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A MULTI–PLANE MODEL FOR DEFECT NUCLEATION AT CRACKS

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ABSTRACT

A mathematical model (2D) of dislocation generation at cracks on interfaces is presented, which takes into account the role of slip processes on several slip planes in the vicinity of a crack. The work investigates the effects of other incipient dislocations on the nucleation and emission of the primary dislocation that emits first and is responsible for crack-tip blunting on atomic length scales. The modeling makes use of the recently-developed Peierls-Nabarro framework for dislocation nucleation. It is found that there is a moderate increase in the critical load necessary to emit a dislocation, when incipient slip activity is allowed to occur on the prolongation of the crack plane. Furthermore, the slip at the tip, the quantity which characterizes to what extent an incipient dislocation forms before it emits, decreases when the dual slip-plane model is used. Implications for the ductile versus brittle response of Ni are discussed.

INTRODUCTION

This paper reviews recent approaches to modeling the interactions that occur between dislocations and cracks, namely, the generation of a dislocation at a crack in various configurations and loadings. This type of modeling is important for understanding the mechanisms, at least on atomic length scales, that contribute to the relative ductility or brittleness of materials. The basic framework of this discussion is that due to Rice and Thomson [1], who considered the stability of a pre-existing dislocation ahead of a crack. If conditions are found that favor the motion of the dislocation away from the crack before conditions for brittle cleavage can occur (say, according to the Griffith criterion), then the material is said to be intrinsically ductile. Conversely, if conditions are found such that the crack propagates, then the material is said to be intrinsically brittle.

Originally, the problem of dislocation nucleation was modelled by invoking continuum elastic expressions for fully formed dislocations, and then determining a critical load which caused a loss of stability [1]. Such models have evolved until recently [2–7], to treatments that incorporate the Peierls-Nabarro [8,9] description of a dislocation. The advantage of the newer formulations is that they describe the nucleation process of a dislocation core in a physically-acceptable manner. In the same manner as with the Peierls-Nabarro model of a dislocation, the nucleation of an incipient dislocation is described as follows: a discontinuity distribution in the displacement field across a slip plane obeys a periodic law of stress versus displacement, and is embedded in a linear elastic continuum surrounding the crack. The primary advantage to this approach is that the poorly-defined core cutoff parameter from the continuum elastic energy expressions of a dislocation is eliminated. A newly defined parameter γ_{us}, the *unstable stacking energy*, is now the key parameter in the nucleation analysis.

The Peierls treatment has the primary advantage that it does *not* consider an already-formed dislocation, i.e., it gives a realistic physical description (in two-dimensions) of the actual nucleation of a dislocation at a crack. However, when the model is used to actually evaluate the ductile versus brittle behavior of materials, it must be realized that much more is occurring. The model does not take into account other processes which occur on various length scales away from the crack. These include, but are not limited to: incipient dislocation activity on competing slip planes at the crack tip; fully formed dislocations in various arrangements and distances from the crack; other defects such as boundaries and point defects; dislocation mobility; three-dimensional aspects, such as the (physically realistic) nucleation of dislocation loops; other material inhomogeneities; and anisotropy. The primary purpose of the work presented here is to investigate the effects of incipient dislocation activity on planes *other* than the nucleation plane. First, the (2D) Peierls-Nabarro treatment of dislocation generation is briefly reviewed, then a mathematical model that accounts for two slip planes (inclined at different angles with respect to the crack plane) is presented. Preliminary results from that model are discussed. Nickel is chosen as a model material in which to compare results here with other continuum (and atomistic) models of defect nucleation. The model presented here has the potential to include other important factors in the overall problem of ductile versus brittle modeling, e.g., pre-existing dislocations, elastic anisotropy, and bimaterial cracks.

