Strain Localization in Ductile Single Crystals

by R. J. Asaro and J. R. Rice

Division of Engineering

Brown University

Providence, R.I., 02912, USA

April 1977

This regard was prepared as an Jossens of work proportion by the United States Government, Mathewall Research and States Government, Mathewall Research and States and Association of States and States Research Research and Revelopment Acted patriotics, the Economic Research and States Control Revelopment Acted patriotics from Section 2012, not any of shale conservation, superson of mathematical and section and s

This work was supported by the U.S. Energy Research and Development Agency under contract EY-76-S-02-3084.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Abstract

This paper is concerned with an analysis of strain localization in ductile crystals deforming by single slip. The plastic flow is modelled as rate-insensitive and localization, viewed as a bifurcation from a homogeneous deformation mode to one which is concentrated in a narrow "shear band", is found to be possible only when the plastic hardening modulus for the slip system has fallen to a certain critical value, h_{cr} , where h_{cr} is sensitive to the precise form of the constitutive law governing incremental shear. We develop the general form of this constitutive law, incorporating within it the possibility of deviations from the Schmid rule of a critical resolved shear stress, and we show that $h_{
m cr}$ may in fact be positive when there are deviations from the Schmid rule. It is suggested that micromechanical processes such as "cross-slip" in crystals provide specific cases for which stresses other than the Schmid stress may influence plastic response and, further, there is an experimental association of localization with the onset of large amounts of cross-slip. Thus we give the specific form of $h_{\rm cr}$ for a constitutive model that corresponds to the non-Schmid effects in cross-slip, and we develop a dislocation model of the process from which we estimate the magnitude of the parameters involved. The work supports the notion that localization can occur with positive strainhardening, h > 0 , and the often invoked notions of the attainment of an ideally plastic or strain softening state for localization may be unnecessary.

1. Introduction

There are numerous examples in which plastic flow in crystals gives way from a more or less homogeneous mode of deformation to one that is heavily concentrated in a narrow shear band. This localization may occur either before or after the onset of necking in a tension test, and is often a direct precursor to ductile rupture through profuse void formation and growth within the band. Indeed, in crystals which do not cleave, it generally seems that fracture occurs either by necking down to a "chisel edge" separation or by rupture within such concentrated shear zones. In this article we explore the precise conditions that allow an assumed homogeneous pattern of plastic flow, in a rate-insensitive crystal undergoing single slip, to develop bands of localized plastic deformation.

Our results are given in Section 3, to follow, and take the form of expressions for the critical value, h_{cr}, of the plastic strain hardening modulus h, in that localization occurs when h has fallen in magnitude to h_{cr}. As revealed in a preliminary analysis of the problem by Rice (1976), h_{cr} is dependent on constitutive parameters which correspond to deviations from the Schmid rule of a critical resolved shear stress, as a criterion for continued plastic shearing. Deviations from the Schmid rule are specific examples of deviations from the "normality flow rule" of continuum plasticity, and it has recently been shown (Rudnicki and Rice, 1975; Rice, 1975) that such deviations from normality allow the possibility of a positive, versus an essentially zero (i.e., non-hardening state) or negative (i.e., strain softening state), value of h_{cr} at localization.

In the next sub-section we discuss some perspectives on localized flow which explain our approach in light of existing empiricism and analyses, and

follow, in Section 2, with a precise formulation of the incremental constitutive law for single slip. This enables us to calculate $h_{\rm cr}$ in Section 3, and in Section 4 we introduce a dislocation model for non-Schmid effects at the onset of cross slip in fcc crystals, as a means of estimating some of the continuum parameters on which $h_{\rm cr}$ is found to depend.

1.1 Perspectives on localized flow

Discussions of localized plastic deformation in the experimental literature have generally associated shear localizations with traction maxima, Whether brought on by strain softening (e.g., Argon, 1973; Hornbogen and Gahr, 1975), adiabatic heating effects (Chin, Hosford and Backofen, 1964) or the attainment of ideal or non-hardening plastic states (Argon, 1.73; Lutjering and Weissman, 1970). There are many examples which suggest such associations. For example, the shearing of coherent precipitates in age hardened alloys of aluminum (Calabrese and Laird, 1974), iron (Hornbogen and Gahr, 1975), nickel (Gell and Leverant, 1968) and titanium (Blackburn and Williams, 1969) seems to be greatly augmented within localized shear bands as illustrated in the micrographs of Blackburn and Williams (1969). Radiation damaged materials are observed to develop soft "channels" with easy slip caused by the sweeping up of point defect debris by moving dislocations (e.g., Wechsler, 1973). Unstable dislocation barriers, which are presumed to break up following an increase in testing temperature, lead to flow localization as reported in the classic work of Cottrell and Stokes (1955). These examples among many others have been interpreted to suggest that localization is in fact caused by degradations in material strength, in the form of a loss of the materials workhardening capacity.

In related studies, Jackson and Basinski (1967) uncovered some interesting examples of localized flow in pure copper tested for latent hardening. When the crystals were sheared on slip planes other than the primary plane of prestraining, the initial deformation was concentrated in intense shear bands which occasionally propagated as Luders bands. Although these subsequently slipped planes were only rarely observed to strain soften, they were characterized by low workhardening rates. Howe and Elbaum (1961) tested aluminum crystals at elevated temperatures where the workhardening rates often approached zero and observed that the flow was decidedly non-uniform, consisting of coarse shear bands. The fact that these shear bands are, in many cases, persistent lends support to their association with material changes or imperfections which lower the strength level or workhardening capacity. But whether or not persistence is actually a result of ensuing substructural changes in the post localized state, rather than a manifestation of preexisting imperfections, is usually unknown. Indeed, there are important examples for which explanations based on an approach to ideal plasticity or strain softening do not seem appropriate.

For example, Elam (1925) and later Karnopp and Sachs (1928) found that age hardened alloys of aluminum displayed pronounced shear instabilities following uniform deformation. Beevers and Honeycombe (1962), followed by Price and Kelly (1964), made careful studies of this phenomena and found that the bands, which sometimes formed within diffuse necks, lead directly to a ductile shear type fracture. But Price and Kelly observed that these localizations occurred with increasing load (positive workhardening), identically in tension and compression, and thus without attendant ideal plastic or non-workhardening states. Furthermore, they pointed out that the

bands, just after forming, were <u>not persistent</u>, although continued straining would induce rupture within them. Indeed, unloading and polishing away the slip steps followed by reloading caused subsequent localization, but "... the bands never occupied the same place as before polishing ..."

The situation in pure face centered cubic crystals may be similar.

Saimoto et al. (1965) found that crystals of pure copper fractured, after some diffuse necking, along shear bands whose pattern closely resembled the ideally plastic slip line field given by Onat and Frager (1954) with its velocity and, hence, plastic strain discontinuity. However, as shown by hardness probes, the shear zones contained material that continuously hardened and thus, in this case, there did not seem to exist an ideally plastic state.

In view of the above experimental observations, it seems prudent to examine the possibility that localized plastic deformation may, in some circumstances, arise for reasons other than worksoftening or related local degradations in strength. Specifically, we explore, as stated previously, the possibility that localization is the result of a constitutive instability and is predictable from the prelocalized constitutive law relating stress increments to strain increments. The basic mechanics of this approach to localization was developed in the context of finite elasticity by Hadamard (1903) and extended to elastic-plastic solids, modelled as rate-insensitive, by Thomas (1961), Hill (1962) and Mandel (1966). Further, the specific calculations by Rudnicki and Rice (1975) for frictional solids, and by Rice (1976) for a wide class of ductile material models, including single crystals, reveal that localizations can occur with positive hardening when there are deviations from the normality flow rule.

In the present context, it is well to note that experimental observations link the onset of localization to the ease of cross slip or similar micromechanical

processes that allow microscopic obstacles to slip to be overcome. This association with cross slip was suggested by Price and Kelly (1964) in their work on aluminum alloy crystals, and profuse cross slip has long been associated with the onset of the so-called stage III deformation, during which coarse shear bands develop in pure single crystals (Cahn, 1951). As Rice (1976) noted, the stress-state dependence of conditions for the onset of cross-slip should, in general, entail deviations from the Schmid rule of critical resolved shear stress, and hence from the normality flow rule. In this sense there is a strong theoretical basis for a wider exploration of cross-slip and like processes as a basis for localization, via the destabilizing effect of non-normality. We explore this connection here.

Our materials are considered to be explicitly rate insensitive with piecewise linear incremental stress strain relations. As such, we preclude from the present study not only strain rate effects but also the possibility that new physical mechanisms of deformation set-in abruptly and degrade the strength. Clearly there are cases where unstable flow is influenced by imperfections or initial non-uniformities of material properties, but these are also omitted from present considerations. The localization criteria are worked out for an assumed class of materials that essentially obey Schmid's rule but display modest departures from it.

Standard notations are used throughout. Bold face symbols denote tensors or dyads, the order of which is indicated by the text. The magnitude of a vector, such as b, or any of its components, such as b_d , is denoted as b or b_d and similarly for the elements of higher order tensors. The summation convention is used and comma's imply differentiation with respect to the corresponding spatial variable, e.g., $t_{ij,i} = \partial t_{ij}/\partial x_i$. For brevity we

use dots and double dots to indicate the following products:

$$\underline{\mathbf{p}} \cdot \underline{\mathbf{n}} = \mathbf{P}_{ij}^{n}_{ij}$$
 , $\underline{\mathbf{q}} : \underline{\mathbf{q}} = \mathbf{Q}_{ji}^{\sigma}_{ij}$;

also

$$L: P = L_{ijk} P_{ik}$$
, $g \cdot P = \sigma_{ij} P_{jk}$

Constitutive Relation for a Crystal Undergoing Single Slip

The constitutive relation governing an increment of deformation is formulated in accord with the general analysis of crystalline slip by Hill and Rice (1972). With reference to fig. 1, in the increment of time dt an element of the crystal deforms from the configuration at the lower left of the figure to that at the upper right. The infinitesimal strain and rotation of the element are $\mathbb Q$ dt and $\mathbb Q$ dt, respectively, where $\mathbb Q$ is the symmetric rate of stretching tensor and $\mathbb Q$ the antisymmetric spin tensor. We observe that the corresponding change of a line element $\delta \mathbb X$ that connects material points of the crystal is

$$d(\delta x) = (Ddt + Ddt) \cdot \delta x \tag{2.1}$$

and, further, that in terms of gradients of the velocity vector v ,

$$2D_{ij} = v_{i,j} + v_{j,i}$$
 , $2\Omega_{ij} = v_{i,j} - v_{j,i}$. (2.2)

Now, as illustrated in fig. 1, the strain D dt and rotation Q dt can be realized by the following sequence: (i) The material is given a plastic shear relative to the lattice of amount dy under conditions for which lattice orientations and spacings are held fixed. This shear takes place on a family of crystal planes having the unit normal m, and has the direction of a unit vector & lying in one of the slip planes, so that the alteration of the

material line element ox is

$$d(\delta_{\underline{X}}) = (d\gamma_{\underline{A}\underline{M}}) \cdot \delta_{\underline{X}} . \qquad (2.3)$$

(ii) Next, the lattice and material deform as one with the infinitesimal strain $\hat{\mathbb{D}}$ dt and rotation $\hat{\mathbb{D}}$ dt , accomplishing the further alteration

$$d(\delta x) = (p^{\dagger}dt + p^{\dagger}dt) \cdot \delta x \qquad (2.4)$$

of the line element. We refer to \underline{D}^{*} and $\underline{\Omega}^{*}$ as the rates of <u>lattice</u> stretching and spin, respectively. In general, they are non-compatible and hence not derivable from a velocity field.

Observing that deformation (2.1) is equivalent to the sum of (2.3) and (2.4), and defining $\dot{\gamma}$ by dy/dt, we have Taylor's (1938) relations

We assume that elastic response properties, phrased relative to directions embedded in the lattice, are unaffected by slip. Then, following Hill and Rice (1972), the stress rate is related to $\mathbb{R}^{\frac{1}{2}}$ by an expression of the kind

$$g^{*} + g \operatorname{tr}(g^{*}) = L g^{*}. \tag{2.6}$$

Here ϱ is the Cauchy (or "true") stress tensor whereas g^{*} is its corotational, or Jaumann, rate formed on axes which spin with the <u>lattice</u>. Specifically,

where g is the ordinary time-rate of g following the material element, and the Cartesian components of g^{*} are the ordinary time-rates of the components of g on axes that rotate rigidly at the lattice spin rate g^{*} . The <u>trace</u>

operator $\text{tr}(\underline{p}^*)$ gives D_{kk}^* . The tensor \underline{L} (= L_{ijkk}) of incremental elastic moduli is symmetric in the indices i,j and k,* and, further, has the symmetry

$$L_{ijkl} = L_{klij} \tag{2.8}$$

when a strain energy function exists for elastic response.

