A Peierls Criterion for Deformation Twinning at a Mode II Crack

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Summary. The theoretical criterion for deformation twinning (DT) at a crack tip due to Tadmor and Hai [TH03] is reviewed. The criterion quantifies the competition between slip and DT at a crack tip in terms of the critical stress intensity factors necessary to nucleate a dislocation and a two-layer microtwin there. The analysis is based on Rice's Peierls framework for dislocation emission from a crack tip [Ric92]. It is found that DT at a crack tip is controlled by a new material parameter named the "unstable twinning energy", which plays an analogous role for twinning as Rice's unstable stacking energy plays for slip. The derivation presented in this paper is for the simplest possible special case: a crack with a co-planar slip plane loaded in pure mode II shear along a crystallographic slip direction. The analysis is limited to a face-centered cubic (fcc) crystal. While this derivation contains all of the features in the full derivation in [TH03], the simpler geometry helps to clarify the underlying concepts. Some of the expressions derived for this special case are new.

1 Introduction

In this paper, the Peierls criterion for DT at a crack tip due to Tadmor and Hai [TH03] is reviewed. The criterion is based on Rice's Peierls framework for dislocation nucleation from a crack tip [Ric92].

Consider a crack with a slip plane intersecting the crack front (Fig. 1). The objective of the analysis is to obtain the critical stress intensity factors (SIFs) required to nucleate a dissociated dislocation and a deformation twin from the crack tip. A dissociated dislocation is formed by the emission of a leading partial dislocation followed by a trailing partial dislocation on the same plane. A twin nucleus is formed by the emission of a leading partial dislocation followed by another leading partial dislocation on the plane above the first partial. The competition between slip and twinning can then be formulated in terms of the competition between the two possible secondary partials after the leading partial has been emitted. This is demonstrated in Fig. 2.

This paper presents the derivation of the DT criterion for the simplest possible special case: the slip plane is coplanar with the crack plane (i.e. $\theta = 0$), the crack is loaded in pure mode II, and the slip direction of the leading partial is oriented along the positive x_1 axis (i.e. $\phi_A = 0$). In an fcc crystal this implies that the x_1 lies along a $\langle 112 \rangle$ direction and the x_2 axis lies along a $\langle 111 \rangle$ direction. The trailing partial will form an angle of $\phi_B = 60°$ with the x_1-axis. The objective of this derivation is to clarify the main features of the theory (which are all present here) by reducing as much as possible complications associated with crystallography and loading. The derivation contains new expressions, but it is based entirely on Rice's derivation for the leading and trailing partials in [Ric92], and Tadmor and Hai's derivation for the twinning partial in [TH03].

2 Emission of the leading partial

The solution for the emission of the leading partial is obtained through application of the J-Integral [Ric68]. A displacement discontinuity $\delta = \delta_1 = u_1^+ - u_1^-$ is assumed to exist along the x_1-axis ahead of the crack tip (Fig. 3). Applying the Peierls concept, the shear stress along this line is taken to be a function of the local slip discontinuity, $\tau(x_1) = f(\delta(x_1))$. An interplanar potential $\Phi(\delta) = \int \tau d\delta$ may be defined, such that $\tau = d\Phi/d\delta$. Away from the slip plane the material is assumed to be linear elastic and isotropic with shear modulus μ and Poisson's ratio ν.

Rice [Ric92] pointed out that the potential $\Phi(\delta)$ used in the Peierls model is related (but not equal) to the generalized stacking fault interplanar potential

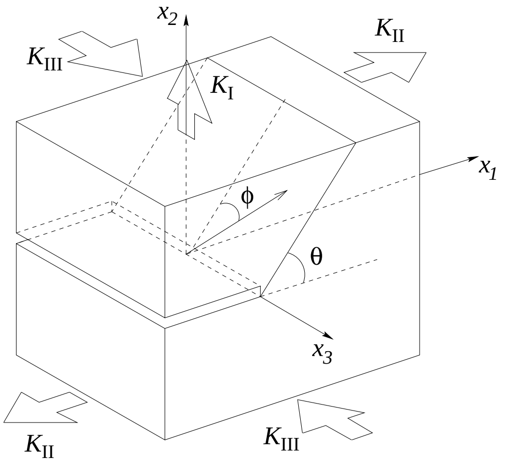

Fig. 1. A schematic diagram of the crack tip region showing the inclined slip plane and slip direction posited by the dislocation nucleation model. Reproduced from [TH03].

