AN ANALYSIS OF CRACKS IN DUCTILE SINGLE CRYSTALS—I. ANTI-PLANE SHEAR

R. Mohan, M. Ortiz† and C. F. Shih
Division of Engineering, Brown University, Providence, RI 02912, U.S.A.

(Received 23 July 1990; in revised form 7 February 1991)

ABSTRACT

The problem of a stationary mathematically sharp semi-infinite crack in an FCC crystal is considered. We adopt a geometrically rigid formulation of crystalline plasticity accounting for finite deformations and finite lattice rotations, as well as for the full three-dimensional crystallographic geometry of the crystal. A comparison of results with earlier small-strain solutions reveals some notable differences. These include the expected development of finite deformations and rotations near the crack tip, but also discrepancies such as a considerable spread of the plastic zones. In addition, nearly self-similar, square-root singular fields are obtained within the portion of the plastic zone where the crystal is in a state of high positive hardening. The results suggest that both finite-deformation and lattice rotation effects, as well as the details of the hardening law, strongly influence the structure of the solution.

1. INTRODUCTION

Microcracks may be induced in polycrystals by dislocation pile-ups (Low, 1954), grain boundary sliding (Lau et al., 1983), and by other mechanisms. Once nucleated, microcracks can propagate as cleavage cracks, as encountered in brittle solids, or be blunted (Vitek and Chell, 1980), depending on such parameters as temperature, crack speed, and the crystallographic geometry of the crack. The question of whether an atomistically sharp crack can remain sharp without spontaneous blunting by dislocation emission is central to the understanding of the brittle and ductile fracture modes of single crystals and polycrystals.

Analyses based on linear elastic dislocation theory have been advanced by several investigators, e.g. Kelly et al. (1967), Rice and Thomson (1974), Vitek (1976), Weertman (1978) and Lin and Thomson (1986) among others [see also the monograph of Weertman and Weertman (1991)]. Bilby et al. (1963) proposed a model, often referred to as the BCS model, based on the theory of continuous distribution of dislocations to examine the length of plastic zone needed to relax the stresses occurring at the tip of a sharp crack under anti-plane deformation. The plastic zone was idealized as a pile up of screw dislocations ahead of the crack tip. The BCS theory has been verified with in situ experiments on thin foils by Ohr and co-workers (Ohr and Narayan, 1980; Kobayashi and Ohr, 1980; Ohr and Chang, 1982). The majority of these studies rely on linear isotropic elasticity theory and envision the solid as

†Author to whom correspondence should be addressed.
deforming in plane strain or anti-plane shear. Furthermore, slip activity is often confined to one or two in-plane slip systems, and thus the precise manner in which these analyses pertain to actual crystallographic geometries is not always entirely clear.

By way of contrast, there remains a paucity of studies based on continuum single crystal plasticity. Rice and co-workers have analyzed the small-strain case with the plastic response assumed to be either ideal (Rice and Nikolic, 1985; Rice, 1987) or to be governed by Taylor power-law hardening (Rice and Saeedvafa, 1988; Saeedvafa and Rice, 1989). The orientations of the crystals and the slip systems presumed active were chosen so as to insure the existence of plane strain or anti-plane solutions. Several limitations of the small-strain formulation were pointed out by Rice and co-workers themselves (Rice and Nikolic, 1985; Rice, 1987). Thus, the small-strain theory does not account for the effect of the finite lattice rotations. As is well known, such lattice rotations may result in geometrical softening or hardening, depending on the sign of the rotations (Asaro, 1983). Deformation modes accompanied by geometrical softening may be more readily induced than those which result in substantial geometrical hardening. This may significantly affect the nature of the solution in cases in which there are several competing modes of deformation. A related issue is the inability of the small-strain theory to differentiate, as regards the computation of the rate of plastic deformation, between the normal to a slip plane and the direction of slip. Thus, deformation modes are treated as indistinguishable which in the finite-deformation theory are quite distinct.

In the present work, we adopt a geometrically rigorous formulation accounting for finite deformations and finite lattice rotations, as well as for the full three-dimensional crystallographic geometry. We consider a stationary mathematically sharp semi-infinite crack in an FCC crystal. To facilitate comparison of results, the geometry of the crack is taken to be identical to that considered by Rice and Nikolic (1985) (henceforth referred to as RN). Thus, in the absence of significant finite deformation effects, and for the loading under consideration, the prevailing deformations are of anti-plane type. We allow, however, for arbitrary generalized-plane solutions, in which the three displacement components may be non-vanishing, but are assumed to be independent of the coordinate direction parallel to the crack front.

The constitutive theory and numerical procedures used in the analysis are defined in Sections 2 and 3. The results of the analysis are presented in Section 4, along with detailed comparisons with the small-strain solutions of RN. Our results show that the finite changes in geometry have a strong effect on the pattern of slip activity near the crack tip, resulting in the loss of the anti-plane character of the deformations. Furthermore, the plastic activity is found to be distributed over finite sectors. This is in contrast with the small-strain solutions of RN, in which all plastic deformations are confined to lines of vanishing thickness. In addition, nearly self-similar, square-root singular fields are obtained within a certain region of the plastic zone. Some tentative explanations for these features are advanced in Section 5.

2. THEORY

Consider a crystal lattice being deformed from its initial undeformed configuration \( \mathcal{R}_0 \) to its current configuration \( \mathcal{R} \), at time \( t \). Locally, the deformation of the crystal is

\[
F = \mathbf{F}^P = \mathbf{F}^P \mathbf{F}^T,
\]

where \( \mathbf{F} \) is the first Piola–Kirchhoff stress tensor, \( \mathbf{F}^P \) is the deformation gradient, and \( \mathbf{F}^T \) is the stress tensor. The stress \( \sigma \) is a stress measure on \( \mathcal{R} \) (Mandel, 1972). In (2) and subsequent equations, the inner product between second-order tensors is implicitly assumed to be a matrix.

