MODE MIXITY EFFECTS ON CRACK TIP DEFORMATION IN DUCTILE SINGLE CRYSTALS

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Abstract—Crack tip deformation and stress fields in ductile single crystals, under mixed mode loading conditions, are examined within the framework of a geometrically rigorous formulation of crystalline plasticity. The theory accounts for finite deformations and finite lattice rotations, as well as for the full three-dimensional crystallographic geometry of the crystal. An experimentally based self-hardening rule exhibiting an initial stage of rapid hardening followed by a saturation stage is used in the analysis. For the orientation of an f.c.c. crystal considered in this study, the geometric nature of slip gives rise to competing deformation modes. Our studies reveal that mode mixity exerts a strong influence on which of these competing deformation modes prevail. It is found that the effects of mode mixity are more complex than those predicted by phenomenological flow theories of plasticity. Finite deformation and lattice rotation effects, as well as the details of the hardening law, strongly influence the structure of the solution.

Résumé—Dans le cadre d’une formulation rigoureuse de la plasticité cristalline, on examine la déformation et les champs de contrainte à l’extrémité d’une fassure en mode de charge mixte. La théorie explique les déformations finies et les rotations finies du réseau, ainsi que la géométrie cristallographique complète à trois dimensions du cristal. Dans cette analyse, on utilise une règle, basée sur l’expérience, d’auto-durcissement qui révèle un stade initial de durcissement rapide suivi d’un stade de saturation. Pour un cristal f.c.c. ayant l’orientation considérée dans cette étude, la nature géométrique du glissement donne lieu à des modes de déformation en concurrence. Nos études révèlent que la mixité du mode exerce une influence forte sur le mode qui va dominer. On trouve que les effets de mixité du mode sont plus complexes que ceux qui prévoient les théories phénoménologiques de l’écoulement plastique. Les effets de déformation finie et de rotation du réseau, ainsi que les détails de la loi de durcissement, influencent fortement la structure de la solution.


1. INTRODUCTION

Mode I and III crack tip fields in single crystals have been extensively studied by analytical [1, 2] and computational methods [3–5]. By contrast, the effect of mode mixity on such fields has received relatively little attention. Lin and Thomson [6] have investigated the competition between cleavage and dislocation emission at the tip of an atomistically sharp crack, based on elastic theory of dislocations. Their results show that dislocation emission is strongly influenced by mode mixity. For example, suppose that a crack subject to Mode I loading can emit dislocations on a slip system having a screw component parallel to the crack front. The addition of a Mode III component of the appropriate sign increases the resolved shear stress on the system and, therefore, promotes dislocation emission. This, in turn, may influence which of the competing mechanisms, i.e. blunting or cleavage, prevails. Within a continuum framework, mode mixity effects have been investigated by Shih [7] and Pan and Shih [8–10], for solids obeying $J_r$ plasticity theory. Their work shows that the transition from pure mode I to mixed

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mode fields occurs gradually, and that the fields depend continuously on the relative ratios of the remote $K_1$, $K_2$, and $K_3$ load components. In contrast, the geometric nature of slip in single crystals gives rise to competing deformation modes. Under such conditions, our results demonstrate that small changes in mode mixity can produce abrupt changes in deformation modes.

The analysis presented here relies on a geometrically rigorous formulation accounting for finite deformations and finite lattice rotations, as well as for the full three-dimensional crystallographic geometry. The stationary crack in an f.c.c. crystal is considered to be initially mathematically sharp. We allow for arbitrary generalized-plane solutions, in which the three components of displacement are assumed to be independent of position along the crack front. For the sake of brevity, only the results corresponding to a specific geometry of an f.c.c. crystal are presented. For this geometry, the deformation fields in the region beyond the zone of finite lattice rotations are symmetric under pure Mode I and Mode III conditions.

The constitutive theory and numerical procedures used in the analysis are described in Section 2. In Section 3, an appropriate normalization of the fields based on the $J$-integral [11] is given. The results of the analysis are presented in Section 4 and a discussion follows in Section 5.

2. THEORY AND NUMERICAL PROCEDURE

Consider a crystal lattice being deformed from its initial undeformed configuration $\mathcal{B}_1$ to its current configuration $\mathcal{B}_t$ at time $t$. The deformation gradient $\mathbf{F}$ fully defines the local deformations of the crystal. Two deformation mechanisms contribute to $\mathbf{F}$: plastic slip, which leaves the lattice invariant, and lattice distortion. Following Lee [12] and others (e.g. [13–17]), this suggests a multiplicative decomposition

$$\mathbf{F} = \mathbf{F}^p \mathbf{F}^p$$

(1)

of $\mathbf{F}$ into elastic and plastic parts $\mathbf{F}^e$ and $\mathbf{F}^p$ respectively. The plastic deformations $\mathbf{F}^p$ define a collection of plastically deformed local configurations which are collectively referred to as the intermediate configuration $\mathcal{B}_t$. The plastic rate of deformation, defined on the reference state lattice, is given by [18]

$$\dot{\mathbf{F}}^p \mathbf{F}^{-1} = \sum_i \gamma^p_i \mathbf{s}^i \otimes \mathbf{m}^i$$

(2)

where $\gamma^p_i$ is the shear strain rate on slip system $\alpha$ and $\mathbf{s}^i$ and $\mathbf{m}^i$ are the slip direction and slip plane normal. The sum ranges over all active slip systems. The slip rate on system $\alpha$, $\gamma^p$, is assumed to depend on stress only through the corresponding resolved shear stress

$$\tau^p = \mathbf{s}^i \cdot (\mathbf{F}^{-1} \dot{\mathbf{F}}^p) \cdot \mathbf{m}^i$$

