{cd} = 0.80 \]

The saddle-point configuration at \( G_{II}/G_{cd} = 0.80 \) in pure mode II loading, \( \beta = 1 \).

Fig. 17
\[ G_{II}/G_{cd} = 0.62 \]

The saddle-point configuration at \( G_{II}/G_{cd} = 0.62 \) in pure mode II loading, \( \beta = 1 \).

It should be carefully noted that the numerical solution underestimates the activation energy owing to the periodicity of the model and the resulting attraction between neighbouring kinks. This effect can be minimized by increasing the period \( T \). The results are insensitive to \( T \) for \( G_{II}/G_{cd} \geq 0.5 \). The activation energy for nucleating an isolated dislocation loop can be estimated by extrapolating the results from several periods to the limit \( T \rightarrow \infty \). The result of this extrapolation is shown as the broken curve in fig. 25. From this estimate it may be concluded that a period of \( T = 32b \) suffices to approximate closely the activation energy of an isolated dislocation loop over a broad range of \( G_{II}/G_{cd} \).
Fig. 18
\[ \frac{G_{II}}{G_{cd}} = 0.43 \]

The saddle-point configuration at \( G_{II}/G_{cd} = 0.43 \) in pure mode II loading, \( \beta = 1 \).

Fig. 19
\[ \frac{G_{II}}{G_{cd}} = 0.99 \]

The saddle-point configuration at \( G_{II}/G_{cd} = 0.99 \) in pure mode II loading, \( \beta = 2 \).

§ 6. TWO-DIMENSIONAL DISLOCATION NUCLEATION UNDER MIXED-MODE LOADING

In this section we investigate a case which illustrates the tension-softening effect on dislocation emission. We envision a semi-infinite crack propping on the (112) slip plane of a b.c.c. crystal as shown in fig. 26. The crack front is parallel to the [110] direction and the Burgers vector is \( \frac{1}{2}[\overline{1}11] \), that is perpendicular to the crack front. The crack is subjected to a combination of mode II and mode I loading. The tension–shear coupling constitutive relations (32a), (32b), (33a), (33b) and (33c) are assumed to apply on the slip plane. We set \( \beta = 1.74 \), which is representative of the system \( \frac{1}{2}[\overline{1}11](112) \) of \( \alpha \)-Fe, and the remaining parameters are taken from the table.

Figure 27 shows the result of two-dimensional calculations giving the dependence of the critical mode II stress intensity factor \( K_{IIIc} \) for dislocation nucleation on the applied mode I stress intensity factor. The application of mode I load small up to values of \( K_I \) of underlying reason for the depicted sequence of consisting of an initial increment in mode II at constant \( K_I \), \( K_I \) decays rapidly away from dislocation core. This effect values of \( K_I \) close to \( K_{IIc} \) is unstable equilibrium concl.
Nucleation of dislocations

Fig. 20

\( G_{II}/G_{cd} = 0.80 \)

The saddle-point configuration at \( G_{II}/G_{cd} = 0.80 \) in pure mode II loading, \( \beta = 2 \).

Fig. 21

\( G_{II}/G_{cd} = 0.62 \)

The saddle-point configuration at \( G_{II}/G_{cd} = 0.62 \) in pure mode II loading, \( \beta = 2 \).

mode I stress intensity factor \( K_I \). The method of analysis is as in §4. Evidently, the application of mode I loading facilitates dislocation nucleation. However, the effect is small up to values of \( K_I \) of the order of 95% of the Griffith cleavage toughness \( K_{IC} \). The underlying reason for the weak mode I–mode II coupling is apparent in fig. 28, which depicts the sequence of opening and shear displacements for a loading program consisting of an initial increase of \( K_I \) from 0 to 0.9\( K_{IC} \) followed by displacement control in mode II at constant \( K_I \). It is observed in this figure that the opening displacement \( \delta_0 \) decays rapidly away from the crack front and does not significantly overlap with the dislocation core. This effectively precludes a strong tension–shear coupling except for values of \( K_I \) close to \( K_{IC} \). The broken curves in fig. 28 represent the two-dimensional unstable equilibrium configurations. The inset gives the variation in \( K_{II} \) with the crack...
The saddle-point configuration at $G_{II}/G_{cd} = 0.45$ in pure mode II loading, $\beta = 2$.

tip inelastic shear displacement at $K_1 = 0.9K_{ic}$. The shear instability occurs at the peak of the curve, which determines the critical value $K_{IIc}$. It is interesting to note that $K_{IIc}$ exhibits a sharp downturn as $K_1$ approaches $K_{ic}$. Our numerical simulations show that, at about $K_1 \approx 0.95K_{ic}$, cleavage and dislocation nucleation occur simultaneously and the crack extends in a steady state.