The work conjugacy relations express the stress–strain relations of the general form

\[
\mathbf{F}^P = \mathbf{F}^P \mathbf{F}^T = \mathbf{F}^P,
\]

where \( \mathbf{F} \) denotes some suitable set of crystal configurations, for which suitable equations are supplied. It should be noted that (4a) implies the rate of plastic deformation and the rate of plastic strains \( \dot{\mathbf{F}}^P \) is invariant with respect to rigid-body rotation, and that equation (4a) is automatically mapped onto the principle of material frame indifference. The principle of material frame indifference is
Furthermore, slip activity is often con-
uously influenced by the precise manner in which these mecha-
nisms is not always entirely clear.

of studies based on continuum single crystal analysis the small-strain case with the Rice and Nikolic, 1983; Rice, 1987) or
(Rice and Saeedvafa, 1988; Saeedvafa, 1988; Saeedvafa and Rice, 1987) crystals and the slip systems presumed to
plane strain or anti-plane solutions. The rotation were pointed out by Rice and co-
(Rice, 1987). Thus, the small-strain shear lattice rotations. As is well known, un
softening or hardening, depending on deformation modes accompanied by a
factor in the simulation of finite strain. As regards the computation of a solution for a slip plane and the direction of the
strain is indistinguishable which in the finite-

rigorous formulation accounting for is as well as for the full three-dimensional the stan-
method of obtaining mathematically sharp semia-
result presented by Rice and Nikolic (1985) the geometry of the
finite deformation are of the generalized-plane solutions, in which non-vanishing, but are assumed to be
in contact with the crack front.

The results used in the analysis are defined are presented in Section 4, along with the sugges-
tions of RN. Our results show that the pattern on the pattern of slip activity near
plane character of the deformations, are distributed over finite sectors. This is
RN, in which all plastic deformations are near add-
addition, nearly self-similar, square-
region of the plastic zone. Some advanced in Section 5.

In its initial undeformed configuration
ually, the deformation of the crystal is fully defined by the deformation gradient field \( F \). The total deformation \( F \) is the result of two main mechanisms of deformation: dislocation motion within the active slip systems of the crystal and lattice distortion. Following Lee (1969), this points to a multiplicative decomposition

\[
F = F^p F^e
\]

of the deformation gradient \( F \) into a plastic part \( F^p \), defined as the cumulative effect of dislocation motion, and an elastic part \( F^e \), which describes the distortion of the lattice. Following Teodosiu (1970) and others (Mandel, 1972; Rice, 1971; Hill and Rice, 1972; Havner, 1973; Asaro and Rice, 1977), we shall assume that \( F^p \) leaves the crystal lattice not only essentially undistorted, but also unrotated. Thus, the rotation of the lattice is contained in \( F^e \). This choice of kinematics uniquely determines the decomposition (1). The plastic part \( F^p \) of the deformation gradients defines a collection of plastically deformed local configurations which are collectively referred to as the intermediate configuration \( \mathcal{B}_0 \).

Further insight into the structure of the constitutive relations can be derived from work conjugacy considerations. By virtue of (1), the deformation power per unit undeformed volume takes the form

\[
\mathbf{P} : \dot{\mathbf{F}} = \dot{\mathbf{F}}^T + \Sigma : \dot{\mathbf{F}}^p,
\]

where \( \mathbf{P} \) is the first Piola–Kirchhoff stress tensor, and

\[
\dot{\mathbf{P}} = \mathbf{F}^p \dot{\mathbf{F}}^p T, \quad \Sigma = \mathbf{F}^T \dot{\mathbf{F}}^e T, \quad \dot{\mathbf{F}}^p = \mathbf{F}^p \mathbf{F}^{-1},
\]

where \( \dot{\mathbf{P}} \) defines the first Piola–Kirchhoff stress tensor relative to the intermediate configuration \( \mathcal{B}_0 \), and \( \Sigma \) is a stress measure conjugate to the plastic velocity gradients \( \dot{\mathbf{F}}^p \) on \( \mathcal{B}_0 \) (Mandel, 1972). In (2) and subsequently, the symbol “:” is used to denote the inner product between second-order tensors, e.g. \( \mathbf{A} : \mathbf{B} = A_{ij} B_{ij} \), where the summation convention on repeated indices is implied. In addition, \( (\cdot)^T \) denotes the transpose of a matrix.

The work conjugacy relations expressed in (2) suggest plastic flow rules and elastic stress–strain relations of the general form

\[
\dot{\mathbf{F}}^p = \mathbf{F}^p (\Sigma, \mathbf{Q}),
\]

\[
\dot{\mathbf{P}} = \overline{\mathbf{P}} (\mathbf{F}^e),
\]

where \( \mathbf{Q} \) denotes some suitable set of internal variables defined on the intermediate configuration, for which suitable equations of evolution, or hardening laws, are to be supplied. It should be noted that (4a) determines uniquely both the rate of plastic deformation and the rate of plastic rotation. Because, by the choice of kinematics, \( \mathbf{F}^e \) is invariant with respect to rigid body motions superimposed on the current configuration, (4a) is automatically material frame indifferent. By contrast, objectivity imposes non-trivial restrictions on the form of (4b). A standard exercise [see, for example, Malvern (1969)] reveals that the most general form of (4b) consistent with the principle of material frame indifference is
Plastically deforming crystals are one of the few classes of solids for which the precise form of the above constitutive equations is known from first principles. From the kinematics of dislocation motion, Rice (1971) showed that (4a) is of the form

$$\mathbf{F}' = \mathbf{F}^\circ \mathbf{S}(C'), \quad C' = F^T F,$$

where $\mathbf{S} = C^{-1} \Sigma$ is the symmetric second Piola–Kirchhoff stress tensor relative to the intermediate configuration $\mathbf{F}'$, and $C'$ is the elastic right Cauchy–Green deformation tensor on $\mathbf{F}'$.

(5)

Plastically deforming crystals are one of the few classes of solids for which the precise form of the above constitutive equations is known from first principles. From the kinematics of dislocation motion, Rice (1971) showed that (4a) is of the form

$$\mathbf{L}' = \sum \gamma^a \mathbf{s}^a \otimes \mathbf{m}^a,$$

where $\gamma^a$ is the shear rate on slip system $a$, and $\mathbf{s}^a$ and $\mathbf{m}^a$ are the corresponding slip direction and slip plane normal. Then, (2) reduces to

$$\mathbf{P} : \mathbf{F}' = \mathbf{P} : \mathbf{F}^\circ + \sum \gamma^a \mathbf{s}^a \otimes \mathbf{m}^a,$$

where

$$\gamma^a = \gamma^a(\tau^a, \mathbf{Q}),$$

(8)

is the resolved shear stress on slip system $a$. We note that $\tau^a$ and $\gamma^a$ are work conjugate.