We note in passing that the left side of (2.6) is the lattice-corotational rate of Kirchhoff stress, defined as $g\rho_0/\rho$ (where ρ is mass density and ρ_0 its value in some reference state), when the reference state is chosen to coincide instantaneously with the current state.

Expressing D^*,Ω^* in terms of D,Ω and γ by (2.5), the constitutive relation (2.6) takes the form

$$g + g tr(p) = L : (p - p')$$
 (2.9)

where

$$P' = P + L^{-1}: (W \cdot g - g \cdot W)$$
 (2.10)

In this, g is the corotational stress rate formed on axes spinning with the <u>material</u> (i.e., it is defined by the right side of (2.7) with g replacing g^{\pm}), and g is the inverse of g and has the same symmetries in its indices as does g itself.

The distinction between \underline{p}' and \underline{p} , pointed out earlier by Hill and Rice (1972), is small and involves $O(\sigma/L)$ terms (where σ and L are representative values of stress and elastic modulus) in comparison to O(1). Nevertheless, it is necessary to retain accuracy of the representation to this order if the critical hardening rate for localization is to be determined to within terms of order σ .

2.1 Plastic shearing with non-Schmid effects

The constitutive description is completed by specification of an expression for $\dot{\gamma}$. We start with less than the necessary precision in observing that the usual description of the incremental slip relation, in accord with the Schmid concept of a critical resolved shear stress, is in the form

$$dY = d\tau_{mA}/h \tag{2.11}$$

(when the slip system is at yield and subjected to an increment of stress causing further yielding) where $\mathrm{d}\tau_{\mathrm{m}\delta}$ is the increment of resolved shear stress and h is the strain hardening modulus. This expression for $\mathrm{d}\gamma$ must be refined and generalized in the following ways: (i) It is necessary to state precisely how $\mathrm{d}\tau_{\mathrm{m}\delta}$ is to be related to a stress increment like g dt . Different ways of computing $\mathrm{d}\tau_{\mathrm{m}\delta}$ (e.g., as an increment of "true" or of "nominal" or of some other kind of shear stress) lead to differences in the $\mathrm{O}(\sigma/L)$ terms, in comparison to the $\mathrm{O}(1)$ terms, in this relation (Hill and Rice, 1972); (ii) Next, as remarked in the Introduction, there are good reasons to suspect that small departures from the Schmid description, in the sense that stress increment components other than $\mathrm{d}\tau_{m\delta}$ affect the shear $\mathrm{d}\gamma$, may be important to the explanation of critical conditions for localization as observed experimentally.

We start with the non-Schmid effects and, letting Z be a unit vector perpendicular to A and M in fig. 1 so that A.M.Z form a right handed triad, we write in place of (2.11)

$$d\gamma = \frac{1}{h} \left(d\tau_{m\delta} + \alpha_{\delta\delta} d\tau_{\delta\delta} + \alpha_{mm} d\tau_{mm} + \alpha_{zz} d\tau_{zz} + 2\alpha_{\delta z} d\tau_{\delta z} + 2\alpha_{mz} d\tau_{mz} \right) . \quad (2.12)$$

Here each a gives the decrement in the Schmid stress required for flow per unit

increase of the corresponding non-Schmid stress, and we will discuss in Section 4 the physical origin of $\alpha_{\Delta Z}$ and α_{mZ} in relation to the process of cross-slip. Further, the relation of the $d\tau$'s to $\overset{\nabla^2}{g}$ dt that we shall adopt will be given shortly, after considering some of the different possible ways of specifying the Schmid increment $d\tau_{mA}$.

In all of these ways we will take τ_{mA} in the form

$$\tau_{mb} = m \cdot g \cdot \xi \tag{2.13}$$

where m and & are unit vectors at the current instant, but different results for dt will arise according to how we choose the vectors dt and mdt identified in fig. 1. The most direct manner of choosing these is perhaps to require that & and m remain orthogonal unit vectors in the deformation, with & remaining in the slip plane as the plane rotates. It is then elementary to show that

$$\dot{\hat{g}} = (\hat{p}^* + \hat{p}^*) \cdot \hat{g} - \hat{g}(\hat{g} \cdot \hat{p}^* \cdot \hat{g}) , \qquad (2.14a)$$

$$\dot{m} = -m \cdot (D^{\Omega} + \Omega^{\Omega}) + m(m \cdot D^{\Delta} \cdot m)$$
, (2.14b)

and the Schmid stress rate $\dot{\tau}_{m\delta}(\Xi d\tau_{m\delta}/dt)$ is

$$\dot{\tau}_{m\Delta} = \dot{m} \cdot \mathcal{Q} \cdot \dot{\mathcal{Q}} + \dot{m} \cdot \dot{\mathcal{Q}} \cdot \dot{\mathcal{Q}} + \dot{m} \cdot \mathcal{Q} \cdot \dot{\dot{\mathcal{Q}}} \\
= \dot{m} \cdot [\dot{\mathcal{Q}}^{\dagger} - \dot{\mathcal{D}}^{\dagger} \cdot \dot{\mathcal{Q}} + \dot{\mathcal{Q}} \cdot \dot{\mathcal{Q}}^{\dagger} \\
+ \dot{\mathcal{Q}} (\dot{m} \cdot \dot{\mathcal{D}}^{\dagger} \cdot \dot{m} - \dot{\mathcal{Q}} \cdot \dot{\mathcal{Q}}^{\dagger} \cdot \dot{\mathcal{Q}})] \cdot \dot{\mathcal{Q}} .$$
(2.14c)

A second alternative in defining the Schmid rate is to convect the vector with the lattice slip plane, so that its length does not remain constant, and to choose m as the "reciprocal base vector" normal to the deformed slip plane:

$$\dot{A} = (D^{+} + \Omega^{+}) \cdot A , \quad \ddot{m} = -m \cdot (D^{+} + \Omega^{+}) .$$
 (2.15a,b)

This gives

$$\dot{\tau}_{\text{mA}} = m \cdot (\ddot{g}^{\pm} - D^{\pm} \cdot g + g \cdot D^{\pm}) \cdot g \qquad (2.15c)$$

for the Schmid rate and, following the discussion of an analogous case by Hill and Rice (1972), we observe that $d\tau_{m\delta}$ can then be written $d\sigma_{\delta}^{m}$ where σ_{δ}^{m} is a mixed component of the tensor g on convected coordinates which deform with the lattice. A third choice is to again convect g with the lattice and to choose g so that it is normal to the deformed slip plane, but of a length which increases in proportion to slip plane area. Then

$$\dot{\underline{A}} = (\underline{D}^{h} + \underline{\Omega}^{h}) \cdot \underline{A} , \quad \dot{\underline{M}} = -\underline{M} \cdot (\underline{D}^{h} + \underline{\Omega}^{h}) + \underline{M} \operatorname{tr}(\underline{D}^{h})$$
 (2.16a,b)

and

$$\dot{\tau}_{m\Delta} = m \cdot [\ddot{g}^{\pm} + g \operatorname{tr}(\dot{g}^{\pm}) - \dot{g}^{\pm} \cdot g + g \cdot \dot{g}^{\pm}] \cdot \dot{g} . \qquad (2.16c)$$

In this case $d\tau_{m\delta}$ is the increment in the product of nominal shear stress on the slip plane and lattice stretch ratio in the slip direction. The case is of special interest because it is this very interpretation of the Schmid stress increment $d\tau_{m\delta}$ which Rice (1971) has shown to lead precisely to normality in work conjugate stress and strain variables. Also, as remarked by Hill and Rice (1972), this expression for $d\tau_{m\delta}$ can alternatively be interpreted as the increment in a mixed component of Kirchhoff stress on convected coordinates, analogous to $d\sigma_{\delta}^{m}$ above.

There are unlimited further generalizations of the Schmid stress, and as a fourth and final illustration we again require & and m to be orthogonal

unit vectors but simply rotate them rigidly at the lattice spin rate:

$$\dot{x} = \Omega^{\hat{x}} \cdot \dot{x} , \dot{y} = \Omega^{\hat{x}} \cdot y .$$
 (21.7a,b)

In this case

$$\dot{\tau}_{m\Delta} = m \cdot \dot{g} \cdot \dot{g} \cdot \dot{g}$$
 (2.17c)

All the above expressions for the Schmid rate have in common the feature that

$$\dot{\tau}_{ms} = m \cdot [\vec{g}^{\hat{n}} + g \operatorname{tr}(\vec{p}^{\hat{n}})] \cdot \underline{\delta} + g : \underline{H} : \vec{p}^{\hat{n}}$$
 (2.18)

where # is some fourth-rank tensor that depends on the precise way in which the base vectors # and # deform with the lattice, and which has components that are O(1). By inverting (2.6), all such rates $\mathring{\tau}_{m\delta}$ can be written in the form

$$\dot{\tau}_{m\Delta} = (\underline{\underline{s}}\underline{m} + \underline{g}; \underline{\underline{H}}; \underline{\underline{L}}^{-1}) : [\underline{\underline{g}}^{2k} + \underline{g} \operatorname{tr}(\underline{\underline{p}}^{2k})]$$

$$= (\underline{\underline{P}} + \underline{g}; \underline{\underline{H}}; \underline{\underline{L}}^{-1}) : [\underline{\underline{g}}^{2k} + \underline{g} \operatorname{tr}(\underline{\underline{p}}^{k})] \qquad (2.19)$$

where, in the last version of the expression, we have observed that the bracketed term is symmetric and have therefore replaced by by the plastic flow direction tensor P of (2.5).

We examine now the specification of the various non-Schmid stress increments of (2.12). Each of these increments is multiplied by an α . If the α 's are small fractions of unity, there will be contributions of negligibly small size, of $O(\alpha\sigma/L)$ in comparison to terms of O(1) or $O(\alpha)$ or $O(\sigma/L)$, made to the bracketed term of (2.12) by specifying precisely (e.g., at the level of choosing a specific $\frac{H}{L}$ in (2.19))the meaning to be given to the rates of non-Schmid stresses like τ_{AB} , τ_{ZM} , etc. On the other hand, looking

ahead to our final result for $h_{\rm crit}$ at localization, if the α 's are <u>not</u> small the correction due to retention of the $O(\sigma/L)$ terms in the non-Schmid stress rates would be negligible anyway. This is a fortunate circumstance, because our current physical understanding of crystalline slip barely enables a definitive choice of the α 's , much less a precise specification of the non-Schmid stress rates. Indeed, even the precise form of the Schmid rate $\dot{\tau}_{mb}$ cannot be specified, according to our present understanding of crystalline slip, although in this case we are helped by the remarkable fact that our result for $h_{\rm crit}$, to the order of accuracy that we determine it, turns out to be independent of how we choose H.