The dependence of the critical energy release rate

$$G_{cd} = \frac{1 - \nu}{2\mu} [K_1^2 + K_{IIc}^2(K_1)]$$

(40)

for dislocation emission on the phase angle

$$\psi = \tan^{-1}\left(\frac{K_{IIc}(K_1)}{K_1}\right)$$

(41)

is shown as the solid curve in fig. 29. For pure mode II loading ($\psi = 90^\circ$), it follows that $G_{cd} = \gamma_{us}$ while, for pure mode I loading ($\psi = 0^\circ$), one has $G_{cd} = 2\gamma_{us}$. On the basis of a shear-only model, Sun et al. (1993) obtained the elegant analytical relation

$$G_{cd} = \frac{\gamma_{us}}{\sin^2\psi} = \frac{1}{\sin^2\psi} \left[ \gamma_{us}^{(s)} - \alpha(\gamma_{us}^{(s)} - \gamma_{us}^{(t)}) \left( \frac{\pi}{2} - \psi \right) \right]$$

(42)

where $\gamma_{us}$ is an effective unstable stacking energy for mixed-mode loading and $\alpha$ is a reduction coefficient which is determined by fitting the coupled shear-tension results. Equation (42) with $\alpha = 0.856$ is plotted as the broken curve in fig. 29. The agreement with the numerical results is remarkably good in the range $\psi \geq 20^\circ$.

§ 7. DISLOCATION NUCLEATION ON INCLINED SLIP PLANES

As a cleavage crack is subjected to a mode I loading, a dislocation may nucleate on a slip plane which is inclined to the plane of the crack. Furthermore, the Burgers vector of the dislocation in general will not be perpendicular to the crack front. A case in point concerns a crack lying in the cleavage plane (001) of an $\alpha$-Fe crystal, its front in the [010] direction, emitting a dislocation of Burgers vector in the $\langle 11 \rangle$ direction
de II loading, $\beta = 2$.

ability occurs at the peak teresting to note that $K_{\text{nd}}$
ally simulations show that, ur simultaneously and the

$$F_{\text{cd}}$$

(40)

ling ($\psi = 90^\circ$), it follows as $G_{\text{cd}} = 2\gamma_s$. On the basis nt analytical relation

$$\psi \right)$$

-mode loading and $\alpha$ is a led shear-tension results.
in fig. 29. The agreement $\psi \geq 20^\circ$.

LIP PLANES

dislocation may nucleate. Furthermore, the Burgers
to the crack front. A case f an $\alpha$-Fe crystal, its front :tor in the $[\overline{1}11]$ direction

$$\frac{\Delta U_{\text{ex}}}{\beta \rho_{\text{in}}} B_n$$

The activation energy for three-dimensional dislocation emission in pure mode II loading scaled by the unstable stacking energy $\gamma_{\text{cd}}$.

$$\frac{\Delta U_{\text{ex}}}{\beta \rho_{\text{in}}} B_n$$

The activation energy for three-dimensional dislocation emission in pure mode II loading scaled by the line tension.
The effect of the size of the periodic cell on the activation energy for three-dimensional dislocation emission in pure mode II loading. The curve for a cell of infinite dimensions is obtained by extrapolation.

on the (101) plane as shown in fig. 30. In general, we shall let $\theta$ denote the angle between the slip plane and the crack surface, and $\phi$ the angle between the Burgers vector and a line perpendicular to the crack front in the slip plane. Using the effective stress intensity factor concept, Rice (1992) estimated the critical energy release rate for dislocation nucleation in two dimensions in an isotropic solid to be

$$G_{cd} = \frac{8}{(1 + \cos \theta) \sin^2 \theta} \gamma_{us}.$$  

(43)

The condition for the propagation of a cleavage crack is, on the other hand,

$$G_{tc} = 2\gamma_s.$$  

(44)

According to these criteria, crack tip blunting by dislocation emission precedes cleavage if $G_{cd} < G_{tc}$, which requires

$$\frac{\gamma_s}{\gamma_{us}} > 4 \frac{1 + (1 - v) \tan^2 \phi}{(1 + \cos \theta) \sin^2 \theta}.$$  

(45)

Since $\gamma_{us}$, which is a measure of interplanar shear resistance, decreases with increasing temperature more rapidly than $\gamma_s$ does, a condition such as eqn. (45) has the potential for explaining the brittle to ductile transition in intrinsically brittle materials. While the simple criterion (45) may help to explain the observed trends, quantitatively accurate predictions require careful consideration of such effects as tension softening (Sun et al. 1993) and the additional resistance due to surface production at the ledge formed when a dislocation is emitted on an inclined slip plane (see the papers by Zhou, Carlsson and Thomson (1994) based on a lattice Green function method, and by Kaxiras and Juan (1994) based on a first-principles approach).

The tension-softening effect can effectively be accounted for through a coupled tension–shear constitutive relation such as that considered in §3. In order to account for the surface production resistance, we resort to the simple model sketched in fig. 31.

Consider a quarter-space block sliding rigidly over a half-plane. Initially, the blocks are
energy for three-dimensional
a cell of infinite dimensions

\( \theta \) denote the angle between
the Burgers vector and
Using the effective stress
energy release rate for

\( \text{(43)} \)

the other hand,

\( \text{(44)} \)
mission precedes cleavage

decreases with increasing
eqn. (45) has the potential
brittle materials. While the
ds, quantitatively accurate
c as tension softening
cc production at the ledge
(see the papers by Zhou,

\( \text{eqn} \) method, and by Kaxiras

\( \text{eqn} \) for through a coupled
in § 3. In order to account
model sketched in fig. 31.