At this point the assumption is commonly made that $\gamma^a$ depends on stress only through the corresponding resolved shear stress $\tau^a$, i.e.,

$$\gamma^a = \gamma^a(\tau^a),$$

(9)

which is an extension of Schmid's rule. If (9) is assumed to hold, then it was shown by Rice (1970) and Mandel (1972) that the flow rule (6) derives from a viscoplastic potential.

The above constitutive framework for crystalline plasticity, or a close variant of it, has been used widely in the past. Some authors prefer to express the elastic response (5) in rate form. Computing the material time derivative of (5) and expressing the result in terms of spatial quantities leads to

$$L' \tau = L^\circ d',$$

(10)

where $\tau$ is the Kirchhoff stress, $L^\circ$ are the (deformation-dependent) spatial tangent moduli

$$d' = (\mathbf{I}' + \mathbf{F}')/2, \quad \mathbf{I}' = \mathbf{F}' \mathbf{F}^{-1},$$

(11)

is the elastic rate of deformation tensor, and

$$L' \tau = \mathbf{I}' \tau - \mathbf{I}^T \tau$$

(12)

is the elastic Lie derivative of $\tau$.† Because $\mathbf{I}' = d' + w'$, (10) can be rewritten by dropping the symmetric component of $\mathbf{I}'$ in the elastic Lie derivative of $\tau$, which thus reduces to the elastic Jaumann rate of $\tau$ (Hill and Rice, 1972), and absorbing the coefficients of that symmetric part into redefined moduli $L^\circ$ having the same symmetries as the original ones. As a simplification, the moduli $L^\circ$ are sometimes taken to be constant, despite the fact that they cannot.

Cracks in solids (Simo and Pister, 1984). For metals, the hardening effect on the outcome of the computational form (5) of the elastic response.

The specific forms of (9) and of the hardening are taken from the work of Peirce et al. (1981) on slip system $a$ to be given by a power-law hardening

$$\gamma^a = \gamma^a(\mathbf{Q}),$$

where $h$ is the strain-rate sensitivity exponent, $\mathbf{Q}$ is the current shear flow stress of system $a$.

The parameter $q$ characterizes the hardening and corresponds to isotropic or Taylor hardening. FCC crystals, Kocks (1970) has determined $q$ to be $1 \leq q < 1.4$. A form of $h(\gamma)$ in (15) is

$$h(\gamma) = h_0,$$

where $h_0$ is the initial hardening rate, $h_0$ is the saturation strength. By way of illustration, the deformed slip implied by (16) is shown in Fig. 13. Similar evidence are given by Asaro (1983). A simple form of the elastic response (5) may be adopted without much loss of (10) as

$$\mathbf{S} = \mathbf{L}^\circ \mathbf{F}'$$

may be adopted without much loss of accuracy. Anisotropic models may be taken to be isotropic to

$$\mathbf{L}^\circ = \lambda \delta \mathbf{I},$$

where $\lambda$ and $\mu$ are the elastic Lamé constants and higher-order moduli have been given.

† For a formal definition of the Lie derivative, see Marsden and Hughes (1983).
\[ F = F^e F^c, \]  
(5)

\[ \varepsilon = \varepsilon^e + \varepsilon^c, \]  
(6)

\[ \sigma = \sigma^e + \sigma^c, \]  
(7)

\[ \mu = \mu^e + \mu^c, \]  
(8)

\[ \eta = \eta^e + \eta^c, \]  
(9)

\[ \nu = \nu^e + \nu^c, \]  
(10)

\[ \gamma = \gamma^e + \gamma^c, \]  
(11)

\[ \chi = \chi^e + \chi^c, \]  
(12)

\[ \hat{\mathbf{F}} = \mathbf{F}^e \mathbf{F}_0^{-1}, \]  
(13)

\[ \hat{\mathbf{E}} = \mathbf{E}^e \mathbf{E}_0^{-1}, \]  
(14)

\[ \hat{\mathbf{S}} = \mathbf{S}^e \mathbf{S}_0^{-1}, \]  
(15)

\[ \hat{\mathbf{E}}^e = \mathbf{E}^e \mathbf{I}, \]  
(16)

\[ \hat{\mathbf{S}}^e = \mathbf{S}^e \mathbf{I}, \]  
(17)

\[ \hat{\mathbf{E}}^e = \mathbf{E}^e \mathbf{I}, \]  
(18)
3. Solution Procedure

The method of solution adopted in the analysis has been discussed in detail elsewhere (MORAN et al., 1990) in the context of flow theories of plasticity. The main extension required here concerns the handling of several simultaneously active slip systems. The constitutive update adopted is based on an implicit treatment of the elastic-plastic kinematics and the elastic response, as defined by (1), (5), (6) and (13), combined with an explicit treatment of the hardening law (14), whereby the plastic modulus (16) is sampled at the start of the time step. This method of discretization results in the following algebraic equations defining the state update:

\[
\begin{align*}
F_{n+1} &= F_{n+1}^T F_{n+1}, \\
C_{n+1} &= F_{n+1}^T C_{n+1} F_{n+1}, \\
(F_{n+1}^p - F_{n+1}^e) F_{n+1}^{e-1} &= \sum \Delta \gamma^p s^p \otimes m^p,
\end{align*}
\]

\[\Delta \gamma^p = \Delta \gamma_0 \text{ sgn}(\tau_{n+1}^z) \left( \frac{|\tau_{n+1}^z|}{C_{n+1}^z} \right)^{\nu_m}, \quad g_{n+1}^p = g_n^p + \sum g_{n+1}^p (q + (1-q)\omega_{n+1}^p)|\Delta \gamma^p|,
\]

\[\tau_{n+1}^z = \Sigma_{n+1} : (s^p \otimes m^p), \quad C_{n+1} = C_{n+1}^c \Sigma_{n+1}, \quad \Sigma_{n+1} = D^e : (C_{n+1}^c - I)/2,
\]

where the subindices ( ) and ( ) refer to the initial and updated values of the state variables, respectively, \(\Delta \gamma^p\) are the incremental slip strains, and \(\Delta t\) is the time increment. In (18), the final deformation gradients \(F_{n+1}\) are to be regarded as given. As noted by MORAN et al. (1990), because the hardening modulus \(h\) is treated explicitly, (18) can be reduced to a system of non-linear equations for the incremental shear strains \(\Delta \gamma^p\). Here, this system is solved by means of a local Newton–Raphson iteration with line searches. Once the \(\Delta \gamma^p\) are known, the remaining state variables follow explicitly from (18). It is noteworthy that, because of the implicit treatment of the 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. Our numerical experiments have demonstrated that, under the conditions of interest here, the equilibrium equations are most efficiently handled by a forward-gradient method of the type proposed by PERCE et al. (1984).