(3)

where $\tau$ is the Kirchhoff stress on $\mathcal{B}_t$. In our calculations we have adopted the power law

$$\gamma^p = \gamma_0 \text{sgn}(\tau^p) \left( \frac{\left| \tau^p \right|}{\sigma^p} \right)^m$$

(4)

proposed by Peirce, Asaro and Needleman [19], where $\gamma_0$ is the reference shear strain rate, $\sigma^p$ is the current shear flow stress on slip system $\alpha$, and $m$ is the material strain-rate sensitivity. For multiple slip, the evolution of the flow stresses may be taken to be governed by a hardening law of the form

$$\sigma^p = \sum_{i} h_{\alpha i} |\gamma^p_i|$$

(5)

for some hardening moduli $h_{\alpha i}$. These in turn are assumed to be of the form

$$h_{\alpha i} = h_0 (q + (1 - q) \delta_{\alpha i})$$

(6)

Here $\gamma = \sum \gamma_\alpha$ is the sum of the accumulated slip strains on all slip systems and $q$ characterizes the hardening behavior. The value $q = 1$, which corresponds to isotropic or Taylor hardening, has been used in our calculations. A form of $h(\gamma)$ in (6) appropriate to Al–Cu alloy crystals [20] is

$$h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_0 - \tau_c} \right)$$

(7)

where $h_0$ is the initial hardening rate, $\tau_0$ is the critical resolved shear stress, and $\tau_c$ is the saturation strength.

The elastic relations for metals may be assumed to be of the simple form

$$\mathbf{S} = \mathbf{D}^e \mathbf{E}^e; \quad \mathbf{E}^e = (\mathbf{C} - 1)/2, \quad \mathbf{C}^e = \mathbf{F}^{-1} \mathbf{F}^e$$

(8)

without much loss of generality. Here, $\mathbf{S}$ is the second Piola–Kirchhoff stress tensor relative to $\mathcal{B}_t$, and $\mathbf{E}^e$ and $\mathbf{C}^e$ are the Green strain tensor and the right Cauchy–Green deformation tensor on $\mathcal{B}_t$, respectively. To a first approximation, the elastic moduli $\mathbf{D}^e$ for the crystals under study may be taken to be isotropic, i.e. of the form

$$\mathbf{D}^e = \lambda \delta_{\alpha \beta} \delta_{\alpha \beta} + \mu (\delta_{\alpha \beta} \delta_{\alpha \beta} + \delta_{\alpha \delta} \delta_{\beta \delta})$$

(9)

where $\lambda$ and $\mu$ are the elastic Lamé constants.

