Dislocation nucleation and emission from crack tip

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Abstract. The problems of dislocation nucleation and emission from a crack tip are analysed based on Peierls model. The concept adopted here is essentially the same as that proposed by Rice. A slight modification is introduced here to identify the pure linear elastic response of material. A set of new governing equations is developed, which is different from that used by Beltz and Rice. The stress field and the dislocation density field can be expressed as the first and second Chebyshev polynomial series respectively. Then the opening and slip displacements can be expanded as the trigonometric series. The Newton–Raphson Method is used to solve a set of nonlinear algebraic equations. The new governing equations allow us to extend the analyses to the case of dislocation emission. The calculation results for pure shearing, pure tension and combined tension and shear loading are given in detail.

1. Introduction

The ductile versus brittle behavior of materials was first demonstrated by Armstrong [1] and Kelly et al. [2]. They postulated the viewpoint that the major factor is the competition between Griffith cleavage and plastic shear at a crack tip. In their pioneer work, Rice and Thomson [3] presented the dislocation emission model to characterize the plastic shear at crack tip and developed a quantitative criterion for ductile versus brittle behavior.

Recently Rice [4], Schoeck [5], Rice et al. [6], Beltz and Rice [7] have reanalyzed the Rice–Thomson criterion on the basis of the Peierls model, in which the fully emitted dislocation is considered as a continuous distribution of infinitesimal continuum dislocations. For mode II case, Rice [4] presented an exact solution for the loading in which nucleation instability was developed and identified a solid-state parameter, the unstable stacking energy γ_{us} , which characterizes the resistance to dislocation nucleation.

Zhou and Carlson [8], Thomson et al. [9] have performed a series of atomistic calculations to evaluate the effects of several physical factors on dislocation emission.

In this paper, dislocation nucleation and emission from a stressed crack tip are analyzed. The concept adopted here is essentially the same as that of [4] and [7]. A periodic relation between shear stress and atomic shear displacement is assumed. A set of new governing equations was developed in this paper, which is different from that of [7]. The new governing equations allow us to extend the analyses to the case of dislocation emission.

2. Mechanical model

Suppose the crack front is contained within one of the possible slip planes in a crystal. As shown in Fig. 1, Δ_x denotes the relative displacement of two atomic planes adjacent to the slip plane. Assume that the τ_x versus Δ_x curve in Fig. 1 is the Frenkel sinusoidal function. We have

$$\tau_x = \tau_{\max} \sin \left(2\pi \frac{\Delta_x}{b} \right). \quad (1)$$

Fig. 1. Shear stress versus shear displacement on a slip plane.

Define δ_x as the slip displacement discontinuity on a mathematical cut coincident with the slip plane. We have

$$\Delta_x = \delta_x + \frac{\tau_x}{\mu}h, \quad (2)$$

where h is the interplanar spacing.

δ_x can be taken as the plastic shearing along the slip plane. According to the crystal plasticity given by Hill [11] and Asaro [12] among others, the plastic shearing will occur when the resolved shear stress reaches the critical shear stress τ_0 . When the resolved shear stress is less than the critical shear stress τ_0 , there is no plastic shearing. Hence (2) becomes

$$\Delta_x = \begin{cases} \delta_x + \frac{\tau_x}{\mu}h, & \tau_x > \tau_0 \\ \frac{\tau_x}{\mu}h, & \tau_x \leq \tau_0 \end{cases}. \quad (3)$$

Let Δ_y denote the relative atomic separation across the slip plane. Similarly the Δ_y can be expressed as

$$\Delta_y = \begin{cases} \delta_y + \frac{\sigma_y}{E}h, & \sigma_y > \sigma_0 \\ \frac{\sigma_y}{E}h, & \sigma_y \leq \sigma_0 \end{cases}, \quad (4)$$

where δ_y is the opening displacement discontinuity on the slip plane, σ_0 is the yield stress, E is the Young's modulus of the crystal.

The corresponding relation for tensile decohesion is taken to be

$$\sigma_y = \sigma_{\max} \frac{\Delta_y}{L} e^{1-(\Delta_y/L)} \quad (5)$$

Fig. 2. Cohesive zone and decohesive zone ahead of a crack tip.

where L is the scaling length of the Thomas–Fermi screening length.