The finite-element mesh is composed of eight-noded isoparametric brick elements. The assumed strain method adopted to prevent locking due to near-incompressibility under conditions of fully developed plastic flow have been presented elsewhere (MORAN et al., 1990). The method generalizes the mean-dilatation approach of NAGTEGAAL et al. (1974) to finite deformations, and consists of postulating a constant deformation Jacobian, \(det(F)\), 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 tip by a single layer of elements and constraining the (three) components of displacement to take equal values on both surfaces of the slice.

For the crack geometry considered in the analysis, a fan-like mesh with exponential grading in the radial direction is used. The ratio of the innermost to the outermost element sizes is of the order of \(10^{-3}\). The angular resolution of the mesh is 12°, and the total number of degrees of freedom is 5748. In order to assess the adequacy of the mesh, we repeated the calculations discussed in Section 4.1 with twice the angular resolution; no significant variation in the solution was observed. Tractions consistent with the linear elastic asymptotic mode I, and increased at increments such as plastified at each step. The rate of approach to the maximum strain rates in the vicinity of the strain rate \(\gamma_0\). This results in modest rate dependency. The values of the material constants \(\lambda = 577\tau_0, \mu = 385\tau_0, \gamma_0 = 10^{-3}\), are typical of Al–Cu alloys (CuAl2) where values of the material constants used in Part II are given here: \(\lambda = 457\tau_0, \mu = 41\tau_0, \gamma_0 = 1.13\tau_0\). These values are typical of

4. Results

Asymmetric as well as full-field calculations of the tip of a stationary crack subjected to an applied load were sought within the small strains, it was shown that the plastic zone was a discrete plane of displacement and strong planes of discontinuity are coincident with the plane and perpendicular to the active slip planes aligned with the slip directions, sweeping out of the crack tip. By way of consequence, it requires a distribution of elongated disclinations. As remarked in the Introduction, the small these two modes of deformation. While, however, shearing along kink bands in which can induce geometrical hardening, bands may be quite different at the tip.

For ease of comparison, we have chosen RN. These cases are subsequently discussed.

4.1. Crack on (111), crack from along (111)

The crack lies on the slip plane (111), as shown in Figure 1(a). Figure 1(b) shows the orientation of the predominantly anti-plane shear crack tip line segment corresponds to a specific predicted by RN are shown in Fig. 1(c) corresponds to spin on the (111)[101]. The length of this plastic zone is \(R = 0.1\). The factor and \(\gamma_0\) is the critical resolved shear stress (111)[101] is represented by the line.
with the linear elastic asymptotic mode III field are distributed over the outer boundary, and increased at increments such that essentially one new ring of elements is plastically deformed at each step. The rate of application of the loads 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 constants used in the calculations are: $\lambda = 577 \tau_0$, $\mu = 385 \tau_0$, $\gamma_0 = 10^{-3}$, $m = 0.005$, $q = 1$, $h_0 = 8.9 \tau_0$, $\tau_1 = 1.8 \tau_0$. These values are typical of Al–Cu alloys (Chang and Asaro, 1981). For completeness, the values of the material constants used in the calculations of BCC crystals discussed in Part II are given here: $\lambda = 547 \tau_0$, $\mu = 418 \tau_0$, $\gamma_0 = 10^{-3}$, $m = 0.005$, $q = 1$, $h_0 = 1.52 \tau_0$, $\tau_1 = 1.13 \tau_0$. These values are typical of Fe–Ti–Mn alloys (Deve et al., 1988).

4. RESULTS OF THE ANALYSIS

Asymptotic as well as full-field calculations of the stress and deformation fields at the tip of a stationary crack subjected to anti-plane loading were performed by RN. The behaviour of the ductile single crystals was modelled as elastic–ideally plastic, and solutions were sought within the small-strain approximation. Under these assumptions, it was shown that the plastic zone at the tip of a stationary crack collapses into discrete planes of displacement and stress discontinuity emanating from the tip. These planes of discontinuity are coincident with the crystal slip planes in some instances, and perpendicular to the active slip planes in others. As noted by RN, the discontinuity planes aligned with the slip directions, termed slip bands, contain screw dislocations sweeping out of the crack tip. By way of contrast, concentrated shearing along the discontinuity planes perpendicular to the slip directions, resulting in a kink band, requires a distribution of elongated dislocation loops of predominantly edge character.

As remarked in the Introduction, the small-strain theory makes no distinction between these two modes of deformation. When finite deformations are taken into account, however, shearing along kink bands is inevitably accompanied by lattice rotations which can induce geometrical hardening or softening. Thus, the behavior of slip and kink bands may be quite different at the present level of description.

For ease of comparison, we have chosen to analyze the same cases considered by RN. These cases are subsequently discussed in turn.

4.1. Crack on (111), crack front along [101]

The crack lies on the slip plane (111) with the crack front along [101] direction. Figure 1(a) shows the orientation of the crystal. The yield surface appropriate to predominantly anti-plane shear conditions is shown in Fig. 1(b), where each straight-line segment corresponds to a specific slip system as marked. The line plastic zones predicted by RN are shown in Fig. 1(c). The plastic zone aligned with the crack plane corresponds to slip on the (111)[101] system, and segment BB' of the yield surface. The length of this plastic zone is $R = 0.385(K/\tau_0)^2$, where $K$ is the elastic stress intensity factor and $\tau_0$ is the critical resolved shear stress. The plastic zone due to slip on system (111)[101] is represented by the lines $R_1$ and $R_2$. These make an angle of 70.54°...
of the computation of the lattice rotations are observed in the vicinities of the crack tip, the slip activity is on the system (111)[101], in agreement with RN’s analysis. By contrast, close to the crack tip, the slip character of the deformation breaks down.

Fig. 2. Contours of lattice rotation.

Fig. 3. Contours of shear strain on slip system.

relative to the crack line. The lengths of these zones are $R_1 = 0.202(K/\tau_0)^2$ and $R_2 = 0.076(K/\tau_0)^2$, respectively. The sectors separated by the line plastic zones are elastic.