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THE PEIERLS–NABARRO APPROACH

To review the Peierls-Nabarro approach [2–7], suppose that *one* of the possible slip planes in a crystal intersects a crack tip (see Figure 1, but ignore, say, slip plane #1). Here we assume the material to be an isotropic elastic solid, that the emergent dislocation is of edge character with respect to the crack tip (i.e., the Burgers vector **b** has no anti-plane components), and that there are no additional dislocations or sources of shielding in the material. Furthermore, we assume the existence of a Peierls-type shear stress τ ($\equiv \sigma_{r\theta}$ acting on the slip plane) as well as a tensile stress σ ($\equiv \sigma_{rr}$ acting normal to the slip plane), which in

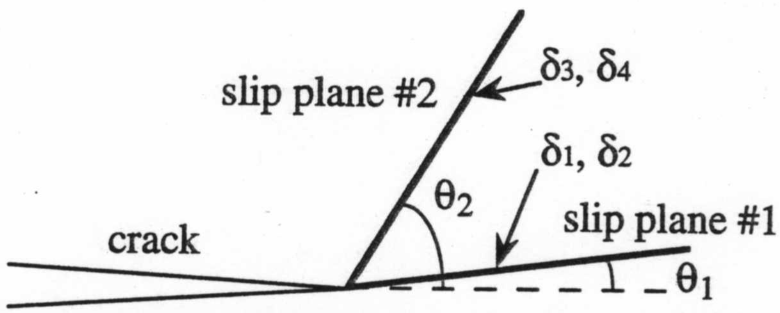

Figure 1. Geometry discussed in this paper – δ_1 and δ_2 denote, respectively, the shear and opening displacements across slip plane #1; δ_3 and δ_4 are the same quantities on slip plane #2. All vary as a function of position along the plane.

turn depend on the relative atomic displacement components Δ_r (sliding parallel to the slip plane) and Δ_θ (opening of the slip plane). The constitutive relations that relate the slip plane stresses to the relative atomic displacements are as follows:

$$\tau = A(\Delta_\theta)\sin\left(\frac{2\pi\Delta_r}{b}\right) \tag{1a}$$

$$\sigma = \left[B(\Delta_r)\,\Delta_\theta - C(\Delta_r)\right] e^{-\Delta_\theta/L} \tag{1b}$$

where

$$A(\Delta_\theta) = \frac{\pi\gamma_{us}}{b} - \frac{2\pi\gamma_s}{b}\left\{q\left(1-e^{-\Delta_\theta/L}\right) - \left(\frac{q-p}{1-p}\right)\frac{\Delta_\theta}{L}e^{-\Delta_\theta/L}\right\} \tag{1c}$$

$$B(\Delta_r) = \frac{2\gamma_s}{L^2}\left\{1 - \left(\frac{q-p}{1-p}\right)\sin^2\left(\frac{\pi\Delta_r}{b}\right)\right\} \tag{1d}$$

$$C(\Delta_r) = \frac{2\gamma_s}{L}\,\frac{p(1-q)}{1-p}\sin^2\left(\frac{\pi\Delta_r}{b}\right) \tag{1e}$$

and are taken from references [4,5]. These forms reduce to the Frenkel sinusoid [10] for pure shearing (i.e., when $\Delta_\theta = 0$) and to the universal bonding correlation of Rose *et al.* [11] for pure opening. The physical properties γ_{us} and $2\gamma_s$ represent, respectively, the maximum energy (per unit area) associated with the unrelaxed (i.e., $\Delta_\theta = 0$) shearing process, and the ideal work of separation (i.e., twice the surface energy). The stress components τ and σ are derivable from a potential $\Psi(\Delta_r, \Delta_\theta)$, that is, they satisfy the Maxwell relation $\partial\tau/\partial\Delta_\theta = \partial\sigma/\partial\Delta_r$. The remaining parameters p, q, and L/b are typically chosen so that the potential Ψ best resembles the same function, as determined via the embedded atom method or density functional theory [5]. Typical values of p and q may be found in Table I; L/b is usually of the order of 1/5.