For the general loadings [7] proposed a generalized constitutive relation ¹

$$\begin{cases} \tau_x = \tau_{\max} A(\Delta_y) \sin\left(2\pi \frac{\Delta_x}{b}\right) \\ \sigma_y = \sigma_{\max} B(\Delta_x) \frac{\Delta_y}{L} e^{1-(\Delta_y/L)} \end{cases}, \quad (6)$$

where

$$A(\Delta_y) = \left(1 + \frac{\Delta_y}{L}\right) e^{-(\Delta_y/L)}, \quad (7)$$

$$B(\Delta_x) = 1 - q \sin^2\left(\pi \frac{\Delta_x}{b}\right), \quad q = \frac{\gamma_{us}}{2\gamma_s}, \quad (8)$$

where γ_s is the surface energy, γ_{us} is the unstable stacking energy.

3. Basic formulas

Figure 2 shows a plane strain or plane stress semi-infinite crack. The crack lies on the negative x axis with its tip at $x = 0$. Let R_1 denote the length of the cohesive zone for slip displacement and R_2 the length of the decohesive zone for opening displacement. Beyond the R_1 , there is no discontinuity for slip displacement, meanwhile beyond the R_2 , discontinuity of the opening displacement vanishes.

According to Atkinson [13] and Loo [14], the traction on the cohesive zone ahead of the crack tip is

$$\sigma_y - i\tau_{xy} = \sigma_y^{(0)} - i\tau_{xy}^{(0)} + \frac{2\mu}{(\kappa + 1)\pi i} \int_0^R \frac{\sqrt{\tau} b(\tau)}{\sqrt{x(x - \tau)}} d\tau, \quad (9)$$

¹ We only consider the case of $r = 0$.

where $\sigma_y^{(0)}$, $\tau_{xy}^{(0)}$ are the singular stress field.

Equation (9) can be represented as

$$\frac{2\mu}{(\kappa+1)\pi} \int_0^{R_1} \frac{\sqrt{\tau} b_x(\tau)}{x-\tau} d\tau = \sqrt{x}[\tau_{xy} - \tau_{xy}^{(0)}], \quad (10a)$$

$$\frac{2\mu}{(\kappa+1)\pi} \int_0^{R_2} \frac{\sqrt{\tau} b_y(\tau)}{x-\tau} d\tau = \sqrt{x}[\sigma_y - \sigma_y^{(0)}]. \quad (10b)$$

Introducing the following nondimensional quantities

$$t_1 = \frac{x}{R_1}, \quad t_2 = \frac{x}{R_2}, \quad s_1 = \frac{\tau}{R_1}, \quad s_2 = \frac{\tau}{R_2},$$

let

$$\begin{cases} F_1(t_1) = \sqrt{t_1} b_x(x) \cdot \frac{\mu}{\kappa+1}, \\ g_1(t_1) = \sqrt{t_1} [\tau_{xy} - \tau_{xy}^{(0)}] \end{cases}, \quad (11)$$

$$\begin{cases} F_2(t_2) = \sqrt{t_2} b_y(x) \cdot \frac{\mu}{\kappa+1}, \\ g_2(t_2) = \sqrt{t_2} [\sigma_y - \sigma_y^{(0)}] \end{cases}, \quad (12)$$

then (10) becomes

$$\begin{cases} -\frac{2}{\pi} \int_0^1 \frac{F_1(s_1) ds_1}{s_1 - t_1} = g_1(t_1) \\ -\frac{2}{\pi} \int_0^1 \frac{F_2(s_2) ds_2}{s_2 - t_2} = g_2(t_2) \end{cases}. \quad (13)$$

The singularity of the dislocation density $b(x)$ is less than $1/\sqrt{x}$ at the crack tip, while the dislocation density $b(x)$ vanishes at the end of the cohesive zone.