\( \text{eqn} \). Initially, the blocks are

Fig. 26

\[
\begin{align*}
[\{111]\] \quad K_\text{I} \\
[110].
\end{align*}
\]

The geometry of a crack under mixed-mode loading.

Fig. 27

\[
\begin{align*}
K_\text{II}/(2\mu\gamma/(1-\nu)) \\
0.0 & 0.2 & 0.4 & 0.6 & 0.8 & 1.0 \\
0.0 & 0.2 & 0.4 & 0.6 & 0.8 & 1.0
\end{align*}
\]

The dependence of the critical \( K_\text{II} \) on \( K_\text{I} \) for the nucleation of a dislocation in the \( 1/2[\{111\}]_{(112)} \)
system of \( \alpha \)-Fe.

Fig. 28

\[
\begin{align*}
\delta_g/b & \\
-25 & -20 & -15 & -10 & -5 & 0 & 5 & 10 & 15 \\
\delta_g/b & \\
-25 & -20 & -15 & -10 & -5 & 0 & 5 & 10 & 15
\end{align*}
\]

The sequence of shear and opening displacements in mixed-mode loading. \( K_\text{I} \) is increased from
0 to 0.9\( K_\text{Ic} \) followed by displacement control in shear. The inset gives the variation in
\( K_\text{II} \) with the crack tip inelastic shear displacement at \( K_\text{I} = 0.9K_\text{Ic}. \)
configured so that the free at the intersection between energy. We define the surfi of the shear resistance $\tau_s$, $\theta$ production resistance show small several atomic spac resistance as the two block by energy conservation, w

\[ \tau_s = \frac{s}{L} \]

which satisfies all the af represents the depth of de concentrated loads at $s = 0$ tension. In the opposite limit uniformly. The value of $\lambda$ is materials than for metallic the inclination $\phi$ of the slip parameter and investigate

We proceed to incorporate potential. By definition of

where $\tau_s$ is the shear resist of the form (31a) and $\theta_s$ is take to be of the form (47). given in §3, we find that

\[ \tau(D_s, \Delta_b; s) \]

\[ \sigma(D_s, \Delta_b; s) \]

and

\[ A'(D_b; s) = \frac{\pi r_m}{b} \]

\[ B'(D_s; s) = \frac{2r_s}{L} \]
configured so that the free boundary is smooth. As the blocks slide, bonds are severed at the intersection between the slip plane and the free boundary at some expense in energy. We define the surface production resistance \( \tau_s \) as the shear resistance in excess of the shear resistance \( \tau_r \) against slip alone in an infinite crystal. Intuitively, the surface production resistance should decrease rapidly from the corner and become vanishingly small several atomic spacings away from the corner. The work done against this resistance as the two blocks slide by one Burgers vector must equal to \( \gamma \mathbf{b} \), as required by energy conservation, which gives the condition

\[
\int_0^\infty \int_0^b \tau_s \, dA_r \, ds = \gamma \mathbf{b},
\]

(46)

where \( s \) is the distance to the corner. Because of the periodicity of the lattice, \( \tau_s \) may reasonably be expected to be itself periodic in \( A_r \), for fixed \( s \). In addition, surface fields are often found to decay exponentially with depth (for example Midlin (1965)). Here again, the precise characterization of \( \tau_s \) requires atomistic modelling. In lieu of this type of information, we postulate the following form:

\[
\tau_s = \frac{\lambda \gamma_s}{b} \exp \left( -\frac{\lambda s}{b} \right) \left[ 1 - \cos \left( \frac{2\pi A_r}{b} \right) \right],
\]

(47)

which satisfies all the aforementioned constraints. In eqn. (47), the parameter \( \lambda \) represents the depth of decay of \( \tau_s \). In the limit of \( \lambda \rightarrow \infty \), eqn. (47) reduces to two concentrated loads at \( s = 0 \), in accordance with the conventional description of surface tension. In the opposite limit of \( \lambda \rightarrow 0 \), the surface production resistance reduces to zero uniformly. The value of \( \lambda \) is expected to be in the range 1–2, and to be larger for covalent materials than for metallic materials. In addition, \( \lambda \) is as yet unknown function of the inclination \( \phi \) of the slip plane. In view of these uncertainties, we shall treat \( \lambda \) as a parameter and investigate its effect by varying it within its expected range.

We proceed to incorporate the surface shear resistance into a conservative interlayer potential. By definition of \( \tau_s \), the total shear resistance \( \tau \) near the surface is

\[
\tau = \tau_r + \tau_s,
\]

(48)

where \( \tau_r \) is the shear resistance against slip in an infinite crystal, which we take to be of the form (31 a) and \( \tau_s \) is the excess shear resistance near the free surface, which we take to be of the form (47). Proceeding as in the treatment of the tension–shear coupling given in § 3, we find that

\[
\tau(A_r, A_\theta; s) = A'(A_\theta; s) \left[ \sin \left( \frac{2\pi A_r}{b} \right) + \frac{\beta - 1}{2} \sin \left( \frac{4\pi A_r}{b} \right) \right]
\]

\[
+ \frac{\rho(s)}{2\pi q} \frac{\rho(s)}{2\pi q} \cos \left( \frac{2\pi A_r}{b} \right),
\]