The next step is to define excess relative displacement quantities. We define δ_r and δ_θ as the displacement discontinuities on a mathematical cut coincident with the slip plane, thus they are related to their counterparts Δ_r and Δ_θ by

$$\delta_r = \Delta_r - \frac{\tau h}{\mu} \tag{2a}$$

$$\delta_\theta = \Delta_\theta - \frac{L^2\sigma}{2\gamma_s} \tag{2b}$$

where h is the interplanar spacing. By adding to the respective displacement discontinuities δ_r and δ_θ across the cut (in what is otherwise considered a linear elastic continuum) the additional "elastic" displacements $h\tau/\mu$ and $L^2\sigma/2\gamma_s$, the relative displacements Δ_r and Δ_θ between atomic planes a distance h apart are approximately simulated. The quantity $2\gamma_s/L$ is an effective modulus for tension across the slip plane and corresponds to the initial slope of the universal bonding correlation.

The final step is to solve for the unknown displacement profiles $\delta_r(r)$ and $\delta_\theta(r)$ along the slip plane as a function of the applied load, and to determine the maximum load for which these solutions are stable. The instability can correspond to dislocation nucleation *or* propagation of a crack-like entity along the slip plane [4,5]. This is perhaps most-straightforwardly achieved by enforcing mechanical equilibrium along the slip plane [4–7], as is demonstrated here for the case of mode I loading:

$$\tau\,[\Delta_r(r), \Delta_\theta(r)] = \frac{K_I}{\sqrt{2\pi r}}\sin\left(\frac{\theta}{2}\right)\cos^2\left(\frac{\theta}{2}\right) - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty g_{11}(r,s,\theta)\frac{d\delta_r(s)}{ds}ds - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty g_{12}(r,s,\theta)\frac{d\delta_\theta(s)}{ds}ds \tag{3a}$$

$$\sigma\,[\Delta_r(r), \Delta_\theta(r)] = \frac{K_I}{\sqrt{2\pi r}}\cos^3\left(\frac{\theta}{2}\right) - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty g_{21}(r,s,\theta)\frac{d\delta_r(s)}{ds}ds - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty g_{22}(r,s,\theta)\frac{d\delta_\theta(s)}{ds}ds \tag{3b}$$

The stresses on the left hand sides of Equations (3a) and (3b) must be expressed as the linear elastic stress components (expressed here in terms of the mode I stress intensity factor K_I) less contributions due to nonlinear relaxation of the slip plane. The kernel functions $g_{ij}(r,s,\theta)$ represent the stresses at distance r due to a unit displacement discontinuity of "gliding" or "climbing" type at position s, and may be found in complex form in [12]. Since the discussion here is limited to mode I loads, the Griffith criterion for relating G and K_I reduces to

$$G = \frac{(1-\nu)}{2\mu}K_I^2 \tag{4}$$

where ν is Poisson's ratio. The solution procedure for the coupled pair of nonlinear integral equations (3a) and (3b) is not discussed here, but may be found in references [4–7]. Some specific critical loads predicted by Equations (3a) and (3b) are given in Table I for $\theta=60°$, $\nu=0.3$, and $L/b=0.2$.

THE EFFECT OF MULTIPLE SLIP PLANES

Consider the situation depicted in Figure 1. Whereas models to date have only considered one incipient dislocation at a crack, here the objective is to account for slip activity on *two* competing slip planes (in what will be hereafter referred to as a *dual-plane* model). A mathematical implementation of the above description of the Peierls-Nabarro scheme for dislocation nucleation would invariably result in a set of four nonlinear, coupled integral equations, which take the following form (for an edge dislocation):

$$\tau_1\,[\Delta_1(r), \Delta_2(r)] = \frac{K_I}{\sqrt{2\pi r}}\sin\left(\frac{\theta_1}{2}\right)\cos^2\left(\frac{\theta_1}{2}\right) - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty \sum_{j=1}^{4} g_{1j}(r,s)\frac{d\delta_j}{ds}ds \tag{5a}$$