Introducing the variable translation: $t_1 = \frac{1}{2}(1 + \cos \theta)$ and $t_2 = \frac{1}{2}(1 + \cos \varphi)$, the functions $F_1(t_1)$ and $F_2(t_2)$ can be expressed as the following sine series

$$\begin{cases} F_1(t_1) = \frac{1}{2} \cdot \sum_{m=1}^{\infty} \alpha_m \sin m\theta, & t_1 = \frac{1}{2}(1 + \cos \theta), \quad 0 \leq \theta \leq \pi \\ F_2(t_2) = \frac{1}{2} \cdot \sum_{m=1}^{\infty} \beta_m \sin m\varphi, & t_2 = \frac{1}{2}(1 + \cos \varphi), \quad 0 \leq \varphi \leq \pi \end{cases}, \quad (14)$$

(14) can be rewritten as

$$\begin{cases} F_1(t_1) = \frac{1}{2} \sqrt{1 - \eta_1^2} \cdot \sum_{m=1}^{\infty} \alpha_m U_m(\eta_1) \\ F_2(t_2) = \frac{1}{2} \sqrt{1 - \eta_2^2} \cdot \sum_{m=1}^{\infty} \beta_m U_m(\eta_2) \end{cases}, \quad (15)$$

Fig. 3. Shear displacement profiles at various levels of applied shear loadings for a pure mode II crack. The solid lines correspond to the present results and the dashed lines correspond to the results by Beltz and Rice [7].

where $U_m(\eta)$ is the second Chebyshev polynomial

$$U_m(\eta) = \frac{\sin m\theta}{\sin \theta}, \quad m = 1, 2, \dots,$$

$$\eta = \cos \theta, \quad t = \frac{1}{2}(1 + \eta).$$

Substituting (15) into (13) and using following formula [15]

$$\frac{1}{\pi} \int_{-1}^1 \frac{\sqrt{1-\xi^2} U_m(\xi) d\xi}{\xi - \eta} = \begin{cases} -T_m(\eta), & -1 \leq \eta \leq 1 \\ -[\eta - \sqrt{\eta^2 - 1}]^m, & \eta > 1 \end{cases}$$

one obtains

$$\begin{cases} g_1(t_1) = \sum_{m=1}^{\infty} \alpha_m \cos m\theta \\ g_2(t_2) = \sum_{m=1}^{\infty} \beta_m \cos m\varphi \end{cases}, \quad (16)$$

where $T_m(\eta)$ is the first Chebyshev polynomial

$$\begin{cases} T_m(\eta) = \cos m\theta \\ \eta = \cos \theta \end{cases}. \quad (17)$$

Fig. 4. Shear stress distributions along the cohesive zone for various pure shear loadings.

Fig. 5. Slip displacement profiles for a pure mode II crack after dislocation emission from the crack tip.

The opening displacement and sliding displacement take the form

$$\delta_x + i\delta_y = \int_x^R b(\tau) d\tau. \quad (18)$$

Fig. 6. Shear stress distributions along the cohesive zone for a pure mode II crack after dislocation emission.

Using (11) and (15), we obtain

$$\frac{\mu}{(\kappa + 1)} \delta_x = \frac{R_1}{4} \cdot \sum_{m=1}^{\infty} \alpha_m V_m(\theta), \quad (19)$$

$$\frac{\mu}{(\kappa + 1)} \delta_y = \frac{R_2}{4} \cdot \sum_{m=1}^{\infty} \beta_m V_m(\varphi), \quad (20)$$

$$V_m(\theta) = \frac{\sin(m - \frac{1}{2})\theta}{m - \frac{1}{2}} - \frac{\sin(m + \frac{1}{2})\theta}{m + \frac{1}{2}}. \quad (21)$$

The singular stress field can be expressed as

$$\sigma_y^{(0)} + i\tau_{xy}^{(0)} = \frac{K}{\sqrt{2\pi r}}, \quad (22)$$

here $K = K_I + iK_{II}$ is the complex stress intensity factor.