With these results by way of background, we now return to the finite-deformation formulation. Absolute values of angles of lattice rotation are shown in Fig. 2. Details
of the computation of the lattice rotations are given in the Appendix. Significant lattice rotations are observed in the vicinity of the crack tip. For \( r \geq 0.02(K/\tau_0)^3 \), by contrast, the lattice rotations are below 1° (\( \approx 0.02 \) rad). At sufficiently large distances from the crack tip, the slip activity is primarily confined to systems \((111)[10\bar{1}]\) and \((1\bar{1}1)[10\bar{1}]\), in agreement with RN's analysis, and the solid ostensibly deforms in anti-plane shear. By contrast, close to the crack tip the pattern of slip activity is far more complex, with non-negligible activity on all systems. By way of example, contours of shear strain on system \((1\bar{1}1)[10\bar{1}]\) are shown in Fig. 3. In addition, the anti-plane character of the deformation breaks down, and the in-plane stress components become

![Fig. 2. Contours of lattice rotations for the geometry given in Fig. 1.](image2)

![Fig. 3. Contours of shear strain on slip system \((1\bar{1}1)[10\bar{1}]\) for the geometry given in Fig. 1.](image3)
non-negligible relative to the out-of-plane shear stresses. For instance, significant levels of hydrostatic stress, \( \tau_k > 1.5 \tau_0 \), are observed in the near-tip region, \( r/(K/\tau_0)^2 < 0.002 \).

Contour plots of computed slip activity for the primary slip systems \( (111)[10\bar{T}] \) and \( (1\bar{T}1)[10\bar{T}] \) are shown in Fig. 4. Plastic straining on slip system \( (111)[10\bar{T}] \) [Fig. 4(a)] concentrates predominantly ahead of the crack tip, whereas the activity on system \( (1\bar{T}1)[10\bar{T}] \) [Fig. 4(b)] is confined mainly to a region behind the crack tip. We note that the plastic zones are fairly diffuse. That this is not a mesh effect is apparent from the fact that the plastic zones span several mesh sectors. The lengths of the plastic zones associated with the primary systems are of the order \( R \approx 0.42(K/\tau_0)^2 \) for system \( (111)[10\bar{T}] \), and \( R_1 \approx 0.31(K/\tau_0)^2 \) and \( R_2 \approx 0.24(K/\tau_0)^2 \) for system \( (1\bar{T}1)[10\bar{T}] \). Because the constitutive model adopted in the calculations lacks a proper elastic domain, the plastic zones are defined as the regions where the reference strain \( \gamma_0 = \tau_0/\mu \). With this definition, they correlate well with RN's predictions.

We have examined the angular variation of the plasticity, \( (K/\tau_0)^{-2} \) also appears to be self-similar. The angular dependence of the shear strain \( J \)-integral using the domain method of LEANDER et al., 1986) were path-dependent within the complex deformation and stress histories.

The angular variation of the Kirchhoff stress by \( K/\sqrt{2\pi r} \) is shown in Fig. 5 for three \( 0.033 \). The self-similarity of the solution for the crack tip in Fig. 1 is the result of the solution.

The angular dependence of the shear strain and SAEEDVAF's (1988) solution for a crack tip in a power-law relation. In contrast to that the crack front is defined by the plane of the crack.

4.2. Crack on \( (0\bar{T}0) \), crack front along \( \{111\} \)

The crack plane coincides with the cube facet, the direction \( [10\bar{T}] \). The geometry of the anti-plane yield surface is depicted in Fig. 1, for the two slip systems which are assumed to yield in the lower-half plane, and to the upper-half plane. The solution for the crack zones make an angle of \( \pm 54.7^\circ \) to the crack front. Owing to the symmetry of the yield surface and the plane of the crack.

Contours of computed slip activity are shown in Fig. 7(a) and (b), respectively. The plastic zones are less diffuse than in all other zones associated with the primary systems, lattice rotations are computed to be small near the crack tip. The shear strain for \( (K/\tau_0)^{-1/2} \) also appear to be organized into distributions of components \( \tau_{ij} \) and \( \gamma_{ij} \), which are self-similar and are reminiscent of the hardening crystal obeying a Taylor–Hill law.

4.3. Crack on \( (0\bar{T}0) \), crack front along \( [111] \)

The crack tip now lies on the cube face, direction \( [00\bar{T}] \), as shown in Fig. 9(a)
plastic zones are defined as the regions where the plastic shear strain exceeds 1% of the reference strain \( \gamma_0 = \tau_0 / \mu \). With this convention, the computed plastic zone lengths correlate well with RN's predictions.

We have examined the angular variation of the ratio \( \gamma / \gamma_0 \), denoted \( \gamma \), for system (111)[10\(\bar{1}\)], for several different radii in the interval \( 0.006(K/\tau_0)^2 \leq r \leq 0.033(K/\tau_0) \), which spans a fair portion of the plastic zone. The strains normalized by \( (K/\tau_0)^{-1/2} \) are roughly self-similar. The shear strain attains a maximum at \( 0^\circ \), in agreement with RN's prediction. The plastic strain for the slip system (111)[10\(\bar{1}\)] normalized by \( (K/\tau_0)^{-1/2} \) also appears to be self-similar. We further note that calculations of the J-integral using the domain method of Shih and co-workers (Li et al., 1985; Shih et al., 1986) were path-dependent within the plastic zone, as a consequence of the complex deformation and stress histories which develop in that region.

The angular variation of the Kirchhoff stress components \( \tau_{13} \) and \( \tau_{23} \) normalized by \( K/\sqrt{2\pi r} \) is shown in Fig. 5 for three different radii \( r/(K/\tau_0)^2 = 0.006, 0.018 \) and 0.033. The self-similarity of the solution within this region is evident from the plots. The angular dependence of the shear stress components is not unlike that for Rice and Saeedvafa's (1988) solution for a rapidly hardening crystal obeying a Taylor power-law relation. In contrast to that solution, however, \( \tau_{13} \) does not exhibit a sharp discontinuity on the plane of the crack.

4.2. Crack on (010), crack front along [10\(\bar{1}\)]

The crack plane coincides with the cube face plane (010), and the crack front with the direction [10\(\bar{1}\)]. The geometry of the crack is shown in Fig. 6(a). The corresponding anti-plane yield surface is depicted in Fig. 6(b). As in the previously considered case, the two slip yield surfaces which are assumed to be active in RN's analysis are (111)[10\(\bar{1}\)], which yields in the lower-half plane, and (1\(\bar{1}\)1)[10\(\bar{1}\)], the activity of which is confined to the upper-half plane. The solution of RN is shown in Fig. 6(c). The line plastic zones make an angle of ±54.7° to the line of crack, with length \( R = 0.292(K/\tau_0)^2 \). Owing to the symmetry of the yield surface, the stress field is symmetric about the line of the crack.