(49a)

\[
\sigma(A_r, A_\theta; s) = \left[ B'(A_r; s) \frac{A_\theta}{L} - C'(A_r; s) \right] \exp \left( -\frac{A_\theta}{L} \right)
\]

(49b)

and

\[
A'(A_\theta; s) = \frac{\pi \gamma_{ys}}{b} \left( 1 + \frac{1}{q} \frac{q - p(s)\xi(s)}{1 - p(s)} \frac{A_\theta}{L} \right) \exp \left( -\frac{A_\theta}{L} \right),
\]

(50a)

\[
B'(A_r; s) = \frac{2\gamma_{ys}}{L} \left( 1 - \frac{q - p(s)\xi(s)}{1 - p(s)} \left[ \sin^2 \left( \frac{\pi A_r}{b} \right) + \frac{\beta - 1}{4} \sin^2 \left( \frac{2\pi A_r}{b} \right) \right] \right)
\]
G. Xu et al.

\[ C' (A_r, s) = \frac{2 \gamma_s \rho(s) \pi(s) - q}{L \left( 1 - p(s) \right)} \left[ \sin^2 \left( \frac{\pi A_r}{b} \right) + \frac{\beta - 1}{4} \sin^2 \left( 2 \pi A_r \right) b \right] \]

\[ + \frac{\rho(s) A_r}{2q b} - \frac{\rho(s)}{4q b} \sin \left( 2 \pi A_r \right) b \]  

(50c)

with

\[ q = \frac{\gamma_{\text{th}}}{2 \gamma_s} \]

(51a)

\[ \rho(s) = \lambda \exp \left( - \frac{\lambda s}{b} \right) \]

(51b)

\[ p(s) = \frac{\Delta \xi(s)}{L} \]

(51c)

\[ \alpha(s) = \frac{4q}{4q + \rho(s)} \]

(51d)

The corresponding tension–shear potential now becomes

\[ \Psi (A_r, A_s; s) = 2 \gamma_s \left[ 1 - \left( 1 + \frac{\Delta \xi}{L} \right) \exp \left( - \frac{\Delta \xi}{L} \right) \right] \]

\[ + \left[ \sin^2 \left( \frac{\pi A_r}{b} \right) + \frac{\beta - 1}{4} \sin^2 \left( 2 \pi A_r \right) b \right] \]

\[ + \frac{\rho(s) A_r}{2q b} - \frac{\rho(s)}{4q b} \sin \left( 2 \pi A_r \right) b \]

\[ \times \left( q + \frac{p q + \rho(s) A_r}{1 - p} \right) \exp \left( - \frac{\Delta \xi}{L} \right) \]  

(52)

Some limitations of the above model should be carefully noted. For instance, our approach does not explicitly account for the effects of local stress concentrations and reconstruction on the interlayer potential. It might also be more appropriate to replace \( A_r \) in eqn. (47) by the inelastic displacement \( \delta \). This, however, complicates the model by, for instance, rendering \( p \) coordinate dependent. Since \( p \) measures the relaxation of shear resistance as atoms move relative to each other, its effect on dislocation nucleation should decrease as the tensile stress increases. In the simple shear case, the critical energy release rate for dislocation nucleation is lowered by about 10% if relaxation is allowed for (Sun et al. 1993). However, this effect may be expected to be lessened in the presence of substantial tension softening, which is always present in situations where dislocation nucleation and cleavage fracture are in competition. For simplicity, in calculations we have set \( p = 0 \), corresponding to no relaxation.

We begin by considering an idealized configuration in which the Burgers vector is perpendicular to the crack front, that is \( \phi = 0^\circ \). We set the ratio of Burgers vector to interplanar spacing \( b/h = 1 \), Poisson’s ratio \( v = 0.3 \) and skewness parameter \( \beta = 1 \). Two slip planes at \( \theta = 45^\circ \) and \( \theta = 90^\circ \) are considered. The crack is subjected to pure mode I loading resulting in a stress intensity factor \( K_1 \). The possible energy release rate from the crack field given by

\[ G_1 = \frac{1 - v}{2\mu} K_1^2 \]

(53)

More precisely, \( K_1^{\text{eff}} \) and \( K_1 \) are indicative of a tendency to a propensity for ductile bel ductile behaviour, while a indeed, the trends revealed \( G_{\text{eff}}/G_{\text{lc}} \) be an increasing f in fig. 32. We note, howe predicted by Rice’s approx effect. The departure from reaches asymptotically a release rate \( G_{\text{eff}}/G_{\text{lc}} \) is required Rice’s relation closely mat In all cases, however, Rio values.

The effect of the shear calculations for \( \lambda = 1 \) and i production shear resistance and therefore causes a sub that, even in nominally di nucleation on inclined s
\[ \frac{\rho(s)}{4\pi q} \sin \left( \frac{2\pi \Delta_r}{b} \right) \]

\[ \frac{1}{2} \pi \frac{\Delta_r}{b} \]

\[ G_e / G_{lc} \]

\[ \lambda = 0 \]
\[ \lambda = 1.0 \]
\[ \text{Rice (1992)} \]
\[ \text{effective cleavage} \]

Dependence of the critical energy release rate \( G_e/G_{lc} \) on \( q \) for dislocation nucleation at 45°.

furnishes an alternative and more meaningful loading parameter. We note for later reference that the effective stress intensity factors acting on the slip plane are

\[ K_1^{\text{eff}} = K_1 \cos^2 \left( \frac{\theta}{2} \right) \]

\[ K_\Pi^{\text{eff}} = K_1 \cos^2 \left( \frac{\theta}{2} \right) \sin \theta. \]

More precisely, \( K_1^{\text{eff}} \) and \( K_\Pi^{\text{eff}} \) are the intensity factors at the tip of a small crack emanating from the crack tip in the direction of the slip plane ( Cotterell and Rice 1980).