$$\sigma_1\,[\Delta_1(r), \Delta_2(r)] = \frac{K_I}{\sqrt{2\pi r}}\cos^3\left(\frac{\theta_1}{2}\right) - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty \sum_{j=1}^{4} g_{2j}(r,s)\frac{d\delta_j}{ds}ds \tag{5b}$$

$$\tau_2\,[\Delta_3(r), \Delta_4(r)] = \frac{K_I}{\sqrt{2\pi r}}\sin\left(\frac{\theta_2}{2}\right)\cos^2\left(\frac{\theta_2}{2}\right) - \frac{\mu}{2\pi(1-\nu)}\int_0^\infty \sum_{j=1}^{4} g_{3j}(r,s)\frac{d\delta_j}{ds}ds \tag{5c}$$

$$\sigma_2 [\Delta_3(r), \Delta_4(r)] = \frac{K_I}{\sqrt{2\pi r}} \cos^3\left(\frac{\theta_2}{2}\right) - \frac{\mu}{2\pi(1-\nu)} \int_0^\infty \sum_{j=1}^{4} g_{4j}(r, s) \frac{d\delta_j}{ds} ds \qquad (5d)$$

where τ_1, σ_1, τ_2, and σ_2 are, respectively, the shear and normal components of stress acting on slip plane #1, and the same components acting on slip plane #2. These in turn are related by some type of nonlinear constitutive law to the shearing and opening displacements along the two cuts (sliding and opening displacements along slip plane #1 are given by δ_1 and δ_2, respectively, and the same quantities for slip plane #2 are denoted by δ_3 and δ_4). The type of constitutive relations used here are the same as used in the previous section, i.e., given by Equations (1a) to (1e). The right hand sides follow from equilibrium: the first terms represent the linear elastic crack field contribution, where K_I is the applied mode I stress intensity factor, and θ_1 and θ_2 are the angles of the two slip planes with respect to the fracture plane. The kernel functions $g_{ij}(r, s; \theta_1, \theta_2)$ are tabulated solutions for a single dislocation in the presence of a crack [12].

Table I. Comparison of the critical loads for instability.

q	p	G/γ_{us} (one plane)	G/γ_{us} (two planes)	fracture?
0.1	0.0	5.95	6.64	no
0.1	0.1	5.24	5.54	no
0.1	0.2	4.07	4.20	no
0.2	0.0	6.03	5.00	yes
0.2	0.1	5.43	5.00	yes
0.2	0.2	4.67	4.37	no
0.2	0.3	3.75	3.99	no
0.3	0.0	5.52	3.34	yes
0.3	0.1	5.21	3.34	yes
0.3	0.2	4.76	3.34	yes
0.3	0.3	4.16	3.34	yes
0.4	0.0	4.41	2.50	yes
0.4	0.1	4.40	2.50	yes
0.4	0.2	4.40	2.50	yes
0.4	0.3	4.13	2.50	yes
0.4	0.4	3.69	2.50	ves

In this study, we restrict ourselves to considering results for the special case of $\theta_1 = 0°$ and $\theta_2 = 60°$ or $70.53°$. The former is a model geometry for which we compare critical loadings to nucleate a dislocation *with* and *without* incipient activity on the plane $\theta = 0°$, under a wide variety of input parameters p and q from Equations (1a) to (1e). It is the same geometry used by Zhou *et al.* [13] in atomistic studies of dislocation nucleation from a crack in a hexagonally-packed 2D structure. The latter geometry is relevant for a crack on a {111} plane in a fcc material, since the most favored slip plane (under a mode I loading) is another {111} type plane inclined at 70.53° with respect to the crack plane. For this particular case, we restrict ourselves to using p and q values appropriate for nickel, as determined via comparison with the embedded atom potential of Foiles *et al.* [14] by Sun *et al.* [5]. As an additional comparison, results here ought to be compared with calculations by Gumbsch [15] on dislocation nucleation in the identical geometry in nickel, using the so-called combined atomistic/finite-element procedure, also based on the same interatomic potential by Foiles *et al.* [14]. Such work is in progress.