Contours of computed slip activity on (111)[10\(\bar{1}\)] and (1\(\bar{1}\)1)[10\(\bar{1}\)] are shown in Fig. 7(a) and (b), respectively. The plastic zones are inclined at ±66° to the plane of crack, which agrees with RN's prediction to within the resolution of the mesh. The plastic zones are less diffuse than in all other cases considered. The lengths of the plastic zones associated with the primary systems are of the order \( R \approx 0.39(K/\tau_0)^2 \). The lattice rotations are computed to be small and confined to the immediate vicinity of the crack tip. The shear strain for the two primary slip systems, normalized by \( (K/\tau_0)^{-1/2} \), also appear to be ostensibly self-similar. Figure 8(a) and (b) show the distributions of components \( \tau_{13} \) and \( \tau_{23} \) of Kirchhoff stress. The fields are roughly self-similar and are reminiscent of Rice and Saeedvafa's (1988) solution for a rapidly hardening crystal obeying a Taylor power-law relation.

4.3. Crack on (010), crack front along [001]

The crack tip now lies on the cube face plane (010) with its tip along the cube edge direction [001], as shown in Fig. 9(a). For this configuration, the anti-plane yield
Fig. 5. Angular variation of the Kirchhoff stress components at several radii [(a) \(\tau_{13}\) and (b) \(\tau_{23}\)] for the geometry given in Fig. 1.

The surface is reduced to a square [Fig. 9(b)]. Each straight-line segment of the yield surface corresponds to two slip systems yielding simultaneously. RN's solution for this geometry is shown in Fig. 9(c). The line plastic zones are inclined at \(\pm 45^\circ\) to the crack line. The plastic zone at \(+45^\circ\) corresponds to the activity on slip systems \((\overline{1}1\overline{1})[1\overline{1}0]\) and \((\overline{1}1\overline{1})[1\overline{1}0]\), whereas the zone at \(-45^\circ\) is the result of activity on systems \((111)[\overline{1}10]\) and \((1\overline{1}1)[\overline{1}10]\). The length of these zones is \(R = 0.104(\frac{K}{\tau_0})^2\).

Contours of computed slip activity and \((\overline{1}1\overline{1})[1\overline{1}0]\), and in Fig. 10(b) for slip zones are observed to be rather diffuse, with the primary systems are of the order of the plastic zone, the strains on slip system maximum at \(\pm 66^\circ\), which is at variance with contours of lattice rotation in Fig. 11. For the crack tip for \(r \leq 0.005(\frac{K}{\tau_0})^2\).
Each straight-line segment of the yield line is inclined at ±45° to the primary systems. The angle of inclination is the result of activity on slip systems inclined at ±45°. The plastic zones associated with the primary systems are of the order of 0.26(K/τo)². At a distance of 0.26(K/τo)². At a fixed distance within the plastic zone, the strains on slip systems indicated in Fig. 10(a) and (b) attain a maximum at ±66°, which is in agreement with RN's prediction of ±45°. From the contours of lattice rotation in Fig. 11, it is seen that significant rotations occur near the crack tip for r < 0.005(K/τo)². For the present geometry, all the remaining slip
systems are found to be active out to considerable distances from the crack tip. As for the geometry considered in Section 4.1, the anti-plane character of the solution is lost in the vicinity of the crack tip, as illustrated by the high levels of hydrostatic stress, \( \tau_h > 1.5 \tau_0 \), which develop in the region \( r/(K/\tau_0)^2 < 0.002 \). The angular variation of the normalized Kirchhoff stress components \( \tau_{13} \) and \( \tau_{23} \) is shown in Fig. 12. A noteworthy feature of these results is the smoothness of all stress components. This behavior is expected in light of the large number of active slip systems, which should bring the solution into closer agreement with the predictions based on the Tresca yield condition (Rice, 1967). As in the first geometry considered, the in-plane stress components \( \tau_{22} \) and \( \tau_{12} \) are non-negligible in the immediate vicinity of the crack tip.

Fig. 7. Contours of shear strain on the most active slip systems [(a) (111)[10\overline{1}], and (b) (111)[10\overline{1}]] for the geometry given in Fig. 6.

Fig. 8. Angular variation of the Kirchhoff stress components in the different geometries.

5. Summary and Conclusions

Numerical results pertaining to three-dimensional crack-tip fields in FCC single crystals have been presented. A geometrically rigorous formulation of the full three-dimensional collection of slip systems is presented, and the results are compared with the predictions of a simplified analytical solution. The agreement is satisfactory, and it is found that the results of the present work are consistent with the predictions of the Tresca yield condition. The angular variation of the Kirchhoff stress components is shown to be smooth, and the in-plane stress components are non-negligible in the immediate vicinity of the crack tip.
Cracks in single crystals—I

Fig. 8. Angular variation of the Kirchhoff stress components at several radii [(a) $\tau_{13}$, and (b) $\tau_{23}$] for the geometry given in Fig. 6.

5. SUMMARY AND CONCLUSIONS

Numerical results pertaining to three different orientations of nominally anti-plane crack-tip fields in FCC single crystals have been presented. The analysis relies on a geometrically rigorous formulation of three-dimensional crystalline plasticity. The full three-dimensional collection of slip systems for FCC crystals is accounted for,
although the displacement solution is constrained to be independent of position along the crack front. Within the small-scale yielding formulation, the only length parameter is \((K/\tau_0)^2\) and, therefore, displacements and quantities with dimensions of length must scale with it. It also follows that the fields can depend on distance only through \(r/(K/\tau_0)^2\) which will be denoted by \(\tilde{r}\). The precise dependence of the stresses and strains on \(\tilde{r}\) is governed by the hardening behavior of the crystal.