We adopt the method of solution given by Moran, Ortiz and Shih [21] in the context of flow theories of plasticity. Here, the method is generalized to handle several simultaneously active slip systems. The constitutive update is based on an implicit treatment of the elastic–plastic kinematics and the elastic response, defined by (1)–(5), (8), and (9), combined with an explicit treatment of the hardening law (6), whereby the hardening modulus (7) is sampled at the start of the time step. This method of discretization results in
stress on $\mathcal{B}$. In our
the power law
\[
\left( \frac{t^*}{g^*} \right)^{1/m} \leq g^*
\]  
and Needleman [19],
strain rate, $g^*$ is the
slip system $a$, and $m$ is
vity. For multiple slip,
may be taken to be of the form
\[
\dot{\gamma}_a \leq g^* \delta \mathcal{B}.
\]  
the accumulated slip
and $q$ characterizes the
are $q = 1$, which corre-
hardening, has been
form of $h(\gamma)$ in (6)
ystals [20] is
\[
\frac{h(\gamma)}{\tau_a - \tau_0}
\]  
elastic hardening rate, $\tau_0$ is the
and $\tau_a$ is the saturation
als may be assumed to
\[
\frac{1}{2m}, \quad C = F^T F
\]  
y. Here, $\mathbf{S} = \mathbf{F}^{-1} \mathbf{t} \mathbf{F}^{-T}$
stress tensor relative
creep strain tensor and
rmination tensor on $\mathcal{B}$,
oramination, the elastic
er study may be taken in
\[
\delta \mathcal{B} = \delta_{s} \mathcal{B} + \delta_{d} \mathcal{B}
\]  
Lamé constants.
section given by Moran,
text of flow theories of
generalized to handle
lip systems. The con-
licit treatment of the
elastic response, 9), combined with an
ning law (6), whereby
ampled at the start of
cretization results in
the following algebraic equations defining the state
update
\[
F_{x+1} = F_{x} , \quad F_{x+1} = \mathbf{F}_{x+1}^T \mathbf{F}_{x+1}, \quad \mathbf{C}_{x+1} = \mathbf{F}_{x+1}^T \mathbf{F}_{x+1} + \Delta t \mathbf{S}_{x+1} \left( \frac{1}{g^*} \right)
\]  
\[
\Delta \gamma = \Delta t \gamma_0 \mathbf{sgn}(\tau_{x+1}^*) \left( \frac{1}{g^*} \right)
\]  
\[
\tau_{x+1}^* = s \mathbf{C}_{x+1} \mathbf{S}_{x+1} \cdot \mathbf{m}
\]  
\[
g_{x+1}^* = g_{x+1}^* + \sum \mathbf{h}(\gamma_a) \left( 1 - q \delta_{s} \right) \Delta \gamma
\]  
\[
\mathbf{S}_{x+1} = \mathbf{F}_{x+1} \mathbf{S}_{x+1} \left( \mathbf{C}_{x+1} - \mathbf{I} \right) / 2
\]  
where the subindices $(\cdot)_{x}$ and $(\cdot)_{x+1}$ refer to the initial
and updated values of the state variables, respecti-
ively, $\Delta \gamma$ are the incremental slip strains, and $\Delta t$ is
the time increment. In (10), the final deformation
gradients $\mathbf{F}_{x+1}$ are to be regarded as given. It is of
interest to note that, since the hardening modulus $h$
is treated explicitly, (10) can be reduced to a system of
nonlinear equations for the incremental shear
strains $\Delta \gamma$ (for details, see [21]). In the pre-
vious analysis, this system is solved by means of a local
Newton–Raphson iteration with line searches. With
the determination of $\Delta \gamma$, the remaining state
variables follow immediately from (10). Owing to the
implicit treatment of the constitutive equations and
the inclusion of the elastic response, the updated
state is always unique even in the rate-independent
limit, provided that the elastic domain is convex. The
integration of equilibrium equations is performed
explicitly, by the forward-gradient method of the type
proposed by Peirce, Shih and Needleman [22].
The finite element mesh is composed of 8-noded
isoparametric brick elements. In order to prevent
locking due to near-incompressibility under condi-
tions of fully developed plastic flow, we employ
an assumed strain method developed by Moran,
Ortiz and Shih [21]. The method generalizes the
mean-dilatation approach of Nagtegaal, Parks and
Rice [23] to finite deformations, and consists of
postulating a constant deformation jacobian $\mathbf{det}(\mathbf{F})$
over each element, the value of which is sampled at
the centroid. The generalized plane condition is
enforced by meshing a slice of the solid perpendicular
to the crack front by a single layer of elements and
constraining the three displacement components to
be equal on both surfaces of the slice.
In the present analysis, a fan-like mesh with
exponential grading in the radial direction and
uniform grading in the circumferential direction is
used. The ratio of the inner-most to the outer-most
element is of the order of $10^{-5}$. The angular reso-
ution of the mesh is $12^\circ$, and the total number of
degrees of freedom is 5939. Tractions consistent with
the linear elastic asymptotic field of appropriate
mode mixity are applied at the outer boundary, and
increased at increments such that essentially one new
ring of elements is plastified at each step. The rate of
load application is chosen such that the maximum
strain rates in the vicinity of the crack tip are of
the order of the reference strain rate $\gamma_0$. This results
in modest or negligible amounts of overstress due
to rate dependency. The values of the material con-
stants used in the calculations of f.c.c. crystals are:
$\lambda = 576.92 \tau_0$, $\mu = 384.62 \tau_0$, $\gamma_0 = 10^{-3}$,
$\tau_0 = 0.005$, $q = 1$, $h_0 = 8.9 \tau_0$, $\tau_0 = 1.89 \tau_0$. These values are typical of
Al–Cu alloys [20].

3. MODE MIXITY AND NORMALIZATION OF FIELDS

Under small scale yielding conditions, the
$J$-integral and the stress intensity factors of
the three crack-tip modes are related by [11]
\[
J = \frac{1}{2 \mu} \left[ (1 - v) K_I^2 + (1 - v) K_{II}^2 + K_{III}^2 \right]
\]  
where $v$ and $\mu$ are the poisson’s ratio and shear
modulus of the solid taken to be elastically isotropic.
It is convenient to define an effective stress intensity
factor, $K$, by
\[
K = \sqrt{2 \mu J}
\]  
Fig. 1. Mode mixities $\psi$ and $\phi$ defined in the $(K_I, K_{II}, K_{III})$
space.

Fig. 2. Crack on (010) cube plane in an f.c.c. crystal with the
crack front parallel to [010] direction.
where $J$ is defined by (11), or equivalently by the path independent value for a contour through the elastic region. This effective stress intensity factor, $K$, proves useful for the purpose of normalizing the mixed mode near-tip fields so as to reveal the trends due to mode mixity.

When all three modes are present, the mode mixity is fully specified by two spherical angles, $\psi$ and $\phi$, in $(K_1, K_{II}, K_{III})$ space,

$$\tan \psi = \frac{K_{II}}{K_1}, \quad \cos \phi = \frac{K_{III}}{(K_1^2 + K_{II}^2 + K_{III}^2)^{1/2}}. \quad (13)$$

The angles $\psi$ and $\phi$ are shown in Fig. 1. An equivalent definition can be given in the space of the traction vector, $\mathbf{t} = (\sigma_{12}, \sigma_{22}, \sigma_{33})$, on the line directly ahead of the crack tip, viz.,

$$\tan \psi = \frac{\sigma_{12}}{\sigma_{22}}, \quad \cos \phi = \frac{\sigma_{33}}{|\mathbf{t}|} \quad \text{as } r \to 0. \quad (14)$$

Here, and subsequently, the axes are chosen such that the crack lies in the $x_1-x_2$ plane, with its front on the $x_1$-axis and growth in the direction of the positive $x_2$-axis. The mode mixity, as defined by (13) and (14), also applies to cracks in anisotropic homogeneous materials, and to a crack along a tilt grain boundary, in which the crack front and the tilt axis are parallel. The concept of mode mixity for an interface crack in general anisotropic solids, which additionally depends on the distance ahead of the crack tip, is discussed at some length by Wang, Shih and Suo [24].
4. RESULTS OF THE ANALYSIS