Results for the case when $\theta_2 = 60°$ are given only in terms of a critical load for defect nucleation, and are summarized in Table I. In all cases, L/b=0.2 (a typical value for most metals) and ν=0.3. When such a configuration is loaded, one of two possibilities can occur first: cleavage along the crack plane or dislocation emission. The former possibility can be directly predicted by the dual-plane model, since crack propagation is an allowed instability mode in Equations (5), and is indicated by a "yes" in the final column of Table I. The single-plane model gives only a load to emit a dislocation on the inclined slip plane, regardless of whether the Griffith cleavage condition is exceeded or not. For example, consider the cases for which q (i.e., $\gamma_{us}/2\gamma_s$) is relatively large, e.g., 0.3 or 0.4. Then the maximum load for which Equations (5) can be solved is (within the accuracy of the numerical procedure) is given by $G=2\gamma_s=(1/q)\gamma_{us}$. The single slip plane model, however, ignores the Griffith cleavage criterion and predicts a dislocation nucleation load which is larger than the realistic maximum-attainable load corresponding to cleavage. Alternatively, the relatively ductile materials (characterized by a relatively low $\gamma_{us}/2\gamma_s$ ratio, e.g. 0.1) involve dislocation nucleation before cleavage, and such a load is predicted by both methods described in this paper. However, the dual-plane model predicts a slightly larger load for emission (approximately 8%) due to the interactions with incipient activity on the prolongation of the crack plane which are taken into account. Intermediate cases, e.g., those with q=0.2 in Table I, can result in dislocation emission or crack propagation, depending on the additional coupling parameter

Table II. Comparison of the critical loads for emission from a {111} crack in nickel. (p = 0.132, q = 0.0879, L/b = 0.271, ν = 0.281) All values are expressed in J/m^2.

Rice-Thomson (1974)	single-plane (isotropic)	dual-plane (isotropic)	single-plane (anisotropic)
1.856	1.135	1.225	1.080