In view of the above remarks it suffices to write expressions of the type $\dot{\tau}_{\text{mZ}} = m \cdot [\overset{\nabla}{g}^{\dot{n}} + g \, \text{tr}(\overset{\dot{n}}{g}^{\dot{n}})] \cdot \overset{\dot{z}}{Z}$, $\dot{\tau}_{\dot{a}\dot{a}} = \overset{\nabla}{g} \cdot [\overset{\dot{a}}{g}^{\dot{n}} + g \, \text{tr}(\overset{\dot{n}}{g}^{\dot{n}})] \cdot \overset{\dot{a}}{Q}$, etc. for the non-Schmid stress increments, since precision of the $O(\sigma D^{\dot{n}})$ terms is unnecessary. Thus, using (2.19), the plastic shear rate of (2.12) can be written

$$\ddot{\gamma} = \frac{1}{h} Q: [\ddot{g}^{+} + g \operatorname{tr}(\ddot{g}^{+})]$$
 (2.20)

where

$$Q = \frac{P}{L} + g : H : L^{-1} + E$$
 (2.21)

and where the tensor g of non-Schmid effects, chosen without loss of generality to be symmetric, has the matrix of components on axes aligned with the triad g, m, z and ordered in the same sense,

$$\mathbf{g} = \begin{bmatrix} \alpha_{\delta\delta} & 0 & \alpha_{\delta Z} \\ 0 & \alpha_{mm} & \alpha_{mZ} \\ \alpha_{\delta Z} & \alpha_{mZ} & \alpha_{ZZ} \end{bmatrix}$$
 (2.22)

The elastic constitutive relation (2.6) and the first of (2.5) may now be called upon to rewrite (2.20) as

$$\dot{Y} = \frac{1}{h} Q: L : (\underline{p} - \underline{p}\dot{Y}) ,$$

and from this we may solve for $\dot{\gamma}$ as

$$\dot{\gamma} = \frac{1}{h + Q: \underline{J}: \underline{P}} \quad Q: \underline{J}: \underline{P} \quad . \tag{2.23}$$

Finally, by substituting this into (2.9) we obtain the form of the constitutive rate relation needed for the localization analysis,

$$\overset{\nabla}{g} + g \operatorname{tr}(\underline{D}) = \left[\underbrace{L}_{-} - \frac{(\underline{L}_{-} : \underline{P}_{-})(\underline{Q} : \underline{L}_{-})}{h + \underline{Q} : \underline{L} : \underline{P}_{-}} \right] : \underline{D} ,$$
 (2.24)

Conditions for Localization

Hill (1962) has presented the general theory of bifurcation of a homogeneous elastic-plastic flow field into a band of localized deformation (or, in Hadamard's (1903) terminology, into a "stationary discontinuity"). There is first the kinematical restriction that for localization in a thin planar band of unit normal \mathbf{p} (see fig. 2) the velocity gradient field $\mathbf{v}_{i,j}$ inside the band can differ from that outside, namely $\mathbf{v}_{i,j}^{0}$, only by an expression of the form

$$v_{i,j} - v_{i,j}^{0} = g_{i}^{n},$$
 (3.1)

In addition, there is the requirement of continuing equilibrium that

$$n_i \hat{\sigma}_{ij} - n_i \hat{\sigma}_{ij}^0 = 0$$
 (3.2)

at incipient localization, where \dot{g} is the stress rate within the band and \dot{g}^0 that outside it (Kill(1962) actually writes this equation in terms of a nominal stress rate but, as remarked by Rudnicki and Rice (1975), the above form is equivalent, given the kinematic restriction which must apply simultaneously).

If the constitutive rate relation is imagined to have the form

$$\hat{\sigma}_{ij} = c_{ijkl} v_{k,l} \tag{3.3}$$

and if the same set of constitutive coefficients g apply both inside and outside the band at incipient localization, then (3.1) and (3.2) will be satisfied simultaneously if

$$(n_i C_{ijkl} n_l) g_k = 0$$
 . (3.4)

Thus the critical condition for localization on a plane of normal $\,\underline{n}\,$ is first met when

$$\det(\underline{n}\cdot\underline{C}\cdot\underline{n})=0 , \qquad (3.5)$$

where $\underline{n} \cdot \underline{C} \cdot \underline{n}$ is considered to be a 2nd rank matrix. Of course, once the critical value of some constitutive parameter, say h, for localization is known as a function of \underline{n} from (3.5), it is then necessary to determine the orientation \underline{n} at which the critical state is first achieved.

To carry the localization calculation out for our single-slip constitutive relation of (2.24), we first identify \underline{C} by rewriting the relation

$$\dot{g} = \left[\underbrace{L - \frac{(\underline{L}:\underline{P}^{1})(\underline{Q}:\underline{L})}{h + \underline{Q}:\underline{L}:\underline{P}}} \right] : \underline{p} + \underline{\Omega} \cdot \underline{g} - \underline{g} \cdot \underline{n} - \underline{g} \operatorname{tr}(\underline{p})$$
 (3.6)

and recognizing that D and Ω can be expressed in terms of the velocity gradient. Indeed, to form the expression analogous to (3.4) we multiply (3.6) from the left with \underline{n} and write

$$\frac{1}{2}$$
 (gn + ng) and $\frac{1}{2}$ (gn - ng)

in place of $\mathfrak Q$ and $\mathfrak Q$, respectively, to obtain

$$Q = \left[(\underline{n} \cdot \underline{L} \cdot \underline{n}) - \frac{(\underline{n} \cdot \underline{L} : \underline{p}')(\underline{Q} : \underline{L} \cdot \underline{n})}{\underline{h} + \underline{Q} : \underline{L} : \underline{p}} \right] \cdot \underline{g} + \underline{A} \cdot \underline{g} , \qquad (3.7)$$

where

$$A = \frac{1}{2} [(\underline{n} \cdot \underline{g} \cdot \underline{n}) \underline{I} - \underline{g} - (\underline{n} \cdot \underline{g}) \underline{n} - \underline{n} (\underline{g} \cdot \underline{n})]$$
 (3.8)

and where \mathbf{I} is the 2nd rank unit tensor, $(\mathbf{I})_{ij} = \delta_{ij}$.

Rather than attempt to set directly the determinant of coefficients to zero in the above equation, we follow a general procedure outlined by Rice (1976, pp. 214-215) which leads more directly to a solution. We let $(\underline{n} \cdot \underline{l} \cdot \underline{n})^{-1}$ denote the 2nd rank tensor having elements which are the matrix inverse of those of $(\underline{n} \cdot \underline{l} \cdot \underline{n})$; this inverse may be assumed to exist since, for all cases of present interest, the <u>elastic</u> response properties are remote from any critical values for localization. Multiplying (3.7) by the inverse,

$$Q = \left\{ [L + (\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} \cdot \underline{A}] - \frac{[(\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} \cdot (\underline{n} \cdot \underline{L} \cdot \underline{p}')](\underline{Q} : \underline{L} \cdot \underline{n})}{\underline{h} + \underline{Q} : \underline{L} : \underline{P}} \right\} \cdot \underline{g} . \tag{3.9}$$

Now, since \underline{A} of (3.8) has elements which are of order σ , the bracketed tensor

differs from the unit tensor only by $O(\sigma/L)$ terms which, in representative cases, are minute fractions of unity. Thus we may assume that this tensor has an inverse and calculate it to any desired degree of accuracy by the series

$$[I + (\underline{n} \cdot \underline{t} \cdot \underline{n})^{-1} \cdot \underline{A}]^{-1} = I - (\underline{n} \cdot \underline{t} \cdot \underline{n})^{-1} \cdot \underline{A}$$

$$+ [(\underline{n} \cdot \underline{t} \cdot \underline{n})^{-1} \cdot \underline{A}] \cdot [(\underline{n} \cdot \underline{t} \cdot \underline{n})^{-1} \cdot \underline{A}] - \dots$$
(3.10)

Thus, when (3.9) is multiplied by this inverse, we have an expression in the form

$$\left[\frac{\mathbf{I}}{\mathbf{I}} - \frac{\mathbf{g}}{\mathbf{h} + \mathbf{Q} : \mathbf{L} : \mathbf{P}}\right] \cdot \mathbf{g} = \mathbf{Q}$$
 (3.11)

where the vectors a and b are given by

$$\mathbf{g} = \left[\mathbf{I} + (\mathbf{n} \cdot \mathbf{L} \cdot \mathbf{n})^{-1} \cdot \mathbf{A} \right]^{-1} \cdot (\mathbf{n} \cdot \mathbf{L} \cdot \mathbf{n})^{-1} \cdot (\mathbf{n} \cdot \mathbf{L} \cdot \mathbf{R}^{\dagger}) ,$$
and $\mathbf{b} = \mathbf{Q} \cdot \mathbf{L} \cdot \mathbf{n} .$ (3.12)

Upon multiplying (3.11) on the left by b^{\centerdot} , we obtain

$$\left(1 - \frac{b \cdot g}{h + Q \cdot L \cdot P}\right)(b \cdot g) = 0. \tag{3.13}$$

Now, in view of (2.23), the term beg cannot vanish for non-zero g unless the bifurcation mode g involves no plastic strain. Thus the only relevant condition allowing a non-zero g is that the coefficient of beg vanish in (3.13),

which gives the critical h at localization as

$$h + Q: L: P = b \cdot a$$
 (3.14)

It is easy to verify from (3.11) that the corresponding bifurcation mode has the form $\mathbf{g} = \mathbf{a}$.

Thus, when we use the expressions for b and a of (3.12), the critical value of b for localization on a plane of normal b is

$$h = -Q: \underline{L}: P + (Q: \underline{L} \cdot \underline{n}) \cdot [\underline{L} + (\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} \cdot \underline{A}]^{-1} \cdot (\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} (\underline{n} \cdot \underline{L}: \underline{P}')$$
 (3.15)

3.1 Expansion to order of σ

To review the origin of the terms appearing in (3.15), P is O(1) and is the plastic flow direction tensor of (2.5). P is defined by (2.10) and differs from P by terms of O(σ /L) which involve the plastic spin direction tensor P of (2.5). P is defined by (3.8) and is O(σ). P is defined by (2.21) and involves the term P, of O(1), a term of O(σ /L) involving the 4th rank tensor P introduced in (2.18) to account for lattice deformation effects on the Schmid stress rate, and the term P of O(σ /L) and (2.22) which accounts for non-Schmid stress effects on yielding. We recall that our specification of P neglected terms of O(σ /L), which, in any event, one would be hard-pressed to specify. For this reason we should delete from the right side of (3.15) all terms of the orders

$$\alpha\sigma$$
 , $\alpha\sigma^2/L$, $\alpha\sigma^3/L^2$, ... , and σ^2/L , σ^3/L^2 , ...

When this is done, with the help of (3.10) and the expressions for P and Q just mentioned, there results

$$h = \{-E: L:E + (E: L\cdot p) \cdot (p \cdot L\cdot p)^{-1} \cdot (p \cdot L:E)\}$$

$$+ \{-g: L:E + (g: L\cdot p) \cdot (p \cdot L\cdot p)^{-1} \cdot (p \cdot L:E)\}$$

$$+ (E: L\cdot p) \cdot (p \cdot L\cdot p)^{-1} \cdot (p \cdot L\cdot p)^{-1} \cdot (p \cdot L:E)$$

$$+ (E: L\cdot p) \cdot (p \cdot L\cdot p)^{-1} \cdot A \cdot (p \cdot L\cdot p)^{-1} \cdot (p \cdot L:E)\}$$

$$- (E: L\cdot p) \cdot (p \cdot L\cdot p)^{-1} \cdot A \cdot (p \cdot L\cdot p)^{-1} \cdot (p \cdot L:E)\} \qquad (3.16)$$

and in this arrangement the first bracket contains terms of O(L), the second of $O(\alpha L)$, and the third of $O(\alpha)$. Indeed, it is convenient to represent these bracketed expressions as the three terms on the right side of

$$h = LF_o(\underline{n}) + \alpha LF_1(\underline{n}) + \sigma F_2(\underline{n}) . \qquad (3.17)$$

Here the functions F are all $\theta(1)$ and L , α , and σ are representative members of the corresponding tensors.

To calculate the most critical orientation \underline{n} , we begin with consideration of the case for which both α and σ/L are sufficiently small that we approximate (3.16) and (3.17) by

$$h = LF_0(\underline{n}) . \qquad (3.18)$$

Upon rewriting the first bracketed term of (3.16), we have

$$LF_{O}(\underline{n}) = -\underline{P} : \underline{N} : \underline{P}$$
 (3.19)

where the 4th rank tensor N is defined by

$$N = L - (\underline{L} \cdot \underline{n}) \cdot (\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} \cdot (\underline{n} \cdot \underline{L})$$
(3.20)

and we observe that N has the same symmetry of indices as does L and, further, that

$$\mathbf{n} \cdot \mathbf{N} = \mathbf{N} \cdot \mathbf{n} = \mathbf{0} \quad . \tag{3.21}$$

In order to draw conclusions from (3.19), we show now that N is merely the tensor of incremental elastic moduli governing plane stress states in a plane perpendicular to N. Specifically, we let the unit vectors N, N and N form a right-handed triad and we make the definitions

$$\underline{d} = 2D_{nu}\underline{u} + 2D_{nu}\underline{v} + D_{nn}\underline{n}$$
 (3.22)

(no sum on repeated indices of form u , v , or n) , and

$$p' = D_{uu}gu + D_{uv}(ux + yu) + D_{vv}yv$$
 (3.23)

where $D_{ij}(i,j=u,v,n)$ are components of an arbitrary rate of stretching tensor \underline{D} on the directions of the corresponding unit vectors. Further, we observe that

$$D = D' + (nd+dn)/2$$
 (3.24)

For an increment of elastic plane stress deformation in the y-y plane, in the sense that the corotational increment of Kirchhoff stress has no components associated with the normal y to that plane, it is evidently necessary that

$$Q = g \cdot L : D = g \cdot L : D' + (g \cdot L \cdot g) \cdot d$$
, (3.25)

and hence that

$$\underline{d} = -(\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} \cdot (\underline{n} \cdot \underline{L} : \underline{p}^{1}) \quad . \tag{3.26}$$

Thus the corotational Kirchhoff rate can be written in terms of the stretching rates $\mathbf{p}^{'}$ in the plane of stressing as

$$g' + g \text{ tr}(D) = L:D = L:D' + (L:D) \cdot g$$

$$= [L - (L:D) \cdot (D:L:D)^{-1} \cdot (D:L)] : D' = M:D' \qquad (3.27)$$

where (3.20) for N has been used. This establishes the interpretation of N as the plane stress elastic moduli tensor and we note that since lattice distortions are small in all cases that we consider, the quadratic form

$$V = p' : N : p'$$
 (3.28)

may be assumed to be positive definite in D.