In this section, results pertaining to a specific geometry of an f.c.c. crystal are presented. The plane of the crack coincides with the (010) cube plane, with the crack front along the [101] direction and growth along the [101] direction, Fig. 2. The complete set of twelve slip systems of the type \{111\}〈110〉 is accounted for in the analysis. Plastic shearing may occur either parallel or perpendicular to an active slip plane. The former type of slip will be termed a shear mode, while the latter will be termed a kink mode. Kink modes of deformation may involve substantial lattice rotations, which may in turn induce geometric hardening or softening depending on the direction of rotation. Different types of dislocation configurations are required to achieve these modes in crystals. Readers are referred to the papers by Rice and Nikolic [1] and Rice [2], where a description of the dislocation configurations required to sustain shear and kink modes under anti-plane strain and plane strain conditions is given.

For ease of reading, the following notation for the slip systems in f.c.c. crystals is adopted [25],

A = (111), B = (111), C = (111), D = (111)
1 = [011], 2 = [011], 3 = [101]
4 = [101], 5 = [101], 6 = [110].

With this notation, the slip systems (111) [101] and (111) [101], for example, are referred to as B4 and C3, respectively.

For the crack geometry and f.c.c. crystal under consideration, crack tip deformation and stress fields under pure Mode III [4] and Mode I [5] have been reported elsewhere. These results are briefly summarized below and the pertinent near-tip fields, normalized by the effective \( K \) as defined in Section 3, are recorded here for later reference.

The fields that evolve have certain features which are common to all load states investigated. These features can be attributed to the constitutive law used in the analysis. The initial portion of the shear stress-slip strain curve rises rapidly and almost linearly, and subsequently flattens out at the saturation level \( t_s \). The nearly linear hardening regime extends up to slip strains of the order 50\( t_s / \mu \), or 0.1. At slip strains of about 0.2, the stress saturates. Thus when the sum of the accumulated slip strains over all slip systems is less than about 0.1, the crystal exhibits a high rate of hardening and the resulting fields are nearly \( 1/\sqrt{r} \) singular. For accumulated slip strains in excess of about 0.2, the crystal behaves like an ideally
4.1. Pure Mode III: \( \phi = \theta \)

Under Mode III loading, the crack is confined to systems B4 and D6, producing plastic zones within the finite strain rotations are small and within the vicinity of the crack tip. The relevant Kirchhoff stress component is given by \( K/\sqrt{2\pi r} \) at \( \dot{r} = r \) (Fig. 3).

4.2. Pure Mode I: \( \psi = \pi/2 \)

Under pure Mode I loading, systems are found to

plastic material. Consequently, two distinct plastic regions exist near the crack tip: an outer region governed by high hardening, and an inner region governed by non-hardening behavior. It should be carefully noted, however, that ideally plastic behavior occurs well within the finite deformation region.

In the interest of space, we have taken advantage of symmetry in presenting the contours of slip activity. For example, under Mode II loading, systems B5 and D6 produce slip activity at +40° and -40° from the crack line, respectively. The slip activity associated with B5, which develops in the upper-half plane, is plotted. Similar slip activity associated with D6, which develops in the lower-half plane, is not shown but the pattern may be inferred by symmetry.

![Fig. 7. Angular variations of the in-plane Kirchhoff stress components at \( \dot{r} = 0.016 \) under pure Mode II loading. The stresses are normalized by \( K/\sqrt{2\pi r} \).](image)

![Fig. 8. Schematic illustration of the orientation of the dominant slip systems with respect to the crack, for the geometry described in Fig. 2.](image)

![Fig. 9. Contours (a) D4 (sh)](image)
4.1. Pure Mode III: $\phi = 0^\circ$

Under Mode III loading, the slip activity is confined to systems B4 and D4. These two systems produce plastic zones which are inclined at $\pm 66^\circ$ to the line of the crack. Within a substantial fraction of the plastic zone, the stresses and slip strains are nearly $1/\sqrt{r}$ singular. The transition from a $1/\sqrt{r}$ type field to one governed by ideally plastic behavior occurs within the finite strain zone. The computed lattice rotations are small and are confined to the immediate vicinity of the crack tip. The angular distributions of the relevant Kirchhoff stress components normalized by $K/\sqrt{2\pi r}$ at $r = r/(K/\tau_0)^2 = 0.016$ are shown in Fig. 3.

4.2. Pure Mode I: $\psi = 0^\circ$

Under pure Mode I loading, three sets of slip systems are found to be operative. The first set involves simultaneous and equal slip on D6 and D1 resulting in an effective shear along an in-plane [121] direction, which contributes to a shear mode at $70^\circ$. The second set involves simultaneous and equal slip on B5 and B2 slip systems resulting in an effective shear along the in-plane direction [121]. This set contributes a kink mode at $40^\circ$ and a less intense shear mode at $130^\circ$. The last set involves equal and simultaneous slip on C3 and A3 systems, giving rise to a kink mode at $112^\circ$. The plastic zones corresponding to these modes are less diffuse than those that develop under Mode III loading. Though significant lattice rotations occur close to the crack tip, the axis of rotation remains parallel to the direction of crack front. This helps to limit the slip activity to the primary systems. The angular variations of normalized Kirchhoff stress components at $r = 0.016$ is shown in Fig. 4. A plot of $(\tau_{11} - \tau_{22})/\tau_0$ vs $\tau_{12}/\tau_0$ spanning the entire angular region of the crack tip, at