The experimentally based constitutive law used in our analysis relates the resolved shear stress \(\tau\) to slip strain \(\gamma\) for single slip. For Al–Cu crystals, the initial portion of the shear stress–slip strain curve rises and flattens out at the saturation level \(\gamma_s\).

\[ y / (K/\tau_0)^2 \]

\[ y / (K/\tau_0)^2 \]

\[ y / (K/\tau_0)^2 \]

\[ y / (K/\tau_0)^2 \]
the shear stress–slip strain curve rises rapidly and almost linearly, and subsequently flattens out at the saturation level \( \tau_s \) (Fig. 13). The initial high hardening regime extends up to slip strains of the order \( 50 \tau_0/\mu \). Our formulation generalizes this relation to multiple slips. When the sum of the accumulated slip strains over all active slip systems is less than about 0.1, the crystal exhibits a high rate of hardening. For accumulated slip strains in excess of about 0.2, the crystal approaches ideally plastic behavior. 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. In addition, because the finite-deformation zone scales with \( K^2/E\tau_0 \), the low initial strength relative to the shear modulus in Al–Cu crystals, \( \tau_0/\mu \approx 2.6 \times 10^{-3} \) (CHANG and ASARO, 1981), suggests that finite-deformation effects can be important.
over physically significant length scales. This contributes to producing near-tip fields which are not readily interpretable within the small-strain theory.

Our results do in fact differ from the RN solution in several notable respects. Thus, despite the fact that deep within the plastic zone saturation is attained and the crystal behaves ideally plastically, the computed plastic zones tend to be more diffuse than those predicted by the RN solution, where they collapse to lines of displacement discontinuity. Other features of the RN solution, such as the asymptotic boundedness of the stresses are not readily identifiable in our calculations.

Several factors may contribute to this disagreement. For the orientations considered here and the hardening behavior of Al-Cu crystals, the near-tip saturated region is strongly affected by finite deformations and lattice rotations. The large lattice rotations contribute to the activation of all slip systems and to the concomitant loss of the anti-plane character of the solution. Indeed, in-plane stress components of magnitude comparable to that of the out-of-plane shear stresses develop in the immediate vicinity of the crack tip. Such effects are not predicted by the small-strain theory. As demonstrated by the results of Section 4.2, when significant lattice rotations are absent the finite and small-strain solutions come into closer correspondence. This trend is reversed in cases where lattice rotations are large (Sections 4.1 and 4.3).

Within the saturation stage, the underlying rate-independent solid may exhibit localization instabilities resulting in loss of ellipticity of the governing equations (ASARO, 1979; PEIRCE et al., 1982). As shown by ABEGARATNE and TRIANTFYLLIDIS (1981), as the solid approaches the point of instability, the effect of small local perturbations on the solution extends out to infinity along the newly emerging characteristic directions. In the present context, this implies that the finite-deformation effects which develop near the tip are not felt locally, as in the case of power-hardening flow theory (MCMEERING, 1977), but rather throughout the saturation region. This may result in significant departures from the RN solution even in cases where the saturation zone extends into the region of small deformations.
contributes to producing near-tip fields in small-strain theory.

tion in several notable respects. Thus, the saturation is attained and the crystal plastic zones tend to be more diffuse than they collapse to lines of displacement, such as the asymptotic boundedness in our calculations.

Fig. 12. Angular variation of the Kirchhoff stress components at several radii [(a) $\tau_{13}$, and (b) $\tau_{23}$] for the geometry given in Fig. 9.

The formation of shear bands in crystals has been studied mainly within the context of two-dimensional idealizations such as the planar double slip model (ASARO, 1979). By contrast, shear banding under conditions of extensive cross hardening in three dimensions has received comparatively little attention. It is conceivable that such conditions, which are found in the near-tip region, may exert a strong influence on the structure of the slip bands, possibly in the sense of broadening them.
Fig. 13. Shear stress, \((r/r_0 - 1)\) vs slip strain, \(\gamma\), for single slip.

In the region \(0.005 < r/(K/r_0)^2 < 0.04\), which extends out to roughly one-quarter of the plastic zone, the calculated stresses nearly collapse onto a single angular distribution when they are normalized by \(K/\sqrt{r}\). The strains also behave in the same way when normalized in a like manner. As shown by Rice and Saedvafa (1988), this type of behavior is to be expected if a high rate of hardening dominates the plastic response. Indeed, an inspection of the computed fields reveals that the sum of the accumulated slip strains over all active systems is less than about 0.1 in the aforementioned region, and hence the crystal is in the high hardening regime. The angular distributions of stress and strain in this region are in fact reminiscent of the corresponding analytical solutions obtained by Rice and Saedvafa (1988) for high hardening crystals.

RN have also considered anti-plane cracks in BCC crystals which, in the context of the small-strain theory, are indistinguishable from the FCC cases analyzed here. Our own calculations of cracks in single crystals subjected to mode I loading (Mohan et al., 1992), however, seem to indicate that cases which are equivalent within the small-strain theory are quite distinct when finite deformations are taken into account. This owes to the fact that slip and kink bands, while indistinguishable within the small-strain theory, may give rise to substantially different lattice rotation patterns. These observations are consistent with the results of Rice et al. (1990).

ACKNOWLEDGEMENTS

The support of the National Science Foundation through the Materials Research Group at Brown University, Grant DMR-8714665, is gratefully acknowledged. The authors are indebted to J. R. Rice for helpful discussions.
which extends out to roughly one-quarter to nearly collapse onto a single angular 
\[ \sqrt{r} \]. The strains also behave in the same 
shown by Rice and Saeedvafa (1988), 
rate of hardening dominates the plastic 
acted fields reveals that the sum of the 
m is less than about 0.1 in the afore-
the high hardening regime. The angular 
region are in fact reminiscent of the cor-
by Rice and Saeedvafa (1988) for high 
BCC crystals which, in the context 
the FCC cases analyzed here. Our 
subjected to mode I loading (Mohan et 
which are equivalent within the small-
formations are taken into account. This 
while indistinguishable within the small-
different lattice rotation patterns. These 
of Rice et al. (1990).

ACKNOWLEDGMENTS

This work has been supported through the Materials Research Group at

The authors are indebted

REFERENCES

Abeyaratne, R. and
Triantafyllidis, N.
Asaro, R. J.
Asaro, R. J.
Asaro, R. J. and Rice, J. R.
Becker, R. and
Panchanadeswaran, S.
Belby, B. A., Cottrell, A. H. and
Swinden, K. H.
Chang, Y. W. and Asaro, R. J.
Deve, H., Harrin, S.,
McCullough, C. and
Asaro, R. J.
Hayner, K. S.
Hill, R. and Rice, J. R.
Kelly, A., Tyson, W. R. and
Cottrell, A. H.
Kobayashi, S. and Ohr, S. M.
Kocks, U. F.
Korn, G. A. and Korn, T. M.
Lau, C. W., Argon, A. S. and
McCintock, F. A.
Lee, E. H.
Li, F. Z., Seith, C. F. and
Needleman, A.
Lin, L.-H. and Thomson, R.
Low, J. R.
McMeeking, R. M.
Malvern, L. E.
Mandel, J.
Marsden, J. E. and
Hughes, T. J. R.
Mohan, R., Ortiz, M. and
Shih, C. F.
Moran, B., Ortiz, M. and
Shih, C. F.
Nagtegaal, J. D., Parks, D. M.
and Rice, J. R.
Ohr, S. M. and Chang, S.-J.
Ohr, S. M. and Narayan, J.
Pierce, D., Asaro, R. J. and
Needleman, A.
Pierce, D., Asaro, R. J.
Pierce, D., Shih, C. F.
and Needleman, A.