On the other hand

by (3.21), and thus the quadratic form V can also be written

$$V = P: \underline{N}: \underline{P} . \tag{3.29}$$

We see, therefore, that V is a positive definite function of \underline{D} but a positive semi-definite function of \underline{D} . In particular,

$$V = \underline{D}: \underline{N}: \underline{D} = 0 \text{ if and only if } \underline{D}' = \underline{0}. \tag{3.30}$$

Making application of these results in (3.18) and (3.19), we see that the critical value of h for localization on a plane of normal n must be either negative or zero, the latter occurring when n is chosen so that n0, defined in (2.5), has no components in the plane perpendicular to n0. It is straightforward to show that there are two, and only two, orientations n1 which allow this condition of n2 and these are given by:

case (i):
$$n = m$$
, and case (ii): $n = 4$. (3.31)

Thus, to summarize, when we approximate (3.17) by (3.18) we find that the critical plastic hardening modulus at the inception of localization is

$$h_{crit} = 0 ag{3.32}$$

and the plane of localization is either the slip plane (i.e., case (i) of n = m) or a plane that we shall refer to as the kink plane (case (ii), n=2).

3.2 Perturbations about slip and kink plane orientations

Now, to study the influence of the terms of order αL and σ in (3.17), we will begin by expanding (3.17) in a series in η , first about $\eta = \eta$ and later about $\eta = \lambda$. In carrying out the work, we wish to be mindful of the fact that σ/L is of the order 10^{-2} or smaller in representative cases, but that the α 's, which we estimate in the next section based on a model for cross slip, may be appreciably larger, perhaps of the order 10^{-1} .

For the perturbation about n = m we write

where g is understood to be small and to be chosen so that g, like g, g, is a unit vector. Also, we define the 2nd rank tensors

$$M = m \cdot L \cdot m , E = m \cdot L \cdot e , H = e \cdot L \cdot e$$
 (3.34)

and we observe that by the representation of (2.5) for $\ { t P}$,

$$P: L \cdot p = A \cdot (M + E) , P: L \cdot P = A \cdot M \cdot A$$
 (3.35)

Further,

$$(g \cdot L \cdot g)^{-1} = (g + g + g^{T} + g)^{-1}$$

$$= [g + g^{-1} \cdot (g + g^{T} + g)]^{-1} \cdot g^{-1}$$
(3.36)

where E^T is the transpose of E and we note that the inverse of a matrix product is the product of matrix inverses, but in inverted order. Since E is small, so also are E and H and the inverse of the bracketed matrix can be expanded in a series to give

$$(\underline{n} \cdot \underline{L} \cdot \underline{n})^{-1} = \underline{M}^{-1} - \underline{M}^{-1} \cdot (\underline{E} + \underline{E}^{T}) \cdot \underline{M}^{-1} - \underline{M}^{-1} \cdot \underline{H} \cdot \underline{M}^{-1} + \dots$$

$$+ \underline{M}^{-1} \cdot (\underline{E} + \underline{E}^{T}) \cdot \underline{M}^{-1} \cdot (\underline{E} + \underline{E}^{T}) \cdot \underline{M}^{-1} + \dots$$
(3.37)

where the deleted terms are of 3rd and higher powers in g.

By using these several results and reading off the various terms of the first bracket of (3.16), comprising $LF_{0}(\underline{n})$, we find after some algebra that

$$LF_{O}(\mathfrak{g}) = -\underbrace{\mathfrak{L}} (\mathfrak{g} - \mathfrak{g}^{T} \cdot \mathfrak{g}^{-1} \cdot \mathfrak{g}) \cdot \mathfrak{L} + O(L\varepsilon^{3})$$
 (3.38)

Next, by using (3.34) for M, M, and M and writing M-M for M, we can write

$$LF_{O}(\underline{p}) = -(\underline{p}-\underline{m}) \cdot (\underline{\lambda} \cdot \underline{M} \cdot \underline{\lambda}) \cdot (\underline{p}-\underline{m}) + O(L|\underline{p}-\underline{m}|^{3})$$
, (3.39)

where the 4th rank tensor M is

$$M = \Gamma - (\Gamma \cdot M) \cdot (M \cdot \Gamma \cdot M)_{-1} \cdot (M \cdot \Gamma)$$
 (3.40)

and corresponds to the tensor N of (3.20) when n is set equal to m.

Since n-m can have no component in the direction of m to the order considered (n and m are unit vectors), we observe from the properties discussed earlier for n that (3.39) for n is a negative definite quadratic form.

Next consider the term $\mathfrak{alF}_1(\mathfrak{g})$ of (3.17), which is defined by the second set of bracketed terms in (3.16). We can write, with (3.20) and (2.5)

$$\alpha LF_{\chi}(\mathfrak{g}) = -g: N: \mathfrak{g} = -(g: N\cdot \mathfrak{m}) \cdot \mathfrak{g} \tag{3.41}$$

and we observe that $\Gamma_1(m) = 0$ since $M \cdot m = 0$. By expanding the expression for $\alpha L \Gamma_1(m)$ with the help of (3.20), (3.33), (3.34) and (3.37), we obtain

$$\alpha LF_{1}(\mathbf{p}) = (\mathbf{p}: M \cdot \underline{\mathbf{p}}) \cdot (\mathbf{p} - \underline{\mathbf{m}}) + O(\alpha L |\mathbf{p} - \underline{\mathbf{m}}|^{2}) . \tag{3.42}$$

Finally, $\sigma F_2(n)$ of (3.17) is given by the last set of bracketed terms in (3.16). We first calculate $F_2(n)$, noting that

$$(m-1-m)^{-1} \cdot (m-1-2) = (m-1-m)^{-1} \cdot (m-1-m) \cdot A = A$$
 (3.43)

so that the terms comprising the last bracketed set of (3.16) give

Observing that the two terms involving # cancel one another, since H_{ijkl} is symmetric in its last two indices, and simplifying the remaining terms, we come to the remarkable conclusion

$$\sigma F_2(m) = 0$$
 , (3.45)

which applies irrespective of the several different generalizations of the Schmid stress rate that we have considered (i.e., the result is independent of $\frac{H}{H}$). We observe, therefore, that for any choice of $\frac{H}{H}$,

$$\sigma F_{2}(\underline{n}) = O(\sigma |\underline{n} - \underline{n}|)$$
 (3.46)

By combining (3.39), (3.42) and (3.46), the formula (3.17) for the value of h at localization on a plane having normal n may now be written

$$h = -(n-m) \cdot (\underline{A} \cdot \underline{M} \cdot \underline{A}) \cdot (n-m) + (\underline{a} \cdot \underline{M} \cdot \underline{A}) \cdot (n-m) + (\underline{a} \cdot \underline{M} \cdot \underline{A}) \cdot (n-m) + (\underline{a} \cdot \underline{M} \cdot \underline{A}) \cdot (\underline{a} \cdot \underline{M}) + O(L|n-m|^3 \cdot \underline{a} \cdot \underline{a}|n-m|^2 \cdot \underline{a} \cdot \underline{a$$

where the order terms include those of (3.39), (3.42), and (3.46) as well as those deleted in writing (3.16) from (3.15). Now, since n-m has no component in the direction of m, to the order considered, and since (with reference to fig. 2)

the mm , &m , and zm components of &.M. & vanish, because

$$\underline{m} \cdot (\underline{\lambda} \cdot \underline{M} \cdot \underline{\lambda}) = (\underline{\lambda} \cdot \underline{M} \cdot \underline{\lambda}) \cdot \underline{m} = \underline{0}$$
 (3.48)

by (3.40), we shall henceforth understand the notation & local to represent a plane 2nd rank tensor. Specifically, this is a tensor which has only components with the indices A4, Az, z4 and zz, and which components agree with those of its 3-dimensional counterpart. The inverse operation to (\frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}

$$(\underline{\delta} - \underline{h} - \underline{\delta}) - \underline{q} = \underline{p}$$
 implies $\underline{q} = (\underline{\delta} - \underline{h} + \underline{\delta})^{-1} - \underline{p}$ (3.49)

for associated vectors p and q lying in the 6-Z plane.

In terms of this inverse, the orientation n which maximizes the right side of (3.47) is

$$\mathbf{p} = \mathbf{g} + \frac{1}{2} \left(\underline{\delta} \cdot \mathbf{h} \cdot \underline{\delta} \right)^{-1} \cdot \left(\underline{\delta} \cdot \mathbf{h} \cdot \underline{\sigma} \right) + O(\alpha^2, \sigma/L)$$
 (3.50)

and when this expression is inserted into (3.47) we find that the critical hardening rate at the onset of localization is

$$h_{crit} = \frac{1}{4} \left(\underline{\alpha} : \underline{\mathbb{M}} \cdot \underline{\delta} \right) \cdot \left(\underline{\delta} \cdot \underline{\mathbb{M}} \cdot \underline{\delta} \right)^{-1} \cdot \left(\underline{\delta} \cdot \underline{\mathbb{M}} : \underline{\alpha} \right) + O(\alpha \sigma, \sigma^2 / L, \alpha^3 L)$$
 (3.51)

A parallel calculation can be carried out for case (ii), in which we perturb about the kink plane n=4. Now the results are given in terms of a tensor

$$\S = L - (L \cdot \&) \cdot (\& \cdot L \cdot \&)^{-1} \cdot (\& \cdot L)$$
 (3.52)

The critical orientation is given by

$$g = \underbrace{\lambda}_{\alpha} + \frac{1}{2} \left(\underbrace{m \cdot \mathcal{L} \cdot m}_{\alpha} \right)^{-1} \cdot \left(\underbrace{m \cdot \mathcal{L} \cdot g}_{\alpha} \right) + O(\alpha^{2}, \sigma/L)$$
 (3.53)

and

$$h_{crit} = \frac{1}{4} (g: g \cdot g) \cdot (g \cdot g \cdot g)^{-1} \cdot (g \cdot g \cdot g) + O(a\sigma, \sigma^2/L, a^3L) . \qquad (3.54)$$

Here $(\underline{m} \cdot \underline{S} \cdot \underline{m})$ is understood as a 2nd rank <u>plane</u> tensor with components in the plane of \underline{m} and \underline{z} , in a sense analogous to that for $(\underline{A} \cdot \underline{M} \cdot \underline{A})$ above.

It is interesting to note from (3.51) and from the result that $\underline{\pi} \cdot \underline{\mathbb{M}} = \underline{0}$, that only the components of $\underline{\alpha}$ in the slip plane (specifically, $\underline{\alpha}_{AA}$, $\underline{\alpha}_{AZ} = \underline{\alpha}_{ZA}$, and $\underline{\alpha}_{ZZ}$) affect the value for \underline{h} for localization, at least to quadratic order in the $\underline{\alpha}$'s. Similarly, from (3.54), only components of $\underline{\alpha}$ in the kink plane affect the result. Also, we see that the critical value of \underline{h} for the onset of localization is indeed <u>positive</u> when the non-Schmid effects, represented by the $\underline{\alpha}$'s, are present.

We note that the terms represented explicitly in (3.51) and (3.54) have the order of $\alpha^2 l$. So long as α is much larger than σ/l , the terms of order $\alpha\sigma$ and σ^2/l represented by $O(\dots)$ in (3.51) and (3.54) will indeed be negligible by comparison to what is retained. On the other hand, the neglected and retained terms are of the same order when the α 's are of the order of σ/l . But in this case $h_{\rm crit}$ will be such a small fraction of σ (say, $10^{-2}\sigma$ or less) that it is to be expected that local necking, setting in when h is of the order of σ , will have long preceded the attainment of conditions for localization. In any event, as we have emphasized in Section 2, it does not seem possible at present to specify the constitutive relation with enough precision to determine suitably the terms of order $\alpha\sigma$ and σ^2/l that we neglect in our expressions for $h_{\rm crit}$.