Figure 32 shows the dependence of the critical energy release rate \( G_e/G_{lc} \) for nucleation at 45° on the parameter \( q = \gamma_a/2\gamma_s \). We recall that a high ratio \( G_e/G_{lc} \) is indicative of a tendency towards brittle behaviour, while a low value of \( G_e/G_{lc} \) denotes a propensity for ductile behaviour. In addition, a small value of \( q \) is expected to favour ductile behaviour, while a large value of \( q \) should promote brittle behaviour. These are, indeed, the trends revealed by eqn. (43) ( Rice 1992). The expectation is therefore that \( G_e/G_{lc} \) be an increasing function of \( q \). Our results do indeed exhibit this trend as shown in fig. 32. We note, however, that the dependence of \( G_e/G_{lc} \) on \( q \) is not linear, as predicted by Rice's approximate relation (43), as a consequence of the tension-softening effect. The departure from proportionality is more severe for large \( q \), where \( G_e/G_{lc} \) reaches asymptotically a constant value. This constant is of the order of the energy release rate \( G_t/G_{tc} \) required to cleave the slip plane, shown in fig. 32 as a broken line. Rice's relation closely matches the computed behaviour for \( \lambda = 0 \) in the range \( q < 0.15 \). In all cases, however, Rice's relation overestimates \( G_e/G_{lc} \) relative to the computed values.

The effect of the shear resistance to surface production is accounted for in the calculations for \( \lambda = 1 \) and is neglected in the results for \( \lambda = 0 \). Interestingly, the surface production shear resistance results in significantly higher values of \( G_e/G_{lc} \) for \( q < 0.2 \) and therefore causes a substantial embrittlement of the material. This result suggests that, even in nominally ductile materials, that is materials with small \( q \), dislocation nucleation on inclined slip planes may not be energetically favoured at low
Dependence of the critical energy release rate $G_{cd}/G_{tc}$ on $q$ for dislocation nucleation at 90°.

Figure 34 shows $G_{cd}/G_{tc}$ for nucleation on slip planes at 90° as a function of $q$. While trends similar to the 45° case are evident from the figure, the rate at which the horizontal asymptote is approached is much slower in the 90° case. The result attest to the considerable difficulty in nucleating a dislocation loop at 90° against the surface production resistance.

The effect of the parameter $\lambda$ on $G_{cd}/G_{tc}$ is shown in fig. 34 for a typical case of $q = 0.125$. As pointed out earlier, the limit of $\lambda \to \infty$ corresponds to a conventional treatment of surface pro-ostensibly attained for $\lambda >$ these values, $G_{cd}/G_{tc}$ is e

We conclude this sect in two representative mat case of a crack lying in t a dislocation of Burgers loading. For Si, we consi in the [110] direction, emi also under the action of:

In both cases, there an on the crack tip. We note unlikely owing to symm the crack front. Once a relaxation makes it more while the dominant disloc by observation (Chiao a displacement hypothesis displacements, and the :direction of the dominant calculations (Yamaguchi 1994).

When slip takes place is not normal to the crac

and accordingly the surf:

$\tau_s = \cdot$

As required, $\tau_s = 0$ when which entails no surface

The material constan table, except that $p$ is set t and Si are $G_{cd}/G_{tc} = 1.42$: with the results of the si relatively insensitive to relatively large $\gamma_{sl}/2\gamma_s$ rat $\alpha$-Fe and Si would be int on the inclined slip sys dislocation nucleation on conclusions. It seems app not intrinsically brittle as cleavage, other rate-limiti the crack tip may cause t observed to play a part semiconductor materials i
treatment of surface production through surface tension. This limiting behaviour is
ostensibly attained for ̂λ > 0.5 in the case of 45°, and for ̂λ > 2 in the case 90°. Beyond
these values, \( G_{dG} / G_{bc} \) is essentially independent of ̂λ.

We conclude this section with a somewhat idealized study of dislocation nucleation
in two representative materials, namely α-Fe and Si. For Fe, we consider as before
the case of a crack lying in the (001) plane with its front in the [010] direction, emitting
a dislocation of Burgers vector \( \frac{1}{2} [111] \) on the (101) plane under the action of mode I
loading. For Si, we consider the case of a crack lying in the (110) plane with its front
in the [110] direction, emitting a dislocation of Burgers vector \( \frac{1}{2} [101] \) on the (111) plane
also under the action of mode I loading.