![Fig. 9. Contours of slip strains corresponding to combined Mode I and Mode III loadings, on systems (a) D4 (shear mode at 70°), (b) D6 (shear mode at 70°) and (c) A3 (kink mode at 112°).](image-url)
\( r = 0.006 \), is shown in Fig. 16(a). For the purpose of reference, the unrotated initial yield and saturated yield surface are also shown in the figure. Such a plot provides information of the prevailing stress state as well as the expected modes of slip on active slip systems, around the tip of the crack. For example, close examination of the plot reveals that around \( \theta = 40^\circ \) and around \( \theta = 130^\circ \) slip systems B5 and B2 are active. Since the former angle coincides with the slip plane normal the resulting mode would be of kink character, and since the latter angle coincides with the effective slip direction a shear mode is implied; both of these are in accordance with our observations. Similar arguments apply to systems D6 and D1, which remain active around \( \theta = 70^\circ \) implying a shear mode and to systems A3 and C3 rendering a kink mode around \( \theta = 112^\circ \). It is also interesting to note that the stress state around the crack tip sweeps the yield surface by two full turns and there are definite elastic sectors surrounding the crack tip. While this is at odds with Rice's [2] analysis, it is consistent with the experimental findings of Shield and Kim [26] for a similar geometry in b.c.c. crystals (cf. [5]).

4.3. Pure Mode II: \( \psi = 90^\circ \)

The slip systems which are operative under Mode I are also operative under Mode II. However the deformation modes, i.e. whether a mode is of shear or kink type, are different under Mode II loading. For example, though the plastic zone associated with slip system B5 is distributed all around the crack tip, the slip activity shown in Fig. 5(a), is suggestive of a kink mode at approx bet to a deformation pattern respect to the crack line. Loading D6 gives rise to activity due to systems B5 and D6, respectively, for systems A3, and the identity of the zone rather diffuse, is suggested in Fig. 5(b). In contrast, N kink mode along \( 112^\circ \) take place close to the cr contours plots in Fig. 6.7 parallel to the crack front of the plastic zone, being nearly \( 1/\sqrt{r} \) singular. The relevant stress compone

![Fig. 10. Angular variations of the Kirchhoff stress components at \( r = 0.016 \) under combined Mode I and Mode III loadings. The stresses are normalized by \( K / \sqrt{2\pi r} \). (a) In-plane stresses and (b) anti-plane stresses.](image)

![Fig. 11. Contours of (a) D4 (shear mode)](image)
is interesting to note that crack tip sweeps and there are definite crack tip. While this is so, it is consistent with the model and Kim [26] for crystals (cf. [5]).

Earlier under Mode II. However the mode is of shear under Mode II loading. The zone is associated with it around the crack tip. (a), is suggestive of a kink mode at approximately 40°. System D6 gives rise to a deformation pattern which is symmetric with respect to the crack line. In contrast, under Mode I loading D6 gives rise to a shear mode at 70°. Slip activity due to systems B2 and D1 are identical to that of B5 and D6, respectively. The slip activity due to system A3, and the identical pattern form C3, though rather diffuse, is suggestive of a shear mode at 0°, Fig. 5(b). In contrast, Mode I loading produces a kink mode along 112°. Significant lattice rotations take place close to the crack tip, as evident from the contours plots in Fig. 6. The axis of rotation remains parallel to the crack front. Within a major portion of the plastic zone, the stresses and strains are nearly 1/√r singular. The angular variations of the relevant stress components at ̂r = 0.016 are shown in Fig. 7. A plot of \((τ_{11}−τ_{22})/τ_0 vs τ_{12}/τ_0\) around the crack tip, at ̂r = 0.006, is shown in Fig. 16(b); also shown are the unrotated initial yield and saturated yield surfaces. It can be seen that systems B5 and B2 remain active around 0° implying a kink mode, since this angle coincides with the slip plane normal. It can also be observed that beyond 0° = 130° the above mentioned systems remain active consistent with our observation of the diffuse nature of the plastic zone due to these systems. Similar arguments apply to systems D6 and D1, which give rise to a kink mode around 0° = 40°, and to systems A3 and C3, which produce a shear mode at 0° = 0°. In contrast to the pure Mode I loading, the stress state around the crack tip, for pure Mode II loading, sweeps the yield surface only by half a turn.

![Contours of slip strain](image)

**Fig. 11.** Contours of slip strains corresponding to combined Mode II and Mode III loadings, on systems (a) D4 (shear mode at 70°), (b) B5 (kink mode at 40°), (c) D1 (shear mode at 70°) and (d) C3 (kink mode at 120°).
4.4. Mode I and Mode III: $\psi = 0^\circ$ and $\phi = 45^\circ$

Consider systems D4, D6 and D1, all of which share the same plane, Fig. 8. Under Mode I loading, D6 and D1 undergo equal and simultaneous slip resulting in an effective in-plane shear along the [121] direction. However, the slip directions of D1 and D6 have components along the positive and negative $x_3$-axis, respectively. The addition of a Mode III load component in the positive $x_3$ direction increases the resolved shear stress on D1 but weakens the resolved shear stress on D6. Consequently, a shear mode associated with D1, as opposed to D6, dominates the deformation pattern. Similar considerations apply to systems B4, B5 and B2. Now consider systems A3 and C3, which share a common slip direction in $x_1$ direction. The normals to these planes have components along the positive and negative $x_3$-axis, respectively. The addition of Mode III loading in the positive $x_1$ direction favors A3, while suppressing C3.