3.3 <u>Isotropic elastic moduli</u>

Suppose that \underline{L} has the isotropic form

$$L_{ijkl} = G(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \Lambda \delta_{ij}\delta_{kl}$$
 (3.55)

where G and Λ are "Lamé moduli", G being the shear modulus. Then we note, e.g., that

$$g: L \cdot \Delta = 2Gg \cdot \Delta + \Lambda \Delta \text{ tr}(g)$$
, $g: L \cdot \Delta = G(I + gg) + \Lambda gg$, $g: L \cdot \Delta = G\Delta g + \Lambda g\Delta$,

where \underline{I} is the unit tensor, $(\underline{I})_{ij} = \delta_{ij}$, and also that

$$(m + 1 + m)^{-1} = G^{-1}(1 + 5mm)$$
, where $\xi = (\Lambda + G)/(\Lambda + 2G)$. (3.56)

With such expressions and (3.40) for M we find

so that its inverse in the sense discussed earlier is

$$(\underline{\&} \cdot \underline{\&} \cdot \underline{\&})^{-1} = G^{-1}[\underline{z}\underline{z} + \underline{\&}\underline{\&}/(4\xi)]$$
 (3.58)

and

$$g: M \cdot A = 2G(\alpha_{ZA} + [(2\xi-1)\alpha_{ZZ} + 2\xi\alpha_{AA}]A).$$
 (3.59)

These last two expressions enable us to carry out the perturbation about p = m, in which case we find from (3.50) that the orientation of the plane of localization is

$$n = m + \alpha_{AZ} z + \frac{1}{4\xi} \left[(2\xi - 1)\alpha_{ZZ} + 2\xi \alpha_{AA} \right] z + O(\alpha^2, \sigma/G) , \qquad (3.60)$$

and from (3.51) the critical hardening rate is

$$h_{crit} = G\{\alpha_{\delta Z}^2 + \frac{1}{4\xi} \left[(2\xi - 1)\alpha_{ZZ} + 2\xi \alpha_{\delta \delta}^{-1} \right]^2 + O(\alpha\sigma_{\sigma}\sigma^2/G_{\sigma}\alpha^3G) . \quad (3.61)$$

In a similar manner, the perturbation about n = 3 leads, from (3.53), to the orientation

$$R = \Delta + \alpha_{mZ} Z + \frac{1}{4\xi} [(2\xi - 1)\alpha_{ZZ} + 2\xi \alpha_{AA}]_{\infty} + O(\alpha^2, \sigma/G)$$
 (3.62)

and, from (3.54), to the critical hardening rate

$$h_{crit} = G \left\{ a_{mz}^2 + \frac{1}{4\xi} \left[(2\xi - 1)a_{zz} + 2\xi a_{mm} \right]^2 \right\} + O(\alpha\sigma, \sigma^2/G, \alpha^3G) . \tag{3.63}$$

The results given thus far are for "small" g. It is possible, however, to write out explicitly the entire expressions for $LF_0(\underline{n})$ and $\mathfrak{al}F_1(\underline{n})$ in the isotropic case. Since such expressions are wanted only when the \mathfrak{a} 's are large, there is no need to retain the terms of order \mathfrak{a} in (3.17) and it suffices to write

$$h = LF_{\sigma}(\underline{n}) + \alpha LF_{\underline{1}}(\underline{n})$$
 (3.64)

(note that since g enters linearly in (3.15), there is no truncation in a in this expression). By using (3.55) in (3.16), and noting that

$$(\mathbf{g} \cdot \mathbf{L} \cdot \mathbf{g})^{-1} = G^{-1}(\mathbf{L} \cdot \xi \mathbf{g})$$
, (3.65)

(3.64) can be written as

h/G = -1 +
$$(p \cdot m)^2$$
 + $(p \cdot a)^2$ - $4\xi(p \cdot m)^2(p \cdot a)^2$
+ $2[p \cdot g \cdot (am + ma) \cdot p - 2\xi(p \cdot m)(p \cdot a)(p \cdot a \cdot p)$
+ $(2\xi - 1)(p \cdot m)(p \cdot a) \cdot tr(g)$. (3.66)

Further, when we choose the coordinate axes as in fig. 2 and use $n_i^n = 1$,

this becomes

$$h/G = -(n_3^2 + 4\xi n_1^2 n_2^2) + 4n_1 n_2 \xi [(1-n_1^2)\alpha_{\delta\delta} + (1-n_2^2)\alpha_{mm} + (1-n_3^2)\alpha_{22}] - 2n_1 n_2 \alpha_{22} + 2n_3 \xi n_2 (1-4\xi n_1^2)\alpha_{\delta2} + n_1 (1-4\xi n_2^2)\alpha_{m2}]$$

$$(3.67)$$

and in general, the most critical orientation must be sought numerically when accuracy greater than that of (3.60) to (3.63) is required.

3.4 Some particular cases

Consider first the possibility of pressure sensitivity of the Schmid stress for the onset of plastic flow. Suppose for example, that

$$(\tau_{m\delta})_{\text{onset}} = \tau_0 + \kappa p$$
 (3.68)

where τ_o is the flow strength at zero pressure, $p=-\sigma_{kk}/3$ is the mean pressure, and κ is a dimensionless parameter. Then the Schmid stress increment $d\tau_{m_A}$ is replaced by

$$d\tau_{m,\delta} + (\kappa/3)(d\tau_{mm} + d\tau_{\delta,\delta} + d\tau_{22})$$

and comparing with (2.12),

$$\alpha_{ij} = \kappa \delta_{ij}/3$$
 (3.69)

This yields the same h_{crit} value, either from (3.61) or (3.63) — by taking $\xi = 2/3$ (corresponding to h = 0) as representative, we have

$$h_{\text{crit}} \approx 0.12 \, \kappa^2 G$$
 . (3.70)

The parameter κ is readily interpreted in terms of the difference between yield strengths in uniaxial tension, σ_{τ} , and in uniaxial compression, $-\sigma_{c}$.

If the slip system is oriented for a maximum resolved shear stress, i.e., at 45° to the tensile axis so that τ_{mA} = $\sigma/2$, then (3.68) gives

$$(\sigma_{\rm e}/2) - (\sigma_{\rm t}/2) = \kappa [(\sigma_{\rm e}/3) + (\sigma_{\rm t}/3)] \ , \label{eq:sigma_e}$$

or

$$\bar{\sigma}_{c} - \bar{\sigma}_{t} = (4\kappa/3)[(\bar{\sigma}_{c} + \bar{\sigma}_{t})/2] , \qquad (3.71)$$

The "strength differential" is $4\kappa/3$ times the mean strength. Hence, making the definition SD = $4\kappa/3$,

$$h_{crit} \approx .07 (SD)^2 G$$
 . (3.72)

Now, localization in crystals is generally observed to take place in the range of hardening between 5×10^{-4} and 5×10^{-3} G and if this is to be explained by a pressure sensitivity of yielding it would be necessary to have values of SD in the range of 0.085 to 0.27. Such values seem considerably larger than most observed strength differentials except perhaps in martensitic high strength steels where SD may approach 0.07 to 0.10 (Spitzig et al., 1975). However, in general, we must surmise that it is unlikely that pressure-sensitivity of yielding has a significant effect on the onset of localization in crystals.

Indeed, as we have emphasized earlier, the experimental association of localization with the onset of cross slip suggests that we examine this and similar cases, in which non-Schmid stresses can aid in "triggering" an increment of plastic flow on the primary slip system, for deviations from normality which may lead to localization. The details of the cross-slip process will be described in the next section but, looking to fig. 3, an increment of the shear stress τ_{mZ} aids the coalescence of the separated partial dislocations comprising a screw dislocation segment, whereas the stress τ_{ZA} aids the driving of the

coalesced screw dislocation segment a small distance along the cross-slip plane, so as to bypass a local obstacle and then continue the shearing of the primary (ms) slip system.

We describe these effects by writing

$$d\gamma = \frac{1}{h} \left[d\tau_{m\delta} + \alpha d\tau_{\delta Z} + \beta d\tau_{mZ} \right]$$
 (3.73)

so that α describes the effect of the stress on the cross slip plane and β the effect of the stress tending to coalesce the partial. Comparing to (2.12),

$$\alpha_{AZ} = \alpha_{ZA} = \alpha/2$$
 , $\alpha_{mZ} = \alpha_{ZM} = \beta/2$ (3.74)

and other components of g vanish. Thus the solutions (3.60) and (3.61) for localization in the neighborhood of the slip plane give

$$p = m + \alpha z/2$$
 , (3.75)

and

$$h_{crit} = (a^2/4)G$$
 (3.76)

(thus reducing to the result of Rice (1976, eq. 30)) whereas the solutions (3.62) and (3.63) for localization in the neighborhood of the kink plane give

$$n = s + \beta z/2$$
, (3.77)

and

$$h_{crit} = (\beta^2/4)G$$
 . (3.78)

Evidently, the largest of the two results for $h_{\rm crit}$ is to be judged as that marking the onset of localization, although the physics of <u>finitely</u> localized deformation would seem to be very different for the slip versus the kink orientation. To fit observations of $h_{\rm crit}$ in the range of 5×10^{-9} to 5×10^{-3} G, it is necessary that the largest of α and β lie in the range from approxi-

mately 0.04 to 0.14. This range of values for hardening rate is chosen to conform to the hardening rates prevailing at the end of stage II deformation in fcc single crystal, $h/G \sim 1/300$ and early stage III.

Our dislocation model of the next section suggests that these ranges do indeed encompass reasonable values for α and β when a crystal is deformed to a state at which profuse amounts of cross slip become possible.

4. Estimate of Non-Schmid Stress Parameters for Cross Slip

One approach to the development of detailed constitutive behavior in metals rests on the premise that plastic micro-processes such as cross slip, particle or forest cutting, etc., are thermally activated events. For purposes of illustration, fig. 3 shows a process like cross slip. As depicted, the critical event requires that extended dislocations first constrict over a finite length and then bow to a critical radius on the cross slip plane, so that the segment can be driven the necessary bypassing distance by the stress on that plane. Depending on the medium and dislocations involved, one of these two processes might dominate in the calculation of the reversible work, AG, required to achieve this transition state; relevant material properties would be lattice structure, stacking fault energy, etc. It is reasonable to assume that this reversible work depends upon all the shearing stresses $\tau_{m\delta}$, $\tau_{\delta Z}$, and τ_{mZ} since they all do work in reaching the critical state. However, for the class of processes we have in mind the reversible work is characterized by a strong stress dependence. For example, for particle cutting in the aluminum-copper alloys discussed earlier, Byrne et al. (1961) found apparent activation volumes, $v = kT\partial \ln \gamma/\partial \tau_{mo}$), of the order $10^2 - 10^3 b_A^3$ where b_A is the Burgers vector.

In these cases plastic flow is observed, as is expected from rate theory, to be sensibly rate insensitive with a correspondingly weak temperature dependence.

We idealize the behavior as explicitly rate insensitive and treat $\Delta G(\tau_{m\delta}, \tau_{mZ}, \tau_{Z\delta}, \rho)$ as a <u>yield function</u>, in the sense that plastic flow occurs at measurable rate when this function falls to a critical value (essentially zero). This leads to a relation among the arguments of ΔG of the form (cf. eqs. (4.13), (4.26))

$$F(\tau_{mA}, \tau_{mZ}, \tau_{ZA}, \rho) = 0$$
 (4.1)

Here p is a <u>structure parameter</u> which increases with straining due to workhardening (see fig. 4), and we write

$$d\rho = \mu d\gamma \tag{4.2}$$

where µ may depend not only on p but also on the stress state under which the shear dy takes place so that eq. (4.2) is, in general, non-integrable. During plastic flow, F must continuously retain its non-zero critical value and thus we have the plastic "consistency" condition

$$d\tau_{m\delta} \frac{\partial F}{\partial \tau_{mA}} + d\tau_{mZ} \frac{\partial F}{\partial \tau_{mZ}} + d\tau_{ZA} \frac{\partial F}{\partial \tau_{ZA}} = -\mu \frac{\partial F}{\partial \rho} d\gamma \qquad (4.3)$$

and this has the same form as eq. (3.73) provided we make the identities

$$h = -\mu \left(\frac{\partial F}{\partial \rho}\right) \left(\frac{\partial F}{\partial \tau_{m\delta}}\right)^{-1}$$

$$\alpha = \left(\frac{\partial F}{\partial \tau_{z\delta}}\right) \left(\frac{\partial F}{\partial \tau_{m\delta}}\right)^{-1}$$

$$\beta = \left(\frac{\partial F}{\partial \tau_{mz}}\right) \left(\frac{\partial F}{\partial \tau_{m\delta}}\right)^{-1}.$$

$$(4.4)$$

Note that if cross-slip resulted in measurable shear on the cross-slip

plane, rather than just that involved in bypassing local obstacles, we would have a $d\gamma_{Z\delta}$ in addition to $d\gamma_{M\delta}$ ($\equiv d\gamma$). A relation like $d\gamma_{Z\delta} = \alpha d\gamma$ would be consistent with plastic normality but this is far too restrictive in general, and so we take $d\gamma_{Z\delta} = 0$.