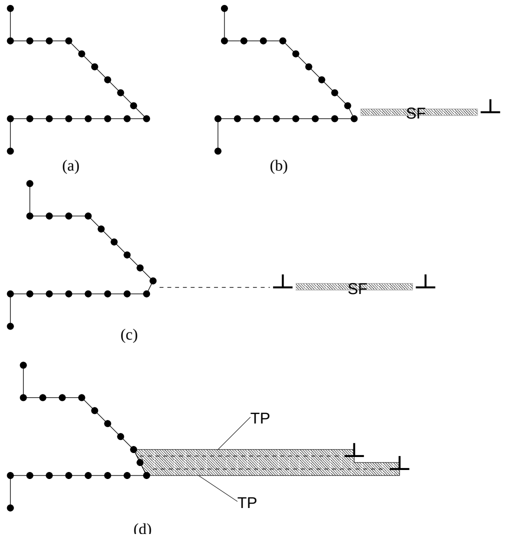

Fig. 2. The competition between slip and twinning at a crack tip. The atomically-sharp crack in (a) is loaded and emits a partial dislocation with a stacking fault (SF) in its wake in (b). As the load continues to increase, the crack will either emit the trailing partial and form a dissociated dislocation in (c), or emit a second leading partial on an adjacent plane forming a two-layer microtwin delimited by twin planes (TP) in (d). Reproduced from [TH03].

$\Psi(\Delta)$ [Vit68]. The difference is that $\Psi(\Delta)$ is the energy obtained by rigidly displacing one half of a crystal relative to the other, where Δ is the disregistry of atoms across the cut plane. For a lattice undergoing a uniform shear γ outside of the slip plane, the disregistry and slip discontinuity are related by $\Delta = \delta + \gamma h$, where h is the interplanar spacing normal to the slip plane. It may be shown that the potentials $\Phi(\delta)$ and $\Psi(\Delta)$ are related according to $\Phi = \Psi - h\tau^2/2\mu$. An important consequence of this relation is that the potentials $\Phi(\delta)$ and $\Psi(\Delta)$ have the same extrema. In particular, the parameter γ_{us}, a maximum on the $\Phi(\delta)$ curve which plays an important role in the nucleation criterion, may be obtained directly from the corresponding $\Psi(\Delta)$ function.

To solve the nucleation problem the path invariance property of the J-integral is utilized, namely that J, given by

$$J = \int_{\Gamma} [n_1 W - n_\alpha \sigma_{\alpha\beta} \partial u_\beta / \partial x_1] \, ds, \tag{1}$$

will be the same for any circuit Γ which does not traverse the crack or the slip zone ahead of it. In (1), $\mathbf{n}$ is the unit normal to the path Γ, W is the strain energy density, $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{u}$ is the displacement field and s is the arc length parameter. Two contours are defined: Γ_{far}, which is far removed

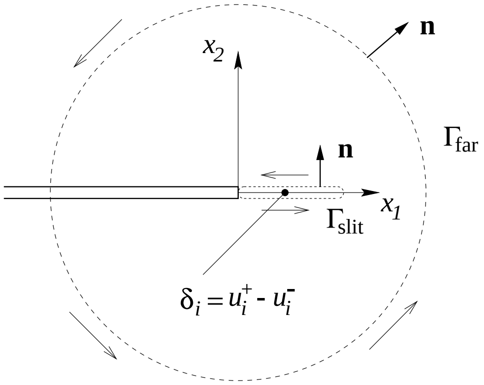

Fig. 3. A schematic diagram of the crack tip loaded in mode II with the slip direction coincident with the loading directions. The J-integral integration contours are indicated.