Figure 9(a) shows the slip activity on system D4. The plastic zone, though slightly more diffuse, bears a strong resemblance to that for pure Mode III loading. System B4 generates a symmetric deformation pattern about the crack line. Slip activity due to system D1, Fig. 9(b), reveals a shear mode at $70^\circ$ resembling the pattern under pure Mode I conditions, Fig. 11(b) of [5]. A less intense kink mode develops along $-40^\circ$, and an even weaker shear mode is formed along $-130^\circ$. Symmetric deformation pattern. Contours of slip activity reveal a strong kink mode is considerably larger than under pure Mode I conditions. The reasons stated earlier, are rendered inoperative.

Under Mode I loading, the strains in D1, B5 and B2, and A3 amount, which results in the addition of a Mode I of breaking this symmetry.

It is noted that, though lattice rotations develop more, the axis of rotation in the $x_1$ direction. The stress is substantial fraction of $K_c/\sqrt{r}$ singular. Relative

![Graph](image-url)

Fig. 12. Angular variations of the Kirchhoff stress components at $r = 0.016$ under combined Mode II and Mode III loadings. The stresses are normalized by $K_c/(2\pi r)$. (a) In-plane stresses and (b) anti-plane stresses.

![Graph](image-url)

Fig. 13. Contours (a) B5 (kr)
common slip direction to these planes have and negative $x_r$-axis, and Mode III loading in the while suppressing C3, activity on system D4, slightly more diffuse, hat for pure Mode III, a symmetric deformation. Slip activity due is shear mode at $70^\circ$ ic Mode I conditions, kink mode develops eaker shear mode is formed along $-130^\circ$. System B5 produces a symmetric deformation pattern with respect to the crack line. Contours of slip activity on systems A3, Fig. 9(c), reveal a strong kink mode at $112^\circ$. The plastic zone is considerably larger than the corresponding one under pure Mode I conditions, Fig. 11(c) of [5]. For the reasons stated earlier, slip systems D6, B2 and C3 are rendered inoperative. It is interesting to note that under Mode I loading, the pairs of systems D6 and D1, B5 and B2, and A3 and C3, slip by the same amount, which results in plane strain deformation. The addition of a Mode III component has the effect of breaking this symmetry.

It is noted that, though not shown here, large lattice rotations develop near the crack tip. Furthermore, the axis of rotation deviates significantly from the $x_r$ direction. The stresses and strains, within a substantial fraction of the plastic zone, are nearly $1/\sqrt{r}$ singular. Relative to those of pure Mode I and Mode III, the angular variations of the inplane and anti-plane stress components at $\hat{r} = 0.016$, are smoother, Fig. 10. The smearing out of Mode I and Mode III features is due to the diffuse nature of the plastic zones and the increased number of active slip systems.

4.5. Mode II and Mode III: $\psi = 90^\circ$ and $\phi = 45^\circ$

In Section 4.4, we have seen that mixed mode loading gives rise to deformation modes which are not found under pure mode loading. This effect is also observed here. Figure 11(a) shows the plastic zone due to slip on system D4, which closely resembles that for pure Mode III loading. A symmetric pattern about the line of crack is contributed by B4. Slip activity on system B5, Fig. 11(b), gives a kink mode at $40^\circ$. This mode is more intense than the corresponding one under pure Mode II conditions, Fig. 5(a). The pattern of slip activity on system D6 is

![Fig. 13. Contours of slip strains corresponding to combined Mode I and Mode II loadings, on systems (a) B5 (kink mode at 40°), (b) D6 (shear mode at 75°) and (c) A3 (shear mode at 0°).](image-url)
similar to that of B5 but reflected about the crack line. It may be noted that the weaker secondary modes which develop under pure Mode II, Fig. 5(a), are suppressed here. The system D1 gives rise to a diffuse plastic zone, suggestive of a shear mode along 70°, Fig. 11(c). The slip activity on B2 is similar to that on D1, but develops on the lower-half plane. This pattern of slip is in contrast to that which develops under pure Mode II, where simultaneous slip on systems D6, D1 and B5, B2 leads to kink modes at ±40°. Contours of slip activity on C3, Fig. 11(d), reveal a kink mode at 120°. A symmetric pattern about the crack line is contributed by A3. Under pure Mode II conditions, this system together with C3 produces a shear mode, Fig. 5(b). Lattice rotations are significant within the finite strain zone (not shown here). Unlike the pure mode cases, the deviation of the axis of rotation from the x3 axis is quite substantial. The stresses and strains are nearly 1/\sqrt{r} singular within a sizeable fraction of the plastic zone. Relative to the pure Mode II and Mode III distribution, the angular variations of the stress components at \( \tilde{r} = 0.016 \), displayed in Fig. 12, are smoother.

4.6. Mode I and Mode II: \( \psi = 45° \) and \( \phi = 90° \)

In preceding sections we have shown that though identical slip systems operate under pure Mode I and Mode II conditions, the resulting deformation modes can be quite different. The main difference are: (i) B5 and B2 give rise to a kink mode at 40° and a shear mode at 130° under Mode I loading, but produce only a kink mode at 40° under Mode II loading; (ii) D6 and D1 produce a shear mode at 70° under Mode I loading, and a kink mode at 140° under Mode II loading; (iii) A3 and C3 give rise to a kink mode at 112° in Mode 1, and a shear mode at 0° under Mode II loading.