Certainly, the approximate experimental validity of Schmid's rule suggests that the terms α and β in (3.73) and (4.4) should be small. However, no estimates are yet available. In the following subsection we make approximate estimates of α and β based on more-or-less standard techniques in dislocation theory as applied to the model illustrated in fig. 3. Before passing to this though, we must bring to mind the approximate nature of the linear elastic continuum theory of dislocations when applied to problems that involve interactions among small segments or closely spaced dislocations. These approximations in the analysis of complex problems are, unfortunately, unavoidable at present.

4.1 A mechanism for cross slip

In face centered cubic crystals the slip systems are of the type $\{111\}$ ($\dot{a}/2$)<110>, {e.g., Hirth and Lothe, 1968); a is the lattice parameter. We consider a screw dislocation gliding on the (111) plane with Burgers vector $\dot{b} = (a/2)[10\bar{1}]$. The two partial dislocations form in the sequence

$$b^{(1)} = (a/6)[2\bar{1}\bar{1}]$$

and

$$\underline{b}^{(2)} = (a/6)[11\overline{2}]$$
.

The slip plane normal is $m = (1/\sqrt{3})[111]$ and the slip direction is $\Delta = (1/\sqrt{2})[10\hat{1}]$; Z, the direction of partial coalescence, is $(1/\sqrt{6})[\hat{1}2\hat{1}]$.

Partial (1) is assumed to be rigidly pinned against a linear barrier and blocks an entire "piled up" array of n such screw dislocations, thus preventing further primary slip. Relaxation takes place by the cross slip excursion of the lead dislocation onto the cross slip plane (whose normal is g), allowing the bypass of the obstacle lying in the primary plane. Since movement of partial (1) on the cross slip plane is energetically prohibited (see Wirth and Lothe, p. 735 for an explanation), cross slip is possible only if the lead dislocation is completely coalesced or if a small dislocation loop with primary Burgers vector is created on the cross slip plane near the tip of the pileup. The first possibility has been discussed by several authors (see Wirth and Lothe, 1968 for a bibliography) while the second has been examined by Avery and Backofen (1963). As it happens, if this secondary dislocation loop is nucleated near the pileup tip our analysis will model both processes as we explain shortly.

Partial dislocation (2) moves to coalesce with (1) under the work performing influence of the normal forces $\tau_{m\delta}b_{\delta}^{(2)}$ and $\tau_{mz}b_{z}^{(2)}$; $b_{\delta}^{(2)} = b_{\delta}^{(2)} \cdot b = a/(2\sqrt{2})$ and $b_{z}^{(2)} = b_{\delta}^{(2)} \cdot z = a/(2\sqrt{6})$ (fig. 3). For the perfect (a/2)[101] dislocation the elastic energy can be written as (Asaro and Hirth, 1973)

$$E = K_{ij}b_ib_j \ln R/r_0$$
 (4.5)

where K is the energy factor matrix and R and r_0 are the so-called outer and inner cutoff radii respectively. The cutoff radii are ill-defined within the continuum theory which makes absolute determinations of our energy terms difficult. K on the other hand, is well defined and for elastic isotropy has the diagonal form $K_{mm} = K_{ZZ} = G/[4\pi(1-\nu)]$ and

 $K_{33} = G/4\pi$. When the two partials are extended a distance δ thus forming an included intrinsic stacking fault the <u>elastic</u> energy is given by (Asaro and Hirth, 1973)

$$E = K_{ij}b_{i}^{(1)}b_{j}^{(1)}kn R/r_{o} + K_{ij}b_{i}^{(2)}b_{j}^{(2)}kn R/r_{o} + 2K_{ij}b_{i}^{(1)}b_{j}^{(2)}kn R/\delta. (4.6)$$

Since the stacking fault has an excess free energy Γ per unit area the total energy of the extended dislocation is augmented by a term $\Gamma(\delta-r_0)$. When $\delta=r_0$ the dislocation is fully constricted and eq. (4.5) is regained if we interpret the inner cutoff for both partials and constricted dislocation as all equal to r_0 . Minimizing E by choice of δ yields

$$\delta = 2E_{12}/\Gamma \tag{4.7}$$

where $E_{12} = K_{ij}b_{i}^{(1)}b_{j}^{(2)}$.

Next we consider the change in <u>total</u> energy as the dislocation extends and include the works done by (or against) the "applied stresses" ,

$$\Delta E = -2E_{12} \ln \delta/r_o + \{\tau_{m\delta}b_{\delta}^{(2)} + \tau_{mz}b_{z}^{(2)}\}(\delta-r_o) + \Gamma(\delta-r_o) . \qquad (4.8)$$

Minimizing &E by choice of & gives

$$\delta = 2E_{1,2}/\tilde{\Gamma} , \qquad (4.9)$$

$$\bar{\Gamma} = \Gamma + \{\tau_{mb}b_{\Delta}^{(2)} + \tau_{m2}b_{z}^{(2)}\}$$
 (4.10)

The total reversible work to be done during constriction of unit length would then be

$$\Delta G = U_c = 2E_{12} \ln (2E_{12} / \bar{\Gamma} r_o e) + \bar{\Gamma} r_o$$
 (4.11)

If the <u>only</u> critical step during cross slip were this constriction process, then U_c would be the ΔG . Furthermore since we assume that there exists an equilibrium pileup of n dislocations driven by $\tau_{m\Delta}$, $\tau_{m\Delta}b_{\Delta}^{(2)}$ should be replaced for an isolated single ended pileup by n $\tau_{m\Delta}$ and $\hat{\Gamma}$ set equal to $\Gamma + n \tau_{m\Delta}b_{\Delta}^{(2)} + \tau_{mz}b_{z}^{(2)}$. β is now computed from its definition in eq. (4.4) to be (maintaining n constant),

$$\beta = b_z^{(2)}/(n b_A^{(2)}) = 0.58/n$$
 (4.12)

The criterion for complete coalescence is obtained by setting $\Delta G = 0$ in (4.11). Taking $r_0 \approx b_4$, as suggested by Hirth and Lothe (1968) for foc metals, and v = 1/3 the criterion is

$$n(\tau_{m\Delta}/G) + 0.58 (\tau_{mz}/G) \approx 1/(8\pi) - 2\Gamma/(Gb_{\Delta})$$
 (4.13)

For fcc metals with intrinsic fault energies less than 150 ergs/cm² $2\Gamma/(Gb) < 1/(8\pi)$; for copper for example $\Gamma/Gb \approx 1/250$ (Hirth and Lothe, 1968) and

$$n(\tau_{mg}/G) + 0.58 (\tau_{mg}/G) \approx .03$$
 . (4.14)

Stress ratios of $3 \times 10^{-2} \rm G$ are never attained in pure metals and are virtually unattainable with alloying either. If $n \approx 10$ then $\tau_{mb} \simeq 3 \times 10^{-3} \rm G$ would in principle be sufficient to induce coalescence and these stress values are only approached in, say, precipitation hardened crystals at the onset of profuse cross slip. Thus we infer that coalescence is at most possible at the stresses prevailing at the latter stages of deformation but probably only over segments restricted in length and aided by thermal activation. Of course, for metals such as pure aluminum where

 $\Gamma/(Gb_4) \geqslant 1/50$ we conclude that partial extensions are not probable or are too small to be modelled in our continuum theory. In what follows we assume that U_C , which may be driven to nearly vanishing values, is the reversible work required to spread the constriction along the linear barrier as the segment of secondary loop bows out on the cross slip plane.

Actually the "applied stresses" should not a priori be interpreted as those applied externally. Lattice frictional resistance should be subtracted and if we are considering the motion of dislocations over distances large compared with the spacing of zones in a zone hardened crystal or the dislocations in a dislocation forest we must account for their frictional resistance as well. In the aluminum-alloy crystals discussed earlier these resistive terms comprise a large fraction of the total flow stress ranging upwards to 1/3. In writing n $\tau_{m_A}b_A$ for the total resolved force on the lead dislocation in the array we have also ignored the interactions among these dislocations and those of nearby glide bands. To include these latter effects we could analyze an infinite sequence shown in fig. (5b) as well as the isolated single pileup shown in fig. (5a). Here $p < \ell$ and typically experiments suggest that $p \sim .12$. If both cases are treated as though the dislocations in the pileup were continuously spread out as a freely slipping shear crack we find that the near tip stress field has the well known form

$$[\tau_{m\phi}, \tau_{Z\phi}] \approx K(2\pi\rho)^{-\frac{1}{2}}[\cos \phi/2, \sin \phi/2]$$
 (4.15)

where the stress intensity factor K is

 $K^2 = 2G \text{ n } \tau_{m_0} b_{\underline{A}} \dots$ isolated single ended pileup $K^2 = \frac{\pi}{2} G \text{ n } \tau_{m_0} b_{\underline{A}} \dots$ isolated double ended pileup $K^2 = G \text{ n } \tau_{m_0} b_{\underline{A}} \dots$ infinite sequence of double ended pileups

For the double ended pileup cases in is interpreted as the number of dislocations of each sign in a length & in a slip line of length 2t . For the three cases respectively, n and the slip line length, & , are related by $n = \pi \tau_{m\Delta} \ell/(Gb_{\Delta})$, $n = 2\tau_{m\Delta} \ell/(Gb_{\Delta})$ and $n \approx \tau_{m\Delta} p/(Gb_{\Delta})$ if p/ℓ is small. In fact, the interactions of the infinite sequence tend to decrease, for a given slip line length, the near tip stresses. Now these inter-glide-band interactions are just the sort that form a basis for most analyses of stage II hardening in single crystals (Nabarro, Basinski and Holt, 1964). The force on the lead dislocation $\tau_1 b_A$ is given by $K^2/(2G)$ (see Rice, 1968, p. 299) and for the infinite sequence case is equal to $n \tau_{md} b_d/2$ which has obvious implications for increased $\tau_{m\delta}$ values in eq. (4.13) for the coalescence criterion. That is, to meet the condition of eq. (4.13), τ_{mA} for the case of an infinite sequence of pileups would have to be a factor $\sqrt{2\pi k/p}$ times as large as it must be for an isolated single ended pileup. The reductions in force on the lead dislocation lead us further toward the **View that coalesence, in most cases, is not completed by the stresses but** through applied stress, and local fluctuations, occurs only along segments with finite size.

Now, with the above in mind, we assume that there exist locally, along the partially constricted dislocation, minute segments that are "pinched" to total constriction: the energy or reversible work involved can be computed in a fashion similar to that used by Stroh (1954). We note that this will yield a work term, U_p , which depends upon the variables and parameters $\tau_{m\delta}$, τ_{mz} and Γ . However, as we shall see this term does not, in our model, contribute to the yield function Γ or to the computations for α or β and hence we will not reproduce the derivation of it here.