from the crack tip where the effects of the nonlinearities associated with the slip can be neglected, and Γ_{slit}, which is coincident with the slipped zone ahead of the crack tip. By equating $J_{\text{far}} = J_{\text{slit}}$, a correspondence between the macroscopic field parameters and the microscopic properties of the slipped zone is obtained. Integrating (1) on the far contour yields the well-known result demonstrating the equivalence between J and the energy release rate G,

$$J_{\text{far}} = (1-\nu)K_{\text{II}}^2/2\mu \equiv G. \tag{2}$$

Integrating (1) on the slit contour turns out to also have a clear significance. The first term in (1) drops out, since $n_1 = 0$, with the result,

$$\begin{aligned} J_{\text{slit}} &= -\int_0^\infty \sigma_{21} \frac{\partial(u_1^+ - u_1^-)}{\partial x_1} dx_1 \\ &= -\int_0^\infty \tau[\delta(x_1)] \frac{\partial \delta}{\partial x_1} dx_1 = \int_0^{\delta_{\text{tip}}} \tau d\delta = \Phi(\delta_{\text{tip}}), \end{aligned} \tag{3}$$

where the relations $\tau = \sigma_{21}$ and $\delta = u_1^+ - u_1^-$ have been used, and where δ_{tip} is the slip discontinuity at the tip of the crack. Equating equations (2) and (3) gives,

$$(1-\nu)K_{\text{II}}^2/2\mu = \Phi(\delta_{\text{tip}}). \tag{4}$$

As K_{II} increases the energy stored in the slipped zone increases and the potential at the crack tip follows the $\Phi(\delta)$ curve. At the first maximum of $\Phi(\delta)$ the system loses stability and a dislocation is emitted. This maximum is defined as the unstable stacking energy γ_{us}. The critical SIF for the nucleation of the leading partial dislocation is thus,

$$K_{\text{II}}^1 = \sqrt{\frac{2\mu\gamma_{\text{us}}}{1-\nu}}, \tag{5}$$

where the superscript "1" indicates that this is the critical load for the emission of the first partial from the crack tip. As soon as $K_{\mathrm{II}} = K_{\mathrm{II}}^{1}$ the leading partial dislocation is nucleated and glides away from the crack tip leaving behind a stacking fault ribbon with energy per unit area γ_{sf}. This sequence of events is demonstrated in Fig. 4 where the interplanar potential $\varPsi(\varDelta)$ is plotted for slip along the leading partial direction. The figure also includes the atomic configurations associated with five points along the curve. The $\varPsi(\varDelta)$ curve was computed using an Embedded Atom Method (EAM) [DB83] potential for aluminum due to Ercolessi and Adams [EA93]. The first part of the curve from I to III is associated with the emission of the leading partial dislocation. The system will lose stability at point II where $\varPhi(\delta_{\mathrm{tip}}) = \varPsi(\varDelta_{\mathrm{tip}}) = \gamma_{\mathrm{us}}$ and emit a partial dislocation. Following the emission, the slip plane behind the partial contains a stacking fault and remains at an elevated energy level γ_{sf} (point III).

The nucleated partial dislocation moves away from the crack tip and settles at an equilibrium distance r_A. This distance is determined by the balance of image and stacking fault forces drawing the dislocation back to the crack tip and the Peach-Koehler force driving the dislocation away,

$$\frac{K_{\mathrm{II}} b_A}{\sqrt{2\pi r_A}} = \gamma_{\mathrm{sf}} + \frac{\mu b_A^2}{4\pi(1-\nu) r_A}, \tag{6}$$

where b_A is the Burgers vector of the leading partial (in an fcc crystal $b_A = a_0/\sqrt{6}$ where a_0 is that lattice parameter). The equilibrium equation in (6) has two roots: a point of unstable equilibrium very close to the origin and a point of stable equilibrium normally at $r_A \gg b_A$. The larger root is the one of interest,

$$r_A = \frac{K_{\mathrm{II}}^2 b_A^2}{8\pi\gamma_{\mathrm{sf}}^2}\left[1 + \sqrt{1 - \frac{2\mu\gamma_{\mathrm{sf}}}{(1-\nu)K_{\mathrm{II}}^2}}\;\right]^2. \tag{7}$$

3 Emission of the trailing partial

As K_{II} continues to increase the incipient slip associated with the trailing partial may begin to form. The critical SIF for the emission of the trailing partial is obtained in a similar manner to the emission of the leading partial. There are, however, several important differences:

(i) The leading partial dislocation that was emitted earlier shields the crack tip and reduces the stress intensity factor from K_{II} to K_{II}^{*},

$$K_{\mathrm{II}}^{*} = K_{\mathrm{II}} - \frac{\mu b_A}{(1-\nu)\sqrt{2\pi r_A}} = \sqrt{K_{\mathrm{II}}^2 - \frac{2\mu\gamma_{\mathrm{sf}}}{1-\nu}}. \tag{8}$$

The final term is obtained after making use of (7) and simplifying.