Under combined mode conditions, the systems B5 and B2, operating simultaneously, give rise to a fairly sharp kink mode at 40°, evident from the contours of slip strain for B5, Fig. 13(a). Contour plots of slip strain on D6 show a somewhat diffuse plastic zone suggestive of a shear mode at about 75°, Fig. 13(b). The system D1 exhibits an identical pattern. Under combined Mode I and Mode II loadings, the deformation patterns are no longer symmetric with respect to the line of the crack and a kink mode corresponding to that in Fig. 13(a) does not develop in the lower-half plane. A shear mode at 12° and a negligible kink mode at 112° from system A3 is evident from Fig. 13(c). An identical deformation mode is produced by C3. Interestingly enough, significant lattice rotations are observed only in the upper-half plane, Fig. 14. This is consistent with the presence of a kink mode in that region.

The accumulated slip strains exceed the saturation threshold of 0.2 over the six innermost rings of elements, which suffers to reveal the transition from a 1/\sqrt{r} type field to one dominated by ideal plasticity.

Angular variations of the Kirchhoff in-plane stress components, normalized by \( K / N_{a} \), are shown in Figs 15(a–c) for \( \tilde{r} = 0.002, 0.006, 0.016 \) and 0.03. It is apparent that the 1/\sqrt{r} variation breaks down for \( \tilde{r} \leq 0.002 \). A plot of (\( \tau_{11} - \tau_{22} \))/\( \tau_{0} \) vs. \( \tau_{12}/\tau_{0} \) around the crack tip, at \( \tilde{r} = 0.006 \), is shown in Fig. 16(c). For the sake of reference, the unrotated initial yield and saturated yield surfaces are also shown in the figure. This plot reveals that in the upper half plane, a kink mode due to systems B5 and B2, a shear mode due to systems D6 and D1 would result. In contrast, in the lower half plane only a shear mode on systems D6 and D1 is implied. This is consistent with our observation of slip modes on these systems. It appears that the nonsymmetric nature of lattice rotations (in this case they are observed only in the upper half plane) significantly affect the stress state, thereby influencing the nature of slip modes. It is also interesting to note that the stress state around the crack tip sweeps the yield surface only by half a turn, as in the case of pure Mode II, though the symmetry of the stress state is lost.

5. DISCUSSION AND CONCLUSIONS

We have presented pure and mixed mode results pertaining to the crack geometry depicted in Fig. 2. Our results indicate that mode mixity exerts a strong influence on competing deformation modes. While our study is limited to a specific geometry in an f.c.c. crystal, similar effects of mode mixity can be expected to the present in other geometries and crystals. The influence of mode mixity on crack tip fields is manifold, and manifests itself in the breaking of symmetries which ensure planar or anti-planar fields in pure modes, in the determination of the
CONCLUSIONS

The mixed-mode results predicted in Fig. 2 illustrate the stress and strain mixity effects on crack propagation modes. While the specific geometry in an SNT specimen can be altered, the overall mixity effect on crack propagation is self-sustained in the planar or anti-planar determination of the

Fig. 15. (a–c) Angular variations of the in-plane Kirchhoff stress components at several radii under combined Mode I and Mode II loadings. The stresses are normalized by $K/\sqrt{2\pi}$. 

magnitude of angles of shear Mode II loadings. Note the upper half-plane of a kink mode on B3 and in the lower half-plane.

Kirchhoff in-plane stress $K/\sqrt{2\pi}$, are shown in 0.006, 0.016 and 0.02. The variation breaks down $\tau_{22}/\tau_0$ vs $\tau_{12}/\tau_0$ around 0.006, as shown in Fig. 16(c). For rotated initial yield and iso shown in the figure, upper half plane, a kink-B2, a shear mode due to a result. In contrast, in the shear mode on systems D6 and in systems 1 is consistent with our observation. It appears that lattice rotations in this plane the upper half plane), thereby influencing also interesting to note as the case of pure try of the stress state is...
dominant slip systems, and in the character of the deformation modes, e.g. whether they are of kink or shear type. The effect of mode mixity is exemplified by the following two cases:

1. Consider systems D4, D6 and D1, all of which share the same plane, Fig. 8. Under Mode I loading, D6 and D1 undergo equal and simultaneous slip, resulting in a shear mode along the [121] direction. However, the slip directions of D1 and D6 have components in the $x_1$ and $-x_1$ directions, respectively. The addition of a Mode III load component in the $x_1$ direction increases the resolved shear stress on D1 but weakens it on D6. Consequently, slip on D1, as opposed to D6, dominates. To make contact with dislocation theories, we note that the mixed dislocations emitted on systems D1 and D6 in pure Mode I loading have opposing screw components which cancel resulting in a dislocation of edge character. However, as observed by Lin and Thomson [6], the addition of a Mode III component favors dislocation emission on D1 while suppressing emission on D6. As a result, the dislocations sweeping through the slip plane have a screw component in the $x_1$ direction. By way of contrast, the anti-plane deformation modes, namely, the shear modes contributed by systems B4 and D4, are relatively unaffected by the addition of a Mode I component. The fact that the dislocations of a purely screw character are operative under pure Mode I loading, the resulting del deficient. For example, shear mode under Mode II is observed under systems A3 and C3 giving rise to slip on D4 and a shear mode on Mode I and a shear mode on D6. The deformation mode and II loading are extremely pure modes under pure mode condition C3 produce a shear mode on D6 while D6 and D1 give rise to slip on D1 case. Unlike the shear mode, the deformation pattern exhibit no symmetries prevalent stress state for modes is illustrated by $\tau_{12}/\tau_0$ spanning the entire range of tip, at $\theta = 0.006$, show initial yield and saturation shown in the figure. Such regarding the prevailing expected modes of slip at the tip of the crack. It is expected slip modes were configured predictions the slip pattern these plots reveal that the state at the crack tip and full turns, while under pure shear only by half a turn. Mode II loading, the slip surface by half a turn a though the stress state is mixed mode loading, the is purely Mode I field about. It appears that the relative dominant. In the previous section, lattice rotations in the $x_1$ plane influence the stress state higher.