In both cases, there are four crystallographically equivalent slip systems converging
on the crack tip. We note, however, that simultaneous emission on all four systems is
unlikely owing to symmetry-breaking thermal fluctuations and heterogeneities along
the crack front. Once a dislocation is nucleated in one system, the attendant stress
relaxation makes it more difficult for the remaining dislocations to be emitted, at least
while the dominant dislocation remains near the crack front. This scenario is borne out
by observation (Chiao and Clarke 1989). We shall therefore adopt the constrained
displacement hypothesis of Rice (1992) and Sun et al. (1993) according to which
displacements, and the attendant shear resistance, take place predominantly in the
direction of the dominant Burgers vector. This conjecture finds support in atomistic
calculations (Yamaguchi, Vitek and Pope 1981, Sun et al. 1991, Kaxiras and Juan
1994).

When slip takes place at an angle \( \phi \neq 0° \), corresponding to a Burgers vector which
is not normal to the crack front, then condition (46) needs to be replaced by

\[
\int_0^\infty \int_0^b \tau_s \, dA_s \, ds = \gamma_s b \cos \phi,
\]

and accordingly the surface production resistance relation (47) becomes

\[
\tau_s = \frac{\lambda \gamma_s}{b} \exp \left( -\frac{\lambda s}{b} \right) \cos \phi \left[ 1 - \cos \left( \frac{2\pi A_s}{b} \right) \right].
\]

As required, \( \tau_s = 0 \) when \( \phi = 90° \). This corresponds to slip parallel to the crack front,
which entails no surface production.

The material constants necessary to evaluate these two cases are taken from the
table, except that \( p \) is set to 0. The calculated dislocation nucleation conditions for α-Fe
and Si are \( G_{dG} / G_{bc} = 1.42 \) and \( G_{dG} / G_{bc} = 1.23 \) respectively. These are in good agreement
with the results of the simulations of Sun et al. (1993). The calculations should be
relatively insensitive to the choice of \( \lambda \) in view of the high tensile stresses and
relatively large \( \gamma_{ss} / 2\gamma_s \) ratios which are involved in both cases. Our results suggest that
α-Fe and Si would be intrinsically brittle if dislocation nucleation were possible only
on the inclined slip systems considered in the analysis. Further consideration of
dislocation nucleation on oblique slip planes is required in order to strengthen these
conclusions. It seems appropriate to emphasize at this point that, even if a material is
not intrinsically brittle as regards the competition between dislocation emission and
cleavage, other rate-limiting effects such as inadequate dislocation mobility away from
the crack tip may cause the material to behave in a brittle manner. These effects are
observed to play a particularly significant role in intermetallic compounds and
semiconductor materials in which dislocation mobility is sluggish. Further large-scale
atomistic simulations and discriminating experimental studies are needed for developing a satisfactory understanding of these processes.

§ 8. DISCUSSION

In the present paper we have employed the variational boundary integral method of Xu and Ortiz (1993) to study dislocation nucleation from atomically sharp cracks under combined mode I—mode II loading. In addition, we have extended the tension–shear potential of Rice et al. (1992) so as to allow for skewness of the shear resistance curve and to incorporate a surface production resistance which accompanies ledge formation. As a consequence of the skewness effect, our potential decouples the unstable stacking energy from the shear modulus.

Our simulations of dislocation nucleation in two dimensions using a sinusoidal shear resistance are in full agreement with the analytical results of Rice and Beltz (1994), which attests to the accuracy of the numerical procedure. With a shear resistance curve appropriately skewed so as to represent Fe, we find significant departures from the results based on Frenkel’s sinusoidal relation, particularly as regards activation energies normalized by the unstable stacking energy. However, a considerable convergence of results is obtained where activation energies are normalized by line tension.

Our three-dimensional simulations of dislocation nucleation under pure mode II loading yield dislocation configurations which closely match the first-order perturbation results of Rice and Beltz (1994) near the critical point \( G_{II} = G_{cd} \), that is in the range of validity of the perturbation analysis. However, the computed dislocation configurations depart sharply from the Rice–Beltz solution elsewhere. We find that the Schöck–Püschl (1991) unrelaxed approximate solution qualitatively captures the overall trends revealed by our analysis. When a mode I component is added to the loading, we find that tension softening facilitates dislocation nucleation, although significantly so only when \( K_1 \) exceeds 0.95\( K_{ic} \).

Our simulations show that dislocation nucleation on inclined slip planes under mode I loading is impeded by surface production resistance, especially for low unstable stacking-energy–surface-energy ratios. For large ratios, tension softening is the dominant effect. Calculations tailored to \( \alpha \)-Fe and Si suggest that dislocation emission on inclined slip planes is not operative at low temperatures.

The recent developments initiated by Rice and Beltz and by Schöck and Püschl have established that the activation configuration of a dislocation nucleating from the tip of a cleavage crack is made up of a fractional dislocation core, and that as a result the large discrepancy that existed in the energy predictions of the original Rice–Thompson (1974) model has been radically reduced. While the results of the present analysis, still based on continuum line notions of dislocations given in fig. 23 and fig. 24 are somewhat less favourable than those of either the Rice–Beltz (1994) or the Schöck–Püschl (1991) models, none of these has yet been able to close the gap.