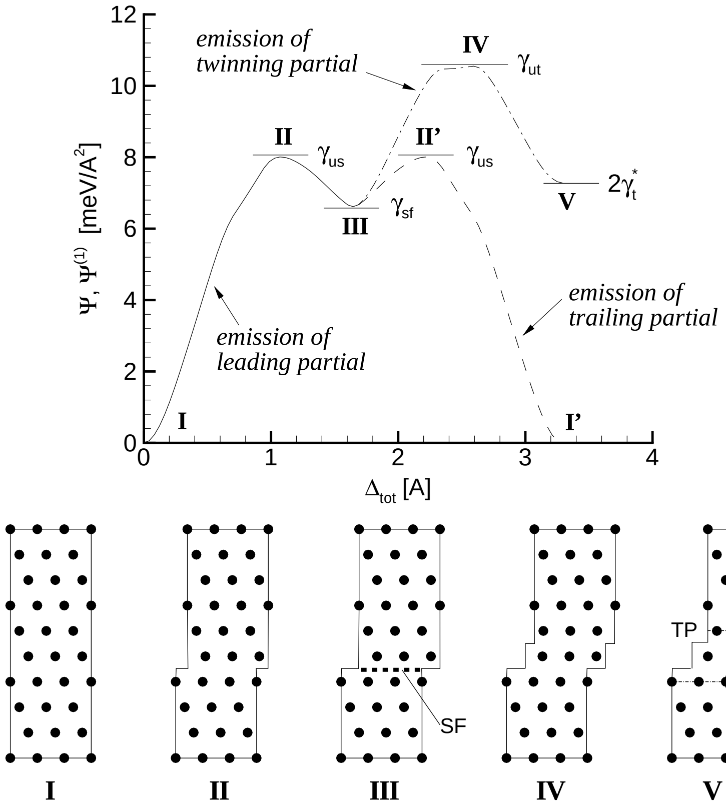

Fig. 4. The interplanar potential $\Psi(\Delta)$ for aluminum for the emission of a leading partial (solid line), trailing partial (dashed line) and a twinning partial (dash-dot line) along with the atomic arrangements associated with points I to V on the $\Psi(\Delta)$ curve. Reproduced from [TH03].

(ii) The slip associated with the trailing partial is no longer aligned with the loading direction. This means that in general there are three independent components of the slip at the crack tip $\boldsymbol{\delta}_{\text{tip}}$ to be determined and a criterion of the form of (4) cannot be used. An approximate closed-form solution may be obtained by neglecting shear-tension coupling (i.e. setting $\delta_2 = 0$) and constraining the slip at the crack tip to coincide with the partial dislocation direction ($\delta_1 = \delta \cos \phi_B$, $\delta_3 = \delta \sin \phi_B$). As a result the crack tip singularity is not fully relaxed and residual SIFs $K_{\text{II(tip)}}$ and $K_{\text{III(tip)}}$ remain at the crack tip.

(iii) The ground level energy is no longer zero, but rather $\gamma_{\rm sf}$. Thus the barrier to dislocation emission is $\gamma_{\rm us} - \gamma_{\rm sf}$. This can be seen in Fig. 4 where the dashed line continuing from point III corresponds to the emission of the trailing partial. At the end of the emission the slip plane behind the resulting dissociated dislocation is undisturbed with zero energy penalty.

Given the factors listed above, reevaluating the J-integral along the far and slit contours gives,

$$J_{\rm far} = (1-\nu)K_{\rm II}^{*2}/2\mu = (1-\nu)K_{\rm II}^{2}/2\mu - \gamma_{\rm sf}, \tag{9}$$

$$J_{\rm slit} = \left[(1-\nu)K_{\rm II(tip)}^{2} + K_{\rm III(tip)}^{2}\right]/2\mu + \Phi(\delta_{\rm tip}) - \Phi(\delta_{\rm sf}), \tag{10}$$

where $\delta_{\rm sf}$ is the slip discontinuity associated with the stacking fault left in the wake of the leading partial, such that $\Phi(\delta_{\rm sf}) = \gamma_{\rm sf}$.