The framework of adopted here tacitly a dislocation generation which may not be realized was that the slip shear or kink modes source of dislocations appear abundant internal dislocation accommodate a kink such internal sources are available in the continuum. It is developed if the appropriate prediction is correct the sources are indeed available.
To make contact with that the mixed dislocation emission on D6, we should keep in mind that the dislocations emitted on D4 and B4 are of a purely screw character.

2. We have shown that, while the same slip systems are operative under pure Mode I and Mode II loading, the resulting deformation patterns are quite different. For example, systems D6 and D1 produce a shear mode under Mode I loading, whereas a kink mode is observed under Mode II loading. Similarly, systems A3 and C3 give rise to a kink mode in Mode I and a shear mode under Mode II loading. The deformation modes under combined Mode I and II loading are reminiscent of those observed under pure mode conditions. In particular, A3 and C3 produce a shear mode, as in the Mode II case, while D6 and D1 give a shear mode as in the Mode I case. Unlike the pure mode cases, however, the deformation patterns under mixed mode loading exhibit no symmetries about the crack line. The prevalent stress state for the pure and mixed-in-plane mode is illustrated by the plots of $\tau_{11} - \tau_{22}$ vs $\tau_{12}/\tau_0$ spanning the entire angular region of the crack tip, at $\phi = 0.006$, shown in Fig. 16. The unrotated initial yield and saturated yield surfaces are also shown in the figure. Such a plot provides information regarding the prevailing stress state, as well as the expected modes of slip on active slip systems, around the tip of the crack. It was discussed earlier that the expected slip modes were consistent with our observations of the slip patterns. Interestingly enough, these plots reveal that under pure Mode I, the stress state at the crack tip sweeps the yield surface by two full turns, while under pure Mode II the yield surface is swept only by half a turn. Under mixed Mode I and Mode II loading, the stress state sweeps the yield surface by half a turn as in the case of pure Mode II, though the stress state is no longer symmetric for the mixed mode loading. Thus, addition of Mode II to a purely Mode I field abruptly changes the stress state. It appears that the resulting stress state becomes Mode II dominant. In addition, as was discussed in the previous section, the nonsymmetric nature of lattice rotations in the mixed mode case can strongly influence the stress state and the precise nature of slip modes.

The framework of continuum crystal plasticity adopted here tacitly assumes that the sources of dislocation generation are distributed uniformly, which may not be realistic in an actual crystal. It has been noted that the slip processes give rise to either shear or kink modes. The crack tip is an efficient source of dislocations for shear modes. By contrast, abundant internal dislocation sources are required to accommodate a kink mode. Since, by assumption, such internal sources of dislocations are readily available in the continuum formulation, kink modes develop if the appropriate conditions are met. This prediction is correct only if abundant dislocation sources are indeed available in the crystal. When kink modes do develop, they are accompanied by extensive lattice rotations, which may in turn induce geometric hardening or softening depending on the direction of rotation, as noted by Asaro [27]. Indeed, Figs 14 and 13(a) show that substantial lattice rotations occur in the upper-half plane when a kink mode develops at $40^\circ$.

We have shown that the fields that evolve possess certain features which are common to all the load cases investigated. These features can be traced to the constitutive law used in our analysis. The initial portion of the shear-stress-slip strain curve rises rapidly, and almost linearly, for slip strains up to about $50\tau_0/\mu$ or 0.1. At slip strains of about 0.2, the stress saturates at the level $\tau_s$. Consequently, two distinct plastic regions exist near the crack tip: an outer region, with slip strains less than about 0.1, governed by high hardening, and an inner region, with slip strains exceeding 0.2, governed by ideal plasticity. In the outer high hardening region, the stresses and strains are nearly $1/\sqrt{r}$ singular. The transition from the $1/\sqrt{r}$-type field to one governed by non-hardening response occurs within the finite deformation zone. The in-plane stresses appear to deviate more strongly from $1/\sqrt{r}$-type field than the out-of-plane stresses. In addition, due to finite lattice rotations, numerous slip systems are activated by mixed mode loading, with the result that the angular stress distributions are smoother than those which develop under pure mode loading.

Shih [7] and Pan and Shih [8–10] have obtained mixed mode fields for solids obeying $J_2$ flow theory of plasticity. Their numerical solutions show that the transition from pure mode fields to mixed mode fields occurs smoothly. For example, when a small amount of Mode II load is superimposed on a primarily Mode I load, the crack-tip field acquires some Mode II features but its original Mode I character is essentially retained. As the amount of Mode II loading is increased, the crack-tip field gradually changes over to Mode II type. By contrast, the near-tip field in a single crystal may change abruptly with small changes in mode mixity. In particular, the type of the modes, i.e. whether they are of a shear or kink character, is especially sensitive to variations in mode mixity. As an example, a complete reversal of the type of deformation mode occurs when the load changes from pure Mode I to pure Mode II. These features can be traced to the strongly geometric nature of slip in single crystals.

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