Substituting (22) into (11) and (12), we obtain

$$\begin{cases} \tau_{xy} = \frac{1}{\sqrt{t_1}} \left[g_1(t_1) + \frac{K_{II}}{\sqrt{2\pi R_1}} \right] \\ \sigma_y = \frac{1}{\sqrt{t_2}} \left[g_2(t_2) + \frac{K_I}{\sqrt{2\pi R_2}} \right] \end{cases}. \quad (23)$$

The Barenblatt's formula [16] can be expressed as

$$\begin{cases} \frac{K_{II}}{\sqrt{2\pi R_1}} = \frac{1}{\pi} \int_0^\pi \sqrt{t_1} \tau_{xy} d\theta = \frac{1}{\pi\sqrt{R_1}} \int_0^{R_1} \frac{\tau_{xy}}{\sqrt{R_1-x}} dx \\ \frac{K_I}{\sqrt{2\pi R_2}} = \frac{1}{\pi} \int_0^\pi \sqrt{t_2} \sigma_y d\varphi = \frac{1}{\pi\sqrt{R_2}} \int_0^{R_2} \frac{\sigma_y}{\sqrt{R_2-x}} dx \end{cases} \quad (24)$$

Formulas (11), (14)–(16) and (23), (24) are the basic formulas of this paper.

4. Calculation methods

The unknown coefficients $\{\alpha_m\}$ and $\{\beta_m\}$ are chosen as the basic unknown quantities. The infinite series in (14) and (16) can be approximated with a sufficient degree of accuracy by the corresponding truncated series.

The cohesive zone $0 \leq x \leq R_1$ is discretized into M elements. The elements are chosen to vary in size along the region. The nodal points are given by the following expression

$$x_i = \frac{1}{2} R_1 \left[1 + \cos \left(\frac{(i-1)\pi}{M} \right) \right]. \quad (25)$$

Similarly the decohesive zone $0 \leq x \leq R_2$ is divided into N elements. The nodal points are given by the formula

$$x_j = \frac{1}{2} R_2 \left[1 + \cos \left(\frac{(j-1)\pi}{N} \right) \right]. \quad (26)$$

The governing equations are transformed into a set of nonlinear algebraic equations

$$\begin{cases} \sum_{k=1}^M a_{ik} \alpha_k - \tau_{\max} A(\Delta_{yi}) \sin \left(2\pi \frac{\Delta_{xi}}{b} \right) = 0, & i = 1, 2, \dots, M \\ \sum_{k=1}^N b_{jk} \beta_k - \sigma_{\max} B(\Delta_{xj}^*) \frac{\Delta_{yj}^*}{L} e^{1-(\Delta_{yj}^*/L)} = 0, & j = 1, 2, \dots, N \end{cases}, \quad (27)$$

where

$$\begin{cases} a_{ik} = \frac{[\cos(k\theta_i) - \cos(k\pi)]}{\sqrt{t_{1i}}} \\ b_{jk} = \frac{[\cos(k\varphi_j) - \cos(k\pi)]}{\sqrt{t_{2j}}} \\ \theta_i = \frac{(i-1)\pi}{M}, \quad \varphi_j = \frac{(j-1)\pi}{N} \end{cases}, \quad (28)$$

Δ_{xi} , Δ_{yi} are the shearing and opening displacements at $x_i = R_1[1 + \cos \theta_i]/2$, Δ_{xj}^* , Δ_{yj}^* are the shearing and opening displacements at $x_j = R_2[1 + \cos \varphi_j]/2$.

Equations (27) is solved by the Newton–Raphson method. The iterating convergence is guaranteed after five to ten iterations. Most calculations in this paper were carried out with five digits of accuracy for stress fields in the cohesive zone.

Fig. 7. Displacement profiles for a combined mode crack after dislocation emission from the crack tip for the case of $R_1/b = 190$ and $R_2/b = 142.5$.

5. Calculation results

Calculation was carried out with materials parameters $h/b = 1$, $L/b = 0.2$, $\tau_0/\mu = 0.01$, $\sigma_0/E = 0.008$, $\nu = 0.3$, $\tau_{\max}/\mu = 0.159$, $\sigma_{\max}/E = 0.0766$, and $M = 180$, $N = 180$.

5.1. PURE SHEARING LOADING

In our calculation, the controllable parameter is the length R_1 of the cohesive zone. The calculation starts from a low value of R_1/b . As the R_1 increases, the nondimensional stress intensity factor $K_{II}/\sqrt{2\pi b}\tau_0$ also increases. When the ratio of R_1/b arrives at 234.5, the applied G is equal to $1.0004\gamma_{us}$ and the Peierls dislocation [10] is fully formed at the crack tip.

