EFFECT OF T-STRESS ON EDGE DISLOCATION FORMATION AT A CRACK TIP UNDER MODE I LOADING

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1. Abstract

We calculate the effect of the nonsingular stress acting parallel to a crack (the "T-stress") on edge dislocation nucleation at a crack loaded in Mode I. We find that this leads to crack size effect – that is, for small cracks (of order 100 atomic spacings or less), the T stress causes the critical load for dislocation nucleation (expressed in terms of the applied stress intensity factor) to deviate from the classical T = 0 result. Specific results are discussed for the case of a finite crack subject to remote tension, where it is shown that the threshold for dislocation nucleation is reduced.

2. Introduction

In the continuum modeling of atomic-scale phenomena at crack tips, an important feature of the asymptotic representation of the stress field is often overlooked. Following the work of Williams [1], the expansion of the stress field in cylindrical coordinates about the tip (see Figure 1) may be generally written as

$$\sigma_{ij} = \frac{K\,S_{ij}(\theta)}{\sqrt{2\pi}} r^{-1/2} + T_{ij}(\theta) + U_{ij}(\theta) r^{1/2} + \ldots \qquad (1)$$

where K is the well-known "applied" stress intensity factor, and $S_{ij}(\theta)$, $T_{ij}(\theta)$, etc. represent the angular variation of the field. The first term is singular in r, the second term remains finite in the vicinity of the tip, and the remaining terms vanish as $r \to 0$. Linear elastic fracture mechanics is based on the reasonable notion that fracture processes that occur close to the tip are only affected by the singular contribution; hence, only the first term of Equation (1) is acknowledged as a valid descriptor of the stress field in a vast majority of the fracture literature. The second term has a particularly simple form – that is, it can be shown [1] that T_{11}, T_{33}, and T_{13} (= T_{31}) must be constant in θ in order to satisfy the field equations of elasticity, and the remaining components must vanish in order to preserve the traction-free boundary condition on the crack faces. We will exclusively deal with plane strain for the remainder of this discussion, thereby rendering T_{11} the only component of interest. Then, the asymptotic representation of the stress field around a crack, ignoring terms of $r^{1/2}$ and higher, takes the form

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{bmatrix} = \frac{K}{\sqrt{2\pi r}} \begin{bmatrix} S_{11}(\theta) & S_{12}(\theta) \\ S_{21}(\theta) & S_{22}(\theta) \end{bmatrix} + \begin{bmatrix} T & 0 \\ 0 & 0 \end{bmatrix} \tag{2}$$

The constant term $T_{11} = T$ is commonly known as the "T-stress."

Several researchers have demonstrated that the T-stress has a significant influence on the shape and size of the plastic zone that develops at a crack in a ductile material [2-5] as well as the directional stability of an advancing crack in a brittle solid [5-8]. The latter effect can be qualitatively understood by imagining a slight upward perturbation of the crack path (see Figure 1): if $T > 0$, the crack tip will continue to undergo opening forces, and will continue to veer away from the x_1-axis. If $T < 0$, the crack opening forces tend to decrease, such that the only way for the crack to continue to propagate is for it to remain on the x_1-axis.

Here, we will focus on the effect of T-stress on the threshold for dislocation nucleation. The basic framework for analysis will be that due to Peierls [9] and Nabarro [10], as introduced by Rice [11] for dislocation formation at a crack. We directly calculate the critical stress intensity factor K_{crit} for dislocation nucleation as a function of T, and comment on the situations for which this effect could be most significant.

3. Peierls Framework for Dislocation Nucleation at a Crack

The Peierls framework for dislocation formation at a crack assumes that the dislocation/crack system can be thought of as two elastic semispaces separated by a common plane (the crack plane and slip plane) on which there is a discontinuous jump in the displacement fields [11]. There exists a periodic relationship between shear stress and slip displacement along the slip plane, with traction free surfaces along the crack plane, as shown schematically in Figure 1. Prior to dislocation nucleation, there

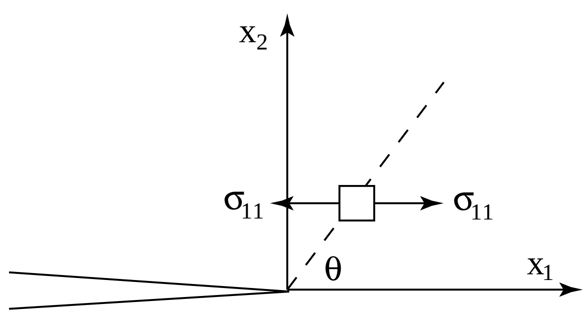

Figure 1. Schematic of crack and slip plane (dashed) inclined at angle θ. The T-stress gives a contribution to σ_{11} in addition to the classical K field result. A positive T-stress decreases the resolved shear stress on the slip plane, while a negative T-stress increases the resolved shear stress.

is a distribution of slip discontinuity along the slip plane that ultimately reaches a point of instability with increased applied load and results in the nucleation of a dislocation. Using this theory, the critical stress intensity factor for various fixed values of the T-stress may be determined, thus establishing a locus of *K* and *T* values at which nucleation occurs.