To demonstrate the magnitude of the remaining gap, we consider the brittle-to-ductile transition as a thermally activated dislocation nucleation event, for which the event probability should scale with a given ratio of \( \Delta U_{act}/kT \) as follows:

\[
\frac{\Delta U_{act}}{kT} = \frac{\alpha \mu b^3}{(1 - v) kT} = C, \tag{57}
\]

where \( C \) depends on the particular scenario of the brittle to ductile transition event and is typically of the order of 10 as we show for a specific case in the Appendix, and where \( \alpha \) will depend on \( G_{II}/G_{cd} \).

In eqn. (58) we have taken in a first-order sense with \( \mu b^3/(1 - v) k = T_0 = 1.2 \times \) transition temperature \( T_{bl} \)

The results in fig. 24 do not production resistance for reservations, it is interesting crack. As we demonstrate on a \{112\} plane where \( \zeta \) propagating with a velocity roughly a factor of ten above.

While the present for inclined planes could it the crystal and the actual are unlikely to be decisive. governing conditions must plays a smaller role and a of the experimental obser It is clear, however, that \( t \) approaches for which the the atoms making up the certain phase of the brittle by dislocation nucleation resistance is governed by well understood, at least.

This research was supported by ONR under Contract No. No0014-92 and discussions with Professors and Dr. R. Thomson of computations were carried out at the Massachusetts Institute of Technology, the guidance of Pr. atomic scale.
studies are needed for
boundary integral method
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we have extended the
or skewness of the shear
ance which accompanies
r potential decouples the
ions using a sinusoidal
results of Rice and Beltz
re. With a shear resistance
significant departures from
rly as regards activation
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that as a result the large
original Rice–Thompson
f the present analysis, still
3 and fig. 24 are somewhat
he Schöck–Püschl (1991)
consider the brittle-to-duct-
event, for which the event
ows:

\[ \frac{\mu b^3}{(1 - \nu)k} = \frac{\mu b^3}{(1 - \nu)k} \left( 1 - \eta \frac{T}{T_m} \right). \]  

(58)

In eqn. (58) we have taken note of the temperature dependence of the shear modulus in a first-order sense with \( \eta \), typically being 0.5, where \( T_m \) is the melting point. For \( \alpha \)-Fe, \( \mu b^3/(1 - \nu)k = T_0 = 1.2 \times 10^5 \) K, and \( T_m = 1809 \) K. Then the expected brittle-to-ductile transition temperature \( T_{BD} \) is related to \( \alpha \)(\( G_{th}/G_{cd} \)) by

\[ \frac{T_{BD}}{T_0} = \left( \frac{C}{\alpha} + \eta \frac{T_0}{T_m} \right)^{-1}. \]  

(59)

The results in fig. 24 do not consider the effect of tension–shear coupling nor the surface production resistance for nucleation on inclined slip planes. Not withstanding these reservations, it is interesting to estimate the \( T_{BD} \) for the arrest of a propagating cleavage crack. As we demonstrate in the Appendix for a realistic case of nucleation of a loop on a \{112\} plane where \( G_{th}/G_{cd} = 0.593 \), the \( T_{BD} \) necessary to arrest a cleavage crack propagating with a velocity of, say, 1 cm s\(^{-1}\) on a (100) cleave should be 2630 K, or roughly a factor of ten above experimental expectations of \(-10^4\) C.

While the present form of continuum analysis using the Peierls approach on the inclined planes could incorporate additional refinements such as anisotropy of the crystal and the actual geometry of the active Burgers vector in the slip plane, these are unlikely to be decisive. The present results have already demonstrated that the actual governing conditions must apply on the oblique slip planes where the surface production plays a smaller role and are most probably influenced by local heterogeneities as most of the experimental observations have indicated. Such analyses are now in progress. It is clear, however, that the final gap can only be closed by resorting to fully atomistic approaches for which the present method of analysis can furnish initial coordinates for the atoms making up the saddle-point configuration. Nevertheless, it is clear that a certain phase of the brittle to ductile transition in cleavage fracture which is controlled by dislocation nucleation as should be the case in b.c.c. metals (where the lattice resistance is governed by double kink nucleation and not by kink mobility) is now quite well understood, at least, semiquantitatively.

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APPENDIX

ESTIMATE OF THE BRITTLE-TO-DUCTILE TRANSITION TEMPERATURE

It is of interest to evaluate the present findings in terms of their predictive capability for the estimation of the brittle-to-ductile transition temperature, for example in \( \alpha \)-Fe.

A number of different scenarios can be constructed to describe a brittle-to-ductile transition. We consider here a relatively precise process described by Argon (1987) in which a brittle cleavage crack in \( \alpha \)-Fe propagates up a temperature gradient with a given constant velocity \( v \) until at a certain temperature \( T_{BD} \) it is arrested by a cascade of ductile processes initiated by the critical event of nucleation of a dislocation loop (or segment) from the crack tip. In this scenario the probability of activation of a transition event must be equal to the Mach number \( m = v/c \) (\( c \) is the velocity of a sound wave) of a propagating crack, that is

\[
\exp \left( -\frac{\Delta U_{\text{act}}}{kT_{BD}} \right) = m = \frac{v}{c}, \quad (A.1)
\]

Thus

\[
\frac{\Delta U_{\text{act}}}{kT_{BD}} = \frac{a \mu b^3}{(1 - v)kT_{BD}} = C = \ln \left( \frac{1}{m} \right), \quad (A.2)
\]

where \( a = a(G_{II}/G_{cd}) \) is given in fig. 24 for \( \beta = 2.0 \) (appropriate for \( \alpha \)-Fe).