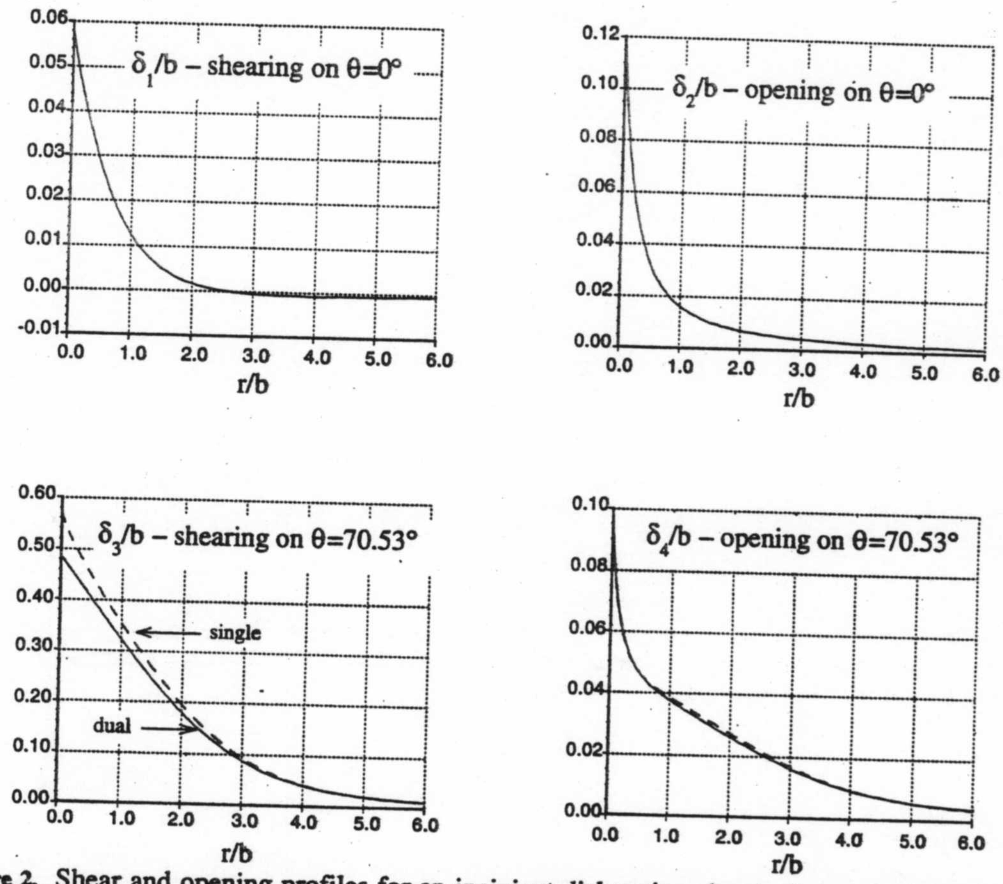

Figure 2. Shear and opening profiles for an incipient dislocation ahead of a crack situated on a {111} type slip plane in nickel.

p. I.e., for such an intermediate case, the larger p, the more likely there is to be dislocation nucleation before cleavage. Note that there is no definitive trend regarding the effect of the additional plane: The critical load for dislocation nucleation for q=p=0.2 is *smaller* in the dual-plane model, unlike other cases when dislocation emission is preferred.

Results for the {111} orientation in nickel are given in Figure 2 and Table II. Specific relative displacement profiles from the continuum model are given in Figure 2, each corresponding to the critical instability load. As expected, the shearing displacement component along the slip plane (i.e., δ_3/b) is significant, as well as the opening component along the slip plane (δ_2/b); but the shearing along the crack plane is not that significant. Note that the shear displacement of the dislocation at instability (i.e., δ_3/b evaluated at $r = 0$) is somewhat smaller in the dual slip-plane model. Such a trend has also been noted in the Lattice Green's function calculations of Zhou *et al.* [13] for hexagonal lattices (i.e., they note a smaller slip displacement at the crack tip just prior to dislocation emission). However, the magnitude of that effect is somewhat larger than the effect seen here, and is likely related to the slip ledge that appears at the crack tip when the dislocation is forming. In the continuum sense, there is a retarding force associated with this creation of energy; however, no sensible means for incorporating this into a continuum model have become apparent [15,16].

Table II gives a comparison of the critical load to emit a partial dislocation in nickel from the {111} orientation already discussed. In addition to the values presented here from the single and dual slip-plane models, predictions from the Rice-Thomson model [1], as well as the single-plane model with full elastic anisotropy taken into account [7], are presented for comparison. Consistent with most of the cases presented in Table I, there is a slight increase in the critical load for nucleation (about 8%) in the dual plane model, compared with the single-plane version (isotropic formulations). All the values are less than the critical G for cleavage [5], which would imply that Ni (at least in the orientation examined) is intrinsically ductile.

SUMMARY

A model for dislocation formation and emission in the presence of *two* competing slip planes has been presented, which builds upon recent advances in the modeling of dislocation nucleation at a crack tip based on the Peierls–Nabarro concept [2–7]. It is found that there is generally a modest increase in the load required to emit a nucleation under a mode I load, when incipient displacement activity is allowed to occur on the prolongation of the crack plane. Furthermore, the amount of slip at the crack tip just prior to emission of the dislocation is found to be slightly less than when one slip plane is taken into account. The model has been specialized to the case of Shockley partial dislocation formation ahead of a crack on a {111} plane in nickel.

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