Before the nucleation criterion can be obtained it is necessary to find $K_{\rm II(tip)}$ and $K_{\rm III(tip)}$. One equation for these quantities may be obtained from the solution for the effect of a slip distribution along the x-axis on the stress intensity factor,

$$K_{\rm II(tip)} - K_{\rm II}^{*} = \frac{\mu\cos\phi_B}{\sqrt{2\pi}(1-\nu)}\int_0^\infty \frac{1}{\sqrt{x_1}}\frac{d\delta(x_1)}{dx_1}dx_1, \tag{11}$$

$$K_{\rm III(tip)} = \frac{\mu\sin\phi_B}{\sqrt{2\pi}}\int_0^\infty \frac{1}{\sqrt{x_1}}\frac{d\delta(x_1)}{dx_1}dx_1. \tag{12}$$

Note that even for pure mode II loading, a mode III component exists at the tip. Rearranging (11) and (12) and equating between gives,

$$(1-\nu)\sin\phi_B\left[K_{\rm II(tip)} - K_{\rm II}^{*}\right] - \cos\phi_B K_{\rm III(tip)} = 0. \tag{13}$$

A second equation relating $K_{\rm II(tip)}$ and $K_{\rm III(tip)}$ is obtained by requiring that the shear stress in the direction of the slip be bounded. The shear stresses ahead of the crack tip are $\sigma_{21} = K_{\rm II(tip)}/\sqrt{2\pi r}$ and $\sigma_{23} = K_{\rm III(tip)}/\sqrt{2\pi r}$. The resolved shear stress in the slip direction is $\tau = \sigma_{21}\cos\phi_B + \sigma_{23}\sin\phi_B$. The condition for bounded shear stress at the crack tip is then,

$$\tau|_{r\to 0} = \frac{1}{\sqrt{2\pi r}}\left[\cos\phi_B K_{\rm II(tip)} + \sin\phi_B K_{\rm III(tip)}\right] < \infty. \tag{14}$$

Since ϕ_B, $K_{\rm II(tip)}$ and $K_{\rm III(tip)}$ are not functions of r, this condition can only be satisfied if,

$$\cos\phi_B K_{\rm II(tip)} + \sin\phi_B K_{\rm III(tip)} = 0. \tag{15}$$

This is the second equation for $K_{\rm II(tip)}$ and $K_{\rm III(tip)}$. By solving (13) and (15) together the tip SIFs are obtained,

$$K_{\rm II(tip)} = \frac{(1-\nu)\sin^2\phi_B}{\cos^2\phi_B + (1-\nu)\sin^2\phi_B}K_{\rm II}^{*}, \tag{16}$$

$$K_{\mathrm{III(tip)}} = -\frac{(1-\nu)\cos\phi_B \sin\phi_B}{\cos^2\phi_B + (1-\nu)\sin^2\phi_B} K^*_{\mathrm{II}}. \tag{17}$$

Substituting (16) and (17) into (10) and equating with (9), the critical SIF for the emission of the trailing partial and the generation of the dissociated dislocation is obtained, after some simplification, as

$$K^{\perp}_{\mathrm{II}} = \sqrt{2\mu\left[\frac{1}{1-\nu} + (1-\frac{\gamma_{\mathrm{sf}}}{\gamma_{\mathrm{us}}})\tan^2\phi_B\right]\gamma_{\mathrm{us}}} = \lambda_{\mathrm{crit}} K^{1}_{\mathrm{II}}, \tag{18}$$

where

$$\lambda_{\mathrm{crit}} = \sqrt{1 + (1-\nu)(1-\frac{\gamma_{\mathrm{sf}}}{\gamma_{\mathrm{us}}})\tan^2\phi_B}, \tag{19}$$

characterizes the additional load necessary to nucleate the trailing partial relative to the leading partial.

4 Emission of the twinning partial

Once the leading partial dislocation has been emitted (and before the emission of the trailing partial) there is a competition between two possible modes of deformation. The system will either nucleate the trailing partial of the dissociated dislocation as discussed in the previous section or it will nucleate another partial dislocation of the leading type on an adjacent plane and form a microtwin. Two quantify this competition, the critical SIF required to nucleate the twinning dislocation is computed and compared to the trailing partial nucleation criterion in (18). Since the nucleation of the microtwin involves the emission of a partial dislocation, exactly as in the previous cases, a Peierls analysis may be applied here as well. The derivation of the twinning criterion closely follows the derivation for the trailing partial in the previous section with two main exceptions:

(i) The twinning partial dislocation has the same orientation as the leading partial, so $\phi_B = \phi_A = 0$.