The final part of our analysis is concerned with the process of bowing of the constricted (or free) segment to critical conditions on the cross slip plane. We assume that the dislocation takes on a roughly semi-circular form with radius r. The resolved stresses that do work on the loop are composed of those caused by the pileup and those due to external sources. From eq. (4.15) this stress becomes (fig. 5a)

$$\tau_{ch} = K(2\pi\rho)^{-\frac{1}{2}} \cos \phi/2 + \tau_{ch} \sin \phi$$
 (4.16)

Now as a segment of the lead dislocation begins to move out onto the cross slip plane we will be interested in how the stress field of the array is affected. Figure (Sc) illustrates our argument in 2-dimensions for the case of straight dislocations. We assume the lead dislocation is discrete while the rest of the array is continuously distributed. The value of the stress intensity $K_{\rm net}$ at the end of the distributed array is dependent upon the applied stress, $t_{\rm md}$, and the position of the dislocation at $\xi_0(=re^{i\theta})$ which, as shown, is able to move on the cross slip plane with orientation ϕ . $K_{\rm net}$ is allowed to relax completely, i.e., $K_{\rm net}=0$, and we seek the value for $\rho, \rho_{\rm c}$, at which a=0, $\phi=\theta$ and thus for which no further movement of the continuous array is possible. The problem of a dislocation near a single continuous array or slipping line has been considered for elastically isotropic media by Rice and Thomson (1974) and by Asaro (1975) for generally anisotropic media. From these results we may write for $K_{\rm net}$

$$K_{\text{net}} = K - \frac{Gb_{\delta}}{\sqrt{2\pi r}} \cos (\theta/2)$$
 (4.17)

In order to estimate ρ_c from eq. (4.17) we require an appropriate value for

K; to obtain one, we look ahead to our yield function, eq. (4.26), where we find that, at yield,

$$K \approx \frac{5}{17} \frac{Gb_{\delta}}{\sqrt{er_{O}}} \sec \phi/2$$

when we leave aside the minor contributions due to the terms in U_c and E. Alternatively, if $\phi \approx \pi/2$, t_1/G at yield is .032. Now from eq. (4.17) we may write

$$\rho_{\rm G} = \frac{\rm G}{4\pi\tau_1} \, b_{\rm A} \, \cos^2\phi/2$$

and, if again $\phi \approx \pi/2$, $\rho_c \approx 1.3$ b_d. If $\phi = 0$, $\rho_c \approx 5$ b_d and when $\phi = 70^\circ$, $\tau_1/G = .024$ and $\rho_c \approx 2.25$ b_d. In other words, for $\phi \ge 70^\circ$ (the cases of interest) this "collapse" distance is quite small. We then expect that in our actual bowing process that so long as the segments bow out to distances comparable to or larger than $2b_d$ the trailing array will essentially collapse to the blocking line, and we may then use eq. (4.16) to represent the pileup tip stress field acting on the cross slipping displocation. The interaction of the loop expanding on the cross slip plane with the pileup is modelled following an argument due to Rice and Thomson (1974). Since a straight dislocation is attracted toward the tip of a slipping line with a force given exactly by $K_{1j}b_jb_j/\rho$ (Asaro, 1975), viz the "image force", we assume that the forces exerted by the pileup on a segment has an image form. Then the half loop is acted upon by an image half loop, and this is taken into account by choosing for the energy of loop expansion the energy per unit length of a full circular loop, namely (Kirth and Lothe, 1968)

$$T = Gb_a^2 \frac{2-v}{8\pi(1-v)} \ln \frac{\theta r}{e^2 r_o}$$
 (4.18)

Now the complete free energy change during the bow out is given by (taking $8/e^2 \approx 1$),

$$U = \Phi rin r/r_{o} - g(r^{3/2} - r_{o}^{3/2}) + 2U_{c}r + E(r^{2} - r_{o}^{2}) + U_{p}$$

$$\Phi = Gb_{d}^{2} (2 - v)/[8(1 - v)]$$

$$B = 1.4 \text{ K } b_{d}\cos \Phi/2 \text{ , and}$$

$$E = \pi/2 \tau_{z,b}b_{z}\sin \Phi .$$
(4.19)

The terms containing 8 and E account for the work of the applied stress of $\{4.16\}$; the terms with U_c and U_p are the energy of the constricted segment. As 8 and E are increased the segment traverses configurations, say $r = r_1(8,E)$ for which the free energy is a minimum -- this is diagrammed in fig. (6). AG is defined in the figure as

$$\Delta G = U(r_2, \Phi, B, U_c, E) - U(r_1, \Phi, B, U_c, E)$$
 (4.20)

where ${\bf r_1}$ is the stable loop radius and ${\bf r_2}$ corresponds to the barrier. As we desire the derivatives of ΔG when ΔG itself vanishes, we have both the conditions

$$\partial U/\partial r = 0 (4.21)$$

and

$$\partial^2 U / \partial r^2 = 0$$
 (4.22)

when $r = r_c$, the critical radius.

Equations (4.21) and (4.22) enable us to solve for the critical value of

 8 , corresponding to $_{c}$ = $_{c}$. Given that $_{c}$ / 4 < 1 for representative stress levels, we treat that quantity as a small parameter and solve for $_{c}$ and $_{c}$ to appropriate orders in the parameter. Thus, defining

$$r_1 = er_o \exp(-2U_c/\Phi) \approx er_o$$
 ,

the latter approximation being valid for representative values of $\stackrel{\cup}{c}$, we find for the critical value of $\stackrel{\circ}{B}$

$$B = (4\phi/3r_1^{\frac{1}{2}})(1 - \xi r_1/\phi)$$
 (4.24)

whereas the corresponding critical radius is

$$r_c = r_1(1-2Er_1/\Phi) \approx r_1 \approx er_0$$
 (4.25)

Recognizing from (4.19) that 8 and E are functions of the stresses; the former via the stress intensity K , (4.24) may be regarded as a yield criterion and from it we may compute the non-Schmid factors α and β . Indeed, to write this yield function it is most convenient to square both sides of (4.24), retaining only the same order of accuracy in the small parameter Er_1/Φ , and replacing the K^2 which appears on the left in terms of the stress τ_1 on the leading dislocation, writing $\text{K}^2 = 2G\tau_1b_3$. In this way we obtain the yield condition

$$\tau_{1} = 0.0071 \frac{(2-v)^{2}}{(1-v)^{2}} \frac{Gb_{\delta}}{r_{1}\cos^{2}(\phi/2)} \left[1 - \frac{8\pi(1-v)\tau_{2\delta}r_{1}\sin\phi}{(2-v)Gb_{\delta}} \right]. \quad (4.26)$$

For representative values in fcc crystals, $\nu=1/3$ and $\phi\approx70^\circ$, and with $r_s\approx er_o\approx eb_A$, this becomes

$$\tau_1 + 0.62 \ \tau_{zA} = 0.024 \ G$$
 , (4.27)

Thus recognizing that τ_1 is a function of the primary shear stress $\tau_{m,j}$ and parameters describing the geometry of the pileups (e.g., the slip line length £) we compute the non-Schmid parameter α as

$$\alpha = 0.62/(3\tau_1/3\tau_{mA})$$
 . (4.29)

Hence, pile-up geometries that efficiently concentrate the applied primary shear stress have small non-Schmid effects and conversely.

For the three pileup cases discussed earlier we have

$$\tau_1 = \pi \tau_{m\Delta}^2 \ell/Gb_{\Delta}$$
 , $\pi \tau_{m\Delta}^2 \ell/2Gb_{\Delta}$, $\tau_{m\Delta}^2 p/2Gb_{\Delta}$ (4.29)

respectively. Thus (4.28), simplified with the help of (4.27), yields

$$\alpha = 1.1(b_4/2)^{\frac{1}{2}}, 1.6(b_4/2)^{\frac{1}{2}}, 2.8(b_4/p)^{\frac{1}{2}}$$
 (4.30)

for the three cases of single and double ended isolated pileups and sequences of closely spaced pileups.

Now, £ typically ranges from 10⁻⁵ to 10⁻⁴ cm in stage II and early stage III hardening and $b_{0}\approx2.7\times10^{-8}$ cm. With £ = 10⁻⁵ cm we find α = 0.06 and 0.08 respectively for the model cases of isolated single and double ended pileups whereas for sequential pileups, taking p = 0.5£, we find α = 0.21. Of course, for £ = 10⁻⁴ cm, all the numbers are smaller by approximately 1/3. We note that £ typically decreases with ongoing strain with the implication that the relative importance of $\tau_{Z\delta}$ with respect to $\tau_{M\delta}$, and hence the size of α , increases. Thus, since $h_{crit}\approx\alpha^{2}G/4$, the critical hardening modulus, below which localization occurs, increases with strain in stage II and early stage III hardening, while h itself decreases with the onset of stage III. This pattern

continues until the localization condition is met.

For the case of a single ended pileup, it could also be appropriate in certain circumstances to regard the number of dislocations π , rather than 2, fixed in the differentiation of (4.23). Since $\tau_1 = n\tau_{m\delta}$ for the isolated single ended pileup, this leads to

$$\alpha = 0.62/n = 2.3(b_A/1)^{\frac{L}{2}}$$
 (4.31)

which is approximately twice the value obtained when 1 is instead regarded as the fixed quantity [compare to the first member of (4.30)]. Alternatively, we may choose n = 10 as representative and this suggests $\alpha = 0.06$ in this case.

To compare the predicted critical hardening rate $G\alpha^2/4$ with experimental values we need only remember that near the stage II-stage III transition h/G is of the order $1/300\approx3\times10^{-3}$ and, of course, falling with increasing strain. If $\alpha\simeq0.1$ on the other hand, which is representative of our estimates, $\alpha^2G/4$ is in the range $2.5\times10^{-3}G$. Thus the magnitudes of these non-Schmid effects we have calculated lead to predicted critical hardening rates that are certainly consistent with experimentally measured rates in the later stages of deformation where localization is observed.

From eqs. (4.26,27) it is easily seen that the yield criterion will not generally require stress levels exceeding those involved in the coalescence criterion, eqs. (4.13,14). We have already seen this for $\phi \sim 70^{\circ}$ in the discussion immediately following eq. (4.17). Thus our assumption of incomplete constriction is not violated by our derived yield function.

In fact we may also examine our assumption regarding the magnitude of $U_{\rm c}$ by using the yield criterion and eq. (4.11). For copper with $\Gamma/({\rm Gb}_{\downarrow})\approx 1/250$ we find that $2U_{\rm c}/\Phi\sim .04$ and thus was justifiably neglected in eq. (4.23). Our critical path then, is one for which ΔG vanishes while $U_{\rm c}$ remains positive.

Some final comments on the model are worth making before closing this section. We have seen that the model predicts a vanishing AG with positive \mathbf{U}_{c} . This in turn required that some mechanism operate to initiate a local constriction and we summarized that thermal fluctuations were important. But if thermal activation were involved, the model would of course predict some degree of rate sensitivity that, in the present case, we wish to preclude. We could avoid this by realizing that the perfectly linear barrier heretofore envisioned in our analysis is simplistic and should be replaced by one having irregularities (e.g., forest dislocations) that enable local constrictions to develop before complete constriction. For the present we will not include such refinements since there is no clear way in which to accurately model such details and overly speculative attempts to do so would only detract from the main intent of our calculations. The only further observation we make is that since U_ is positive both the α and β effect exist together whereas if θ_{c} were to vanish, only β would remain, unless some extraneous barrier were present, such as the dislocation forest, restricting the free segment length bowing onto the cross slip plane.

In the case where $U_{\alpha} > 0$ we may recompute β from eq. (4.26), using

(4.23), (4.11), and (4.10) to obtain

$$\beta = \frac{0.3\xi(\delta - r_0)(b_z^{(2)}/b_0) \sec \phi/2}{\sqrt{2\pi r_0}}$$

or

$$\beta = \frac{0.3(\delta - r_0)(b_z^{(2)}/b_{\delta}) \sec \phi/2}{\sqrt{pr_0}} . \tag{4.32}$$

Here $\xi=1$ or $\sqrt{2}$ for the isolated single or double ended pileup respectively. If we assume nearly complete constriction $(6\sim2r_0)$ and use the same numerology that followed eq. (4.30), we find $\beta\sim.01$ for, as an example, the isolated double ended pileup. This can be compared to eq. (4.12) by taking $n\sim10$ as a typical number to observe that β , as obtained from eq. (4.32), is substantially lower than the value .058. Values of β may be computed from eqs. (4.11) - (4.14) for the other cases we have considered and the general conclusion follows that β is smaller than α when both effects coexist.

Discussion

The particular mode of localized deformation considered here seems to be a "limiting" one in the sense that experimentally it is often preceded by other modes, such as necking. In their experiments on underaged aluminum-copper alloys, Beevers and Honeycombe (1962) clearly demonstrated the two modes of inhomogeneous flow. Necking usually preceded localized shearing but the results of these workers taken together with those of Price and Kelly (1964) suggest that it is often localized shearing that occurs first. The two modes seem independent of each other and which occurs first may well be a matter of specimen shape (see, e.g., Hill and Hutchinson, 1975). A thorough analysis of the bifurcation modes coupled with a complimentary experimental study on this system should be most helpful in developing a fuller understanding of inhomogeneous deformation in general. However, it seems to be the localized shearing that leads to rapid failure of these crystals, and we have demonstrated that this is possible with positive workhardening and without worksoftening or non-hardening plastic states.