If the nondimensional stress intensity factor was chosen as the controllable parameter, the determinant of Jacobian matrix of the governing equations will approach to zero at the instability. Thus the governing equations are singular and we are unable to get a solution.

In the present calculation, the issue is different. The determinant of Jacobian matrix of the governing equation is not singular when the Peierls dislocation is fully formed at the crack tip. But the calculation convergence becomes poor due to the fact that the governing equations are ill behaved. The calculation convergence is remarkably improved after introducing the damping coefficient 0.1 into the Newton–Raphson method.

Figure 3 shows the slip displacement profiles for pure shear loading at various load levels up to dislocation nucleation. When the applied energy release rate G is only slightly larger than γ_{us} , the shear displacement δ_x at the crack tip is $\frac{1}{2}b$. It means that the Peierls crystal dislocation is fully formed. The comparison of the present results with the results of [7] is

Fig. 8. Stress distributions along the cohesive zone for a combined mode crack after dislocation emission for the case of $R_1/b = 190$ and $R_2/b = 142.5$.

also shown in Fig. 3. The solid lines correspond to the present results and the dashed lines correspond to the results by [7]. It can be seen that both results are nearly identical.

Figure 4 shows the shear stress τ_{xy} distribution along the cohesive zone. The shear stress arrives at local maximum where δ_x is $\frac{1}{4}b$.

Figure 5 shows the slip displacement profiles for pure shear loading at various load levels after dislocation emission. As the length of the cohesive zone increases, the emitted dislocation moves further away from the crack tip. It is worth noting that there is a well-defined region of fairly 'perfect' crystal between the emitted dislocation and the crack tip. This feature is consistent with the atomistic calculation given by [8].

In the present calculation, the crack is completely shielded from the external loading. After the dislocation emission, the shielding effect produced by the emitted dislocation becomes so strong that the external stress intensity factor will reduce. In Fig. 5, the three curves are corresponding to $R_1/b = 262.5, 302.5$ and 362.5 and $(K_{II}/\sqrt{2\pi b\tau_0}) = 13.7, 4.98$ and 2.65 , respectively. Meanwhile, the centers of the emitted dislocations are located at $x/b = 1.06, 5.4$ and 18.6 , respectively. In the atomistic calculation given by [8], there is a strong pinning point at the end of the cohesive zone. Hence the external load can increase a little bit after dislocation emission.

The shear stress distributions along the cohesive zone are shown in Fig. 6. The shear stress changes drastically around the center of the emitted dislocation.

5.2. COMBINED TENSILE AND SHEAR LOADING

The results for general combined shear and tension loading are given in Figs. 7 and 8. Figure 7 shows the slip and opening displacement profiles after the dislocation emission for the case of $R_1/b = 190, R_2/b = 142.5, K_I/\sqrt{2\pi b\sigma_0} = 10.6$ and $K_{II}/\sqrt{2\pi b\tau_0} = 5.19$. The stress fields ahead of the crack tip are shown in Fig. 8. Both the shear and normal stresses arrive at maximum value at $x/b = 29.6$. The shear and normal stresses actually vanish behind the center of the emitted dislocation due to the large separation Δ_y .

6. Discussion

Based on the concept of Peierls dislocation, the dislocation nucleation and emission from the crack tip were analyzed in this paper. The Rice model was slightly modified to identify the pure linear elastic response of the crystal. This modification is consistent with the theory of the crystal plasticity. It means that there is an internal friction to resist the dislocation movement.

A new calculation approach was developed here. Using this approach both the dislocation nucleation and the dislocation emission were simulated.

Many simplified assumptions have been introduced in the present analysis of dislocation nucleation and emission. The dislocation emission actually takes place in the three dimension geometry by a dislocation loop. Present analysis only concerned the two dimension description. Elastic anisotropy was neglected in our analyses. The significant effect of thermal activation on the dislocation emission has not been accounted for here. We only reported the partial results of dislocation emission in which the emitted dislocation is not far away from the crack tip. The process of the dislocation emission is more complicated since the emitted dislocation will rapidly move far away from the crack tip, leaving behind a 'dislocation-free zone' between the crack and the plastic zone. The length of the 'dislocation-free zone' may be as large as several thousands of Bergers vector b . The present calculation scheme is not suitable for such a situation. Further investigation is needed.

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