For all of the calculations presented here, a simple relationship due to Frenkel [12] between shear stress and slip displacement on the slip plane is assumed,

$$\tau(\delta) = \frac{\mu b}{2\pi h}\sin\left(\frac{2\pi\Delta}{b}\right) = \frac{\pi\gamma_{us}}{b}\sin\left(\frac{2\pi\Delta}{b}\right) \tag{3}$$

where τ is the shear stress, Δ is the relative atomic displacement between two atomic planes, h is the interplanar spacing of those two planes, μ is the shear modulus, b is the Burgers vector, and γ_{us} is the unstable stacking energy (equal to $\mu b^2/2\pi^2 h$ in the Frenkel model). As introduced by Rice [11], the continuum analog to Δ (referred to as δ) is thought of as Δ extrapolated to a cut halfway between the slipping planes and is given by

$$\delta = \Delta - \frac{\tau h}{\mu}. \tag{4}$$

From elastic considerations, the stress along the slip plane can be written as:

$$\tau[\delta(r)] = \frac{K\cos^2\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)}{\sqrt{2\pi r}} - T\sin\theta\cos\theta - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty \sqrt{\frac{s}{r}}\,\frac{\partial\delta(s)}{\partial s}\,\frac{ds}{r-s} \tag{5}$$

where the first two terms on the right hand side give the pre-existing shear stress along the slip plane due to the applied load on the crack geometry (comprising the most singular term, scaled by *K,* as well as the constant term, proportional to *T*), and the third term reflects the stress relaxation that occurs due to sliding along the cut. The kernel in the integral term represents the stress due to a dislocation positioned at *s*, integrated over the entire slip distribution consisting of a continuous array of infinitesimal Burgers vectors $-(\partial\delta/\partial s)\,ds$. We seek a slip distribution $\delta(r)$ such that, for all $r > 0$, $\tau[\delta(r)]$ predicted by the linear elastic formulation, Equation (5), must equal $\tau[\delta]$ provided by the atomic-based shear relation in Equation (3). Using a numerical procedure outlined by Beltz [13]and Beltz and Rice [14], we carry this out for incremental increases in *K*, at a fixed value of *T*, until an instability (i.e., dislocation nucleation) is attained.

4. Results and Discussion

The principal results are shown in Figure 2, where the critical stress intensity factor for dislocation nucleation is plotted as a function of T-stress for several slip plane angles between 0° and 90°. It has been shown in earlier work [11,15] that the parameter $\sqrt{2\mu\gamma_{us}/(1-\nu)}$ is the natural normalization factor for K_{crit}, as it represents the threshold for dislocation nucleation under the simplest geometry of a mode II shear

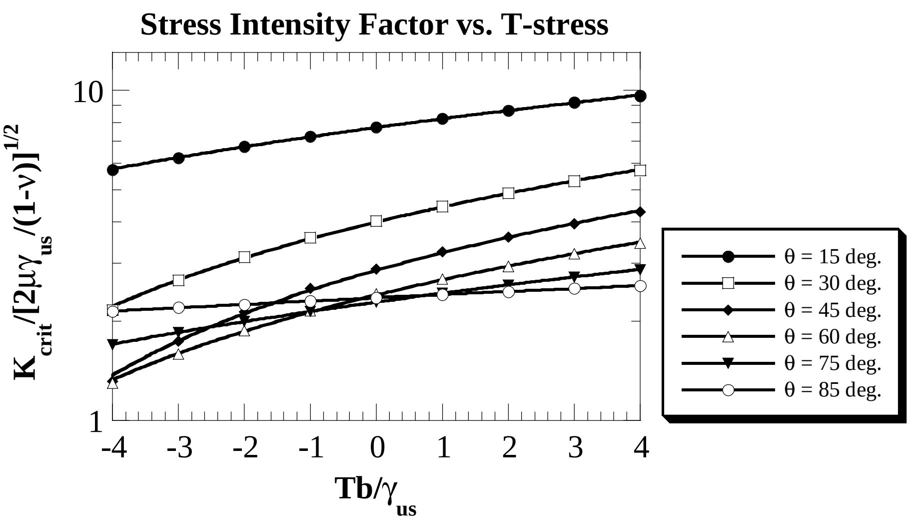

Figure 2. Positive (or tensile) T-stress increases the critical stress intensity for nucleation, while a negative T-stress decreases the critical stress intensity for nucleation.

crack with a non-inclined slip plane. The vertical axis is compressed logarithmically in order to capture results for a wide range of slip plane inclination angles (ranging from 15° to 85°). The general trend is that positive values of *T* increase the threshold for dislocation nucleation, while negative values of *T* lower the threshold. The results for *T* = 0 are consistent with earlier work by Rice *et al.* [15]. For $\theta \to 0$, the critical load would of course become unbounded since the resolved shear stress driving dislocation formation would vanish. The T-stress effect is greatest for intermediate angles, and can cause variations in the critical load by up to approximately 50% for the *T* values considered here, depending on the sign of the T-stress. We note that the T-stress effect is weakest at angles near 0° and 90°, since the resolved shear stress due to the T-stress vanishes.