If account is also taken of the temperature dependence of the shear modulus of iron to first order effects through

\[
\mu = \mu_0 \left( 1 - \eta \frac{T}{T_m} \right), \quad (A.3)
\]

where \( \mu_0 \) is the shear modulus at 0 K and \( \eta \) is typically of the order 0.5 for most metals, we find that

\[
T_{BD} = T_0 \left( \frac{\ln \left( \frac{1}{m} \right)}{\alpha} + \eta \frac{T_0}{T_m} \right)^{-1}, \quad (A.4)
\]

where \( T_0 = \mu b^3/(1 - v) = 1.2 \times 10^5 \) K and \( T_m = 1809 \) K for \( \alpha \)-Fe.

We consider now the critical loop nucleation event to occur on the \( \{112\} \) plane for a \((001)\) cleavage crack propagating in a \((001)\) direction under a crack driving force \( G_I = G_{II}= 2\gamma_s \). For such a crack the momentary driving force \( G_{II}(\theta) \) probing the \( \{112\} \) slip plane should be given by

\[
\frac{G_{II}(\theta)}{G_{II}} = \frac{K_{II}}{K_c} = (\hat{\sigma}_{11}(\theta))^2 \quad (A.5)
\]

where \( \hat{\sigma}_{11}(\theta) \) is the angular factor for a mode I crack, and \( \theta = 35.2^\circ \) for the \( \{112\} \) plane under consideration, for which \( \hat{\sigma}_{11}(\theta) = 0.275 \). Taking \( G_{cd} = \gamma^{(0)}_{cd} = 0.497 \) J m\(^{-2}\) (table) and \( \gamma_s = 1.95 \) J m\(^{-2}\) (Hirth and Lothe 1982), we estimate the driving force ratio \( G_{II}/G_{cd} \) for nucleation of a critical configuration on the inclined \( \{112\} \) plane to be

\[
\frac{G_{II}}{G_{cd}} = \frac{G_{II}}{G_{II}} \frac{G_{II}}{G_{cd}} = (\hat{\sigma}_{11}(\theta))^2 \frac{2\gamma_s}{\gamma^{(0)}_{cd}} = 0.593. \quad (A.6)
\]

From fig. 24 for \( \beta = 2.0 \) we determine that \( a = \Delta U_{\text{act}}(1 - v)/\mu b^3 = 1.0 \) for the above estimate of the driving force ratio. Taking \( m = 4 \times 10^{-6} \), that is \( v = 1 \) cm s\(^{-1}\) we calculated for \( T_{BD} = 2630 \) in relation to an experimen

ARGON, A. S., 1987, Acta me
ARMSTRONG, R. W., 1956, M
BELTZ, G. E., and RICE, J. R., 1987, Theory, Application of the
P. S. Follansbee and (AIME), p. 457.
BOWER, A. F., and ORTIZ, M., 1980, V. v., and LOMER, V
BREDE, M., and HAASEN, P., 1974, Advance
BULATOV, V. V., YIP, S., and CHAO, Y.-H., and CLARKE, I
CLOUGH, R. W., and PLIZZIEL
cotterell, B., and RICE, J. J.,
CURTICHE, L. R., 1972, Ph.D.
FOREMAN, A. J., JASWON, M.,
GEOGE, A., and MICHOT, G.
HUTCHINSON, J. W., and KO
HIRSCH, P. B., and ROBERTS,
HIRSCH, P. B., SAMUEL, J. T.,
HIRTH, J. P., and LOTHE, J. I,
KAXIRAS, E., and DUESBERY,
KAXIRAS, E., and JUAN, Y. Y.
KELLY, A., TYSON, W. R., and
KOESTER, W. T., 1943, Ph.D.
MIDLIN, R. S., 1965, Int. J.
NABARRO, R. W. H., 1947, Pr
NEDELE wee, A., 1990, J. Me
PERRY, R. E., 1940, Proc. F
RICE, J. R., and BELTZ, G. E.,
RICE, J. R., BELTZ, G. E., et
SCHOCK, G., 1991, Phil. Mag
SCHOCK, G., and PUSEHL, W.
SHI, L.-T., and ARGON, A. S.
SIMMONS, G., and WANG, H.
SUN, Y., BELTZ, G. E., and R
SUN, Y., RICE, J. R., and TR
Aloy, Materials
ST JOHN, C., 1975, Phil. Mag.
VINEYARD, G. H., 1957, Phys.
XU, G., and ORTIZ, M., 1993
YANAGUCHI, M., VITEK, V., a
ZHOU, S. J., CARLSSON, A. E.
calculated for $T_{BD} = 2630$ K from eqn. (A 4). This is roughly a factor of ten too high in relation to an experimental temperature that should be around $-10^\circ$C.

REFERENCES

BULATOV, V. V., YIP, S., and ARGON, A. S., 1995, Phil. Mag., A, 72, 453.
RICE, J. R., and THOMSON, R., 1974, Phil. Mag., A, 29, 73.