1979 Acta metall. 27, 445.
1967 Phil. Mag. 15, 567.
1985 Engng Fracture Mech. 21, 405.
1954 In Symposium on Relation of Properties to Microstructures, ASM, p. 163.
1980 Phil Mag. A41, 81.
1982 Acta metall. 30, 1087.
1984 Comp. Struct. 18, 875.
Equation (A8) provides a convenient means of calculating the plastic matrix. An explicit formula for the axis of rotation can be obtained by introducing the four Euler–Rodrigues parameters (KORN and KORN, 1968):

$$
\begin{align*}
\rho &= \cos \frac{\theta}{2}, \\
\lambda &= p_1 \sin \frac{\theta}{2},
\end{align*}
$$

where $p_1$, $p_2$, and $p_3$ are the components of the quaternion representation of rotations. The rotation matrix $R$ can be expressed as

$$
R = \begin{bmatrix}
\lambda^2 - \mu^2 - \nu^2 + \rho^2 & 2(\lambda \mu + \nu \rho) & 2(\lambda \nu - \mu \rho) \\
2(\lambda \mu - \nu \rho) & \mu^2 - \nu^2 + \rho^2 & 2(\mu \nu + \rho \lambda) \\
2(\lambda \nu + \mu \rho) & 2(\mu \nu - \rho \lambda) & \nu^2 - \lambda^2 + \rho^2
\end{bmatrix}
$$

From this representation of $R$ and (A7), the components $p_1$, $p_2$, and $p_3$ of the rotation vector $v$ are given by

$$
\begin{align*}
p_1 &= R_{32} - R_{23}, \\
p_2 &= 2 \sin \theta, \\
p_3 &= 2 \sin \theta
\end{align*}
$$

Within the formulation of finite plasticity by $R'$, i.e. the rotation component of $F'$ in (A7), the identities discussed above were applied to the lattice rotation.

### APPENDIX: COMPUTATION OF LATTICE ROTATIONS

Consider a three-dimensional rotation defined by a proper orthogonal matrix $R$, i.e. one which satisfies the identities

$$
RR^T = I, \quad \det(R) = 1,
$$

where $I$ is the identity matrix. Let the unit vector $p$ defines the axis of rotation. Then:

$$
Rp = R'p = p.
$$

Thus, $p$ is the unit eigenvector of $R$. Let $q$ and $r$ define, in conjunction with $p$, an orthonormal triad. If the angle of rotation is $\theta$, then the rotated vectors $q'$ and $r'$, denoted $q'$ and $r'$, respectively, can be expressed as

$$
q' = Rq = \cos \theta q + \sin \theta r, \quad r' = Rr = -\sin \theta q + \cos \theta r.
$$

From (A2) and (A3), the following scalar products, to be used subsequently, may be deduced:

$$
q \cdot (Rp) = r \cdot (Rp) = p \cdot (Rq) = p \cdot (Rr) = 0, \quad p \cdot (Rp) = 1,
$$

$$
-q \cdot (Rr) = r \cdot (Rq) = \sin \theta, \quad q \cdot (Rq) = r \cdot (Rr) = \cos \theta.
$$

Using the following standard formulas for the first and second invariants of a real matrix:

$$
I_R = \text{trace } R = 1 + p \cdot [(Rq) \times r] + p \cdot [q \times (Rr)],
$$

$$
II_R = (Rp) \cdot [(Rq) \times (Rr)] + p \cdot [(Rq) \times r] + p \cdot [q \times (Rr)]
$$

and (A4) one finds

$$
I_R = II_R = 1 + 2 \cos \theta.
$$
Equation (A8) provides a convenient means of computing angles of rotation from the rotation matrix. An explicit formula for the axis of rotation $p$ may be defined as follows. Start by introducing the four Euler–Rodrigues parameters [see, for example, Becker and Panachadenprasannan (1989)]:

$$
\rho = \cos \left( \frac{\theta}{2} \right), \quad \lambda = p_1 \sin \left( \frac{\theta}{2} \right), \quad \mu = p_2 \sin \left( \frac{\theta}{2} \right), \quad \nu = p_3 \sin \left( \frac{\theta}{2} \right),
$$

(A7)

where $p_1$, $p_2$, and $p_3$ are the components of the axis of rotation $p$. These parameters arise in the quaternion representation of rotations. Then, it is possible to parametrize rotation matrices as

$$
\mathbf{R} = \left[ \begin{array}{ccc} \lambda^2 + \mu^2 - \nu^2 + \rho^2 & 2(\lambda \mu - \nu \rho) & 2(\nu \lambda + \mu \rho) \\ 2(\lambda \mu + \nu \rho) & \mu^2 - \lambda^2 + \rho^2 & 2(\mu \nu - \lambda \rho) \\ 2(\nu \lambda - \mu \rho) & 2(\mu \nu + \lambda \rho) & \nu^2 - \lambda^2 - \mu^2 + \rho^2 \end{array} \right].
$$

(A8)

From this representation of $\mathbf{R}$ and (A7), the axis of rotation follows explicitly as

$$
p_1 = \frac{R_{23} - R_{32}}{2 \sin \theta}, \quad p_2 = \frac{R_{13} - R_{31}}{2 \sin \theta}, \quad p_3 = \frac{R_{12} - R_{21}}{2 \sin \theta}.
$$

(A9)

Within the formulation of finite plasticity given in Section 2, the lattice rotations are defined by $\mathbf{R}^*$, i.e. the rotation component of $\mathbf{F}^*$ in a standard polar decomposition $\mathbf{F}^* = \mathbf{R}^* \mathbf{U}^*$. The identities discussed above were applied to $\mathbf{R}^*$ to determine the corresponding angle and axis of lattice rotation.