As a practical matter, how large is the T-stress for a given geometry? To give some insight, we use a finite crack of length *2a* centered in an infinite solid with remotely applied stress σ (see Figure 3). In this example, the applied stress intensity factor *K* is $\sigma\sqrt{\pi a}$, and *T* is $-\sigma$ [3]. Combining and solving for *T* gives $-K/\sqrt{\pi a}$. We must choose some *K* characteristic of dislocation nucleation, say, $\alpha\sqrt{2\mu\gamma_{us}/(1-\nu)}$, where α is some dimensionless parameter of order unity or moderately larger. Solving for the normalized *T* gives

$$\frac{Tb}{\gamma_{us}} = -2\alpha\sqrt{\frac{\pi h}{a(1-\nu)}} \tag{6}$$

Hence, we see that the T-stress effect may be most severe when the crack size is tens of atomic spacings or less. More specifically, we have plotted the reduction in the threshold for dislocation nucleation (as a percentage, from the uncorrected, or T=0, result) versus crack size for several values of θ in Figure 4. We take b = h and $\nu = 0.3$.

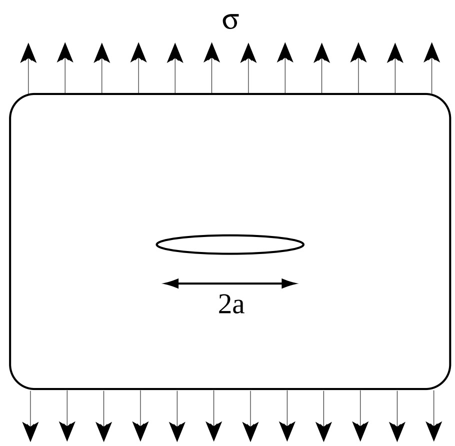

Figure 3. Finite crack of length *2a* in an infinite solid, with remote tensile stress σ. The T-stress for this particular geometry is $-\sigma$; thus, the threshold for dislocation nucleation is less than what would be calculated using the classical K-field result.

For small values of θ as well as for small values of the crack size, the T-stress effect is most significant. Clearly, one should proceed cautiously when applying continuum concepts to cracks as small as, say, 10 atomic spacings; however, we note that the T-stress effect can lead to appreciable reductions in K_{crit} for moderately longer cracks when the slip plane inclination angle is less than about 45°. This could lead to a substantial source of error if trying to reconcile atomistic results for short cracks with continuum-based predictions. If the crack is of some macroscopic dimension, then $T \approx 0$ for this geometry, and the effect can be safely neglected. The results presented here are consistent with the crack size effect on dislocation nucleation as noted by Beltz and Fischer for mode III cracks [16] and Zhang and Li for mode I cracks [17].

We would like to dedicate this paper to Professor James R. Rice, with whom the first author (GEB) had the great fortune to have as a mentor beginning ten years ago. Jim's high standards of scholarship, superb teaching, and supportive and modest personality benefitted all of us who've had the chance to work with him.

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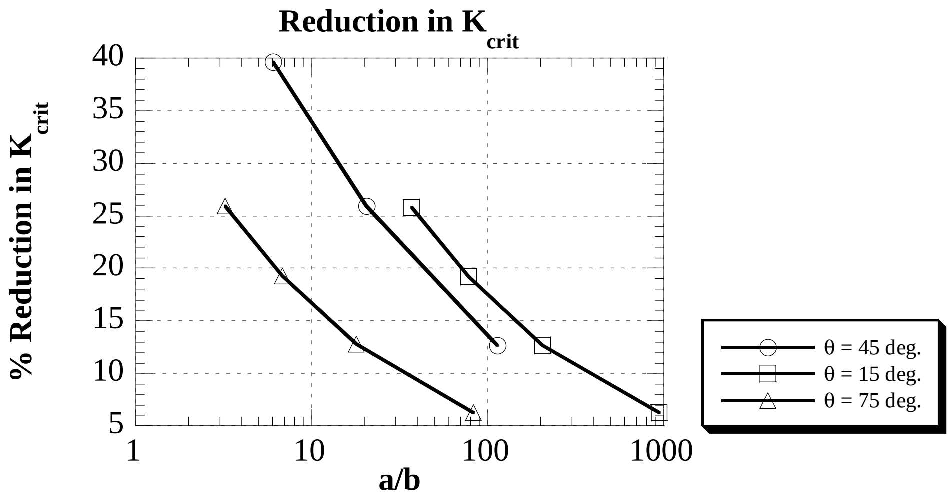

Figure 4. Reduction (from that of the T=0 result) of threshold for dislocation nucleation for a finite crack of length 2a subject to remote tension (see Figure 3).

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