(ii) The maximum barrier which must be overcome to emit the twinning partial is not $\gamma_{\mathrm{us}} - \gamma_{\mathrm{sf}}$ but rather $\gamma_{\mathrm{ut}} - \gamma_{\mathrm{sf}}$. The physical significance of γ_{ut} is explained in Fig. 4 which shows the interplanar potential $\Psi(\Delta)$. As noted earlier, the first part of the curve from I to III corresponds to the emission of the leading partial and the dashed line to the emission of the trailing partial. Consider now instead the case where another leading partial dislocation is emitted on the plane above the plane with the stacking fault. This occurs along the curve from III to V. The energy barrier for this emission $\gamma_{\mathrm{ut}} - \gamma_{\mathrm{sf}}$ depends on the new maximum γ_{ut} (point IV) which is different from γ_{us}. The parameter γ_{ut} is the maximum energy encountered when in a crystal containing an intrinsic stacking fault the part of the crystal one layer above the stacking fault is rigidly displaced along the twinning partial direction. This is demonstrated by atomic arrangements IV and V. After the emission of the second partial a microtwin is formed. An intrinsic stacking fault exists between the two partials and an extrinsic stacking fault (point V) exists behind the second partial. The energy of the extrinsic fault is $2\gamma_{\mathrm{t}}^{*}$ where γ_{t}^{*} is nearly equal to the twin boundary energy γ_{t} except for distant-neighbor interaction effects.

Given the above, the critical mode II SIF for nucleating the twinning dislocation $K_{\mathrm{II}}^{\mathrm{T}}$ is obtained from (18) by simply setting $\phi_B = 0$ and replacing γ_{us} with γ_{ut}, so that

$$K_{\mathrm{II}}^{\mathrm{T}} = \sqrt{\frac{2\mu\gamma_{\mathrm{ut}}}{1-\nu}} = K_{\mathrm{II}}^{1}\sqrt{\frac{\gamma_{\mathrm{ut}}}{\gamma_{\mathrm{us}}}}. \tag{20}$$

Comparing this expression to (5) it is clear that γ_{ut} plays a similar role for twinning as γ_{us} does for dislocation emission. The analysis that follows demonstrates that the unstable twinning energy plays a key role in determining the propensity of a material to twin.

5 Twinning criterion

In the previous sections, the critical mode II SIFs for nucleating the leading partial dislocation K_{II}^{1} (5), the trailing partial dislocation $K_{\mathrm{II}}^{\perp}$ (18) and the twinning partial dislocation $K_{\mathrm{II}}^{\mathrm{T}}$ (20) were obtained. The *twinning tendency* of a material T is defined as the ratio between the SIF for dislocation emission and the SIF for twinning,

$$T = \frac{K_{\mathrm{II}}^{\perp}}{K_{\mathrm{II}}^{\mathrm{T}}} = \lambda_{\mathrm{crit}}\sqrt{\frac{\gamma_{\mathrm{us}}}{\gamma_{\mathrm{ut}}}}. \tag{21}$$

A material will emit a dislocation before twinning if $T < 1$ and will twin first if $T > 1$. This is the twinning criterion. The twinning tendency expression in (21) lends itself to a clear physical explanation. T is affected by two factors: λ_{crit}, which characterizes the additional load necessary to nucleate the trailing partial relative to the leading partial, and $\gamma_{\mathrm{us}}/\gamma_{\mathrm{ut}}$, the ratio of the energy barriers for dislocation emission and DT. For cases where spontaneous emission of the trailing partial does not occur, λ_{crit} will be larger than one. The larger the value of λ_{crit} the larger that of T, signifying that DT is becoming more favorable due to the difficulty in nucleating the trailing partial. The ratio $\gamma_{\mathrm{us}}/\gamma_{\mathrm{ut}}$ will normally be less than one, so this factor tends to reduce T. In particular, the larger the value of γ_{ut} the more difficult it is for the material to twin. For cases where spontaneous emission of the trailing partial occurs, λ_{crit} will be less than one and hence T will also be less than one. The twinning criterion will thus predict dislocation emission in this case, consistent with the behavior of the system.

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