There are several other important aspects of shear localization that require further understanding. We have explicitly considered the effects of non-normality with a smooth yield surface, in the context of slight deviations from Schmid's law for yielding. We recall that with a in the range 0.1, h_{cr}/G is predicted to be of the order, 2 × 10⁻³, and this corresponds quite reasonably with what is expected for the hardening rate shortly after the stage II-stage III transition in face centered cubic crystals (Nabarro et al., 1964). Related studies of localized deformation in polycrystalline sheets (Stören and Rice, 1975) and general solids (Rudnicki and Rice, 1975) have demonstrated the importance of "vertex" structures on yield surfaces. Single crystal yield surfaces contain

vertex like structure at points where the yield surfaces for various slip systems intersect. Indeed, in following the rotations of the tensile axis during straining, Price and Kelly (1964) noted that it "...usually reached or overshot the [001]-[111] boundary ..., and the slip bands (shear bands) belonged to the conjugate system." In all cases the shear bands were closely alligned with the active slip system — a result we reproduce in our analysis. But whether localization is preferred on the conjugate system because of vertex effects in the constitutive law or for the non-Schmid effects explored here, is not as yet clear. Localization is favored by low hardening rates and, if the latent hardening trends documented for pure face centered cubic crystals (Jackson and Basinski, 1967) also apply to these zone hardened crystals, it is expected that the workhardening on the conjugate planes would be correspondingly low. Again, full resolution of this question awaits further study.

Future experiments on shear fracture in single crystals, and notably precipitation hardened single crystals, should prove invaluable for developing more complete analyses of the localization phenomena. Our results suggest that the values of workhardening rates when localization occurs as well as stress level should be determined. The experiments to date, that we have mentioned, have noted that the resolved shear stress, but not shear strain, correlates reasonably well with the appearance of localized shearing, however there may well prove to be an equally good correlation with h, the slip plane hardening rate. Furthermore, the persistence of the shear bands is important in evaluating the role of strain softening. Price and Kelly (1954) seem to be among the few workers who have posed this question and, for the case of zone-hardened crystals, they found no evidence for strain softening. However, there is the possibility that in their aluminum-copper alloys room temperature aging during unloading and

repolishing can complicate the interpretations. Evidently, the point is significant and must be explored further.

Finally, we wish to call attention to the symmetry of our predictions regarding the orientation of the plane for localization: both planes that are nearly coincident with the slip plane and with what we have called the kink plane (normal in the slip direction, &) are predicted. It has, of course, occurred to us that a finite localization of the kink type is kinematically analogous to the phenomenon of "deformation kinking", in which a crystal lattice is observed to bend about an axis along Z in a planar band with normal & (Cahn, 1951). The mechanisms for forming such kinks are not well established and have usually been associated with asymmetries in loading. However, our analysis suggests that a rather different explanation may be possible in certain cases, in that some observed kinking may be explainable as a localization instability.

To conclude this article, we recall its intentions set forth in Section

1. There are numerous examples of highly localized plastic deformation in ductile single crystals that are not easily explained in terms of strain softening or ideal plasticity. We have instead put forth a rather detailed and (we hope) sufficiently precise analysis of the problem in initially homogeneous rate insensitive crystals, which does seem to provide a suitable description of the process. We have given formulae for the critical parameters, and have discussed in detail how they could be related to the micromechanics of slip. Clearly our procedures of section 4 could be applied to other types of "triggered" slip processes. Analytical extensions of our model are appealing, but whether or not our description, or some other, is the correct one in any particular case will probably be determined only by careful experiment of the kind we have suggested.

		·
References		·
Argon, A.S.	1973	The Inhomogeneity of Plastic Deformation, American Society for Metals Pub., ed. R.E. Reed-Hill, 161.
Asaro, R.J.	1975	J. Phys. F: Metal Phys. <u>5</u> , 2249.
Asaro, R.J. and Hirth, J.P.	1973	J. Phys. F: Metal Phys. <u>3</u> , 1659.
Avery, D.H. and Backofen, W.A.	1963	Trans. Met. Soc. AIME <u>227</u> , 835.
Beevers, C.J. and Honeycombe, R.W.	1962	Acta Met. <u>10</u> , 17.
Blackburn, M.J. and Williams, J.C.	1969	Trans. ASM <u>62</u> , 398.
Byrne, J.G., Fine, M.E. and Kelly, A.	1961	Phil. Mag. <u>6</u> , 1119.
Cahn, R.W.	1951	J. Inst. Metals, <u>79</u> , 129.
Calabrese, C. and Laird, C.	1974	J. Mat. Sci. and Engin., <u>13</u> , 141.
Chin, G.Y., Hosford, W.F. and Backofen, W.A.	1964	Trans. AIME <u>230</u> , 437.
Cottrell, A.H. and Stokes, R.J.	1955	Proc. Roy. Soc. <u>A233</u> , 17.
Elam, C.F.	1925	Proc. Roy. Soc. <u>Al09</u> , 143.
Gell, M. and Leverant, G.R.	1968	Acta. Met. <u>16</u> , 553.
Hadamard, J.	1903	Lecons sur la Propagation des Ondes et les Equations de L'Hydrodynamique, Paris, Ch. 6.
Hill, R.	1962	J. Mech. Phys. Sol., <u>10</u> , 1.
Hill, R. and Hutchinson, J.W.	1975	J. Mech. Phys. Sol., <u>23</u> , 239.
Hill, R. and Rice, J.R.	1972	Ibid., 20, 401.
Hirth, J.P. and Lothe, J.	1968	Theory of Dislocations, McGraw-Hill.

Hornbogen, E., and Gahr, K.	, 1975	Metallography $\underline{\theta}$, 181.
Howe, S., and Elbaum, C.	1961	Phil. Mag. <u>6</u> , 37.
Jackson, P.J., and Basinski, Z.S.	1967	Can. J. Phys. 45, 707.
Karnopp, R., and Sachs, G.	1928	Z. Phys. <u>49</u> , 480.
Lutjerling, G., and Weissmann, S.	1970	Acta. Met. <u>18</u> , 785.
Mandel, J.	1966	Rheology and Soil Mechanics, eds., J. Kravtchenko and P.M. Sirleys, Springer-Verlag, 58.
Nabarro, F.R.N., Basinski, Z.S., and Holt, D.B.	1964	Advan. Phys. <u>13</u> , 193.
Onat, E.T., and Prager, W.	1954	J. Appl. Phys. <u>25</u> , 491.
Price, R.J., and Kelly, A.	1964	Acta. Met. <u>12</u> , 974.
Rice, J.R.	1968	Fracture: An Advanced Treatise (Vol. 2, Mathematical Fundamentals), ed. H. Liebowitz, Academic Press, 191.
	1971	J. Mech. Phys. Sol., <u>19</u> , 433.
	1976	Proc. 14th International Congress of Theoretical and Appl. Mechanics, Vol. I, ed. W.T. Koiter, North-Holland Pub- lishing Co., 207.
Rice, J.R., and Thomson, R.	1974	Phil. Mag. <u>29</u> , 73.
Rudnicki, J.W., and Rice, J.R.	1975	J. Mech. Phys. Sol. <u>23</u> , 371.
Saimoto, S., Hosford, W.F., and Backofen, W.A.	1965	Phil. Mag. <u>21</u> , 319.
Spitzig, W.A., Sober, R.J., and Richmond, O.	1975	Acta. Met. <u>23</u> , 885.

•

.

		•
	٠	-54
Stroh, A.N.	1954	Proc. Phys. Soc. <u>B67</u> , 427.
Thomas, T.Y.	1961	Plastic Flow and Fracture of Solids, Academic Press.
Wechsler, M.S.	1973	The Inhomogeneity of Plastic Deformation, American Society for Metals Pub., ed. R.E. Reed-Hill, 19.

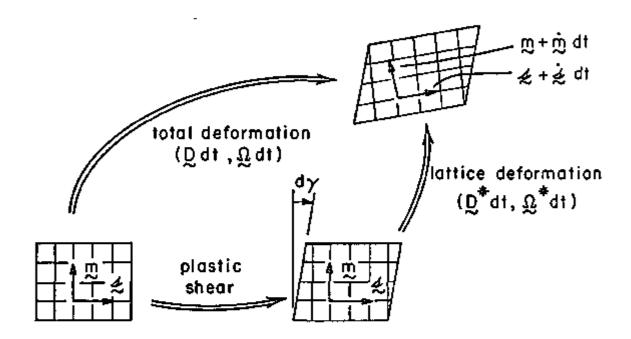


FIGURE 1

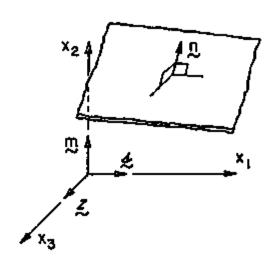


FIGURE 2

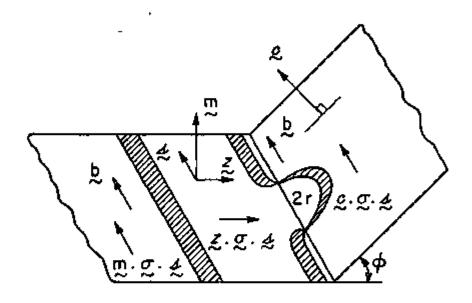


FIGURE 3

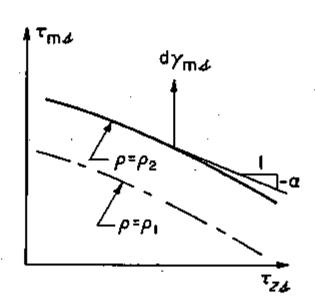


FIGURE 4

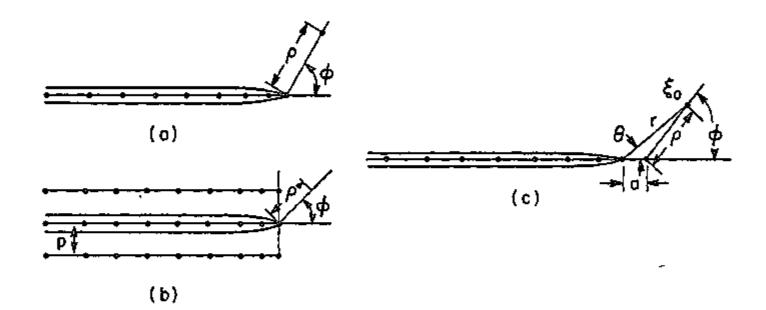


FIGURE 5

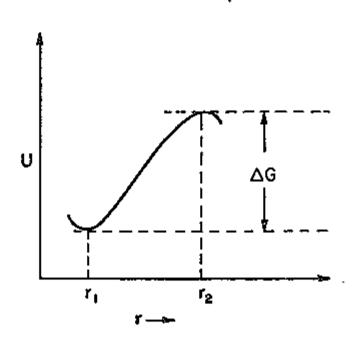


FIGURE 6

Figure Captions

- Figure 1. The total <u>deformation</u> <u>D</u> dt of a crystalline material in the time interval dt can be kinematically decomposed into: (i) A <u>plastic</u> shear dγ, imposed on the material under conditions for which the lattice is rigidly fixed relative to the background reference axes, and (ii) A <u>lattice deformation</u> <u>D</u> dt, imposed under conditions for which the material and lattice deform and rotate identically. The total infinitesimal rotation of the material is <u>Ω</u> dt, but the corresponding lattice rotation is <u>Ω</u> dt.
- Figure 2. Cartesian coordinates aligned with unit vectors of crystal slip system. Surface of localization is shown with unit normal \underline{n} , having components n_1 , n_2 , n_3 .
- Figure 3. Cross slip model. Local obstacle is bypassed by partial segments of a screw dislocation on the primary plane constricting, and moving a small distance on the cross slip plane, before continuing primary slippage.
- Figure 4. The surface $\Delta G \approx 0$, in the space of stresses $\tau_{m\Delta}$, $\tau_{Z\Delta}$, and τ_{mZ} , can be taken as a yield surface. Different yield surfaces correspond to different values of the structure parameter ρ .
- Figure 5. Arrays of discrete dislocations "piled up" at a barrier at the origin. φ is the angle of inclination of the cross slip plane. The dots represent discrete dislocations and the surrounding solid lines the continuous smearing of these dislocations along the slip line for the (a) isolated array, and (b) an infinite sequence of arrays, each separated by a distance p. Sc shows an idealization of an array where the lead dislocation is discrete while the remaining dislocations are continuously distributed.
- Pigure 6. Schematic form of the activation barrier for cross slip.