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ON THE STRAIN LOCALIZATIONS OF DUCTILE SINGLE CRYSTALS UNDERGOING SINGLE SLIP

X. M. SU
Department of Mechanics, Tianjin University, Tianjin, P. R. China

and

W. D. LU
Institute of Applied Mathematics and Mechanics, Shanghai University of Technology, Shanghai, P. R. China

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Abstract—In this paper, shear bands in single crystals undergoing single slip are analyzed. It is suggested that there are thin layers of multiple slip even though the crystals are designed to perform single slip. These multiple slip layers, which either occur as a result of distortion of the crystal lattice, or are induced by pile-up dislocations, provide a location for the shear bands. Using Asaro's plane model, the analysis of a single crystal specimen is presented where thin layers of conjugate double slip account for the formation of kink bands.

This analysis, by supposing that there are conjugate double slip layers in a specimen of single slip, is equal to the analysis of a specimen with imperfections. The calculation of this paper is quite different from those which usually appear in the literature, and is simple and clear.

1. INTRODUCTION

Single crystals deformed homogeneously in tension or compression, always give way to inhomogeneities: shear bands, e.g. kink bands and coarse slip bands, are formed in thin layers (Cahn, 1951; Honeycombe, 1952). These inhomogeneities act as barriers to further slip, contributing to the hardening of the crystal, and on the other hand, supply places for final fractures.

Shear bands are a type of instability. When one uses the classical plasticity theory to account for them, one nevertheless arrives at the conclusion that they can exist only when the crystal is degraded to be zero or minus hardening. This conclusion sometimes contradicts the experimental facts that shear bands also appear in hardening range.

Asaro and Rice (1977) performed an analysis of the strain localizations in ductile crystals undergoing single slip, which is the very problem that we will discuss. With the hypothesis that non-Schmid effects may exist in crystals, they obtained shear bands with a positive hardening rate. Their idea is new and their results agree with experimental conclusions in many respects.

After some careful analysis of experimental results we believe that there are some phenomena which could not be explained by non-Schmid effects. For example, Honeycombe (1952) pointed out that there would be no kink bands if the specimen was performing conjugate double slip. Since there are obviously non-Schmid effects in the conjugate double slip, a kink band, if it exists in the specimen with single slip, has no reason to disappear. Also, Cahn (1951) showed that the higher the temperature, the sparser the kink bands, and the more the cross slip. Cross slips are the signs of non-Schmid effects, according to Asaro and Rice (1977), then it seems that more cross slips should correspond to closer kink bands. This is not easy to explain.

At the same time, we notice from the experimental evidence that there are thin layers of multiple slip in test specimens performing single slip, and these thin layers usually develop into shear bands. And although there may be no signs of secondary slip at sites where kink bands develop later, slips on different sets of planes in the kink band are found after moderate deformation (Honeycombe, 1952).

The formation of shear bands in a specimen with tensile history, especially under the condition of hardening, requires a lower shear modulus than that of elasticity. Classical plasticity, by assuming a normality rule setting strain rate normal to yield surface and the smoothness of the yield surface, gives a shear modulus too stiff to account for experimental results concerning bifurcation (Hutchinson, 1974). To get a lower shear modulus, either the smoothness of the yield surface or the rule of normality has to be abandoned. For the special case of crystal slip, non-Schmid effects introduce deviations from the normality rule and multiple slip will induce singularities on the yield surface. So, the experimental evidence mentioned above leads naturally to the hypothesis that thin layers of multiple slip that exist or are induced in the crystals arranged for single slip are reasons of shear bands, and specifically, layers of conjugate double slip, which are easily created by the rotation of crystal lattice during tests will lead to kink bands.

In the following, we use the plane model of Asaro (1979) to analyze crystals which are arranged for single slip, but are of layers of conjugate double slip. Conditions under which shear band is possible are given, and for the specific case of rigid–plastic crystals, detailed numerical calculations are carried out and compared with existing experiments.

As a rule, summations on repeated indices are assumed unless otherwise indicated. Boldface symbols will be used throughout to denote tensors, and the normal ones with subscripts to denote their components. A dot between tensors means inner product. A dyad is expressed by putting vectors together. Greek indices are ranged from 1 to 2, and Latin ones from 1 to 3.

2. CONSTITUTIVE LAWS

2.1. *Theory of crystal slip* (*Asaro*, 1983)

Let ξ_i $(i = 1, 3)$ be the coordinates of reference configuration, x_i be those of current configuration, **L** the velocity gradient:

$$\mathbf{L} = \mathbf{D}+\mathbf{\Omega} \tag{1}$$

where

$$2\mathbf{D} = \mathbf{L}+\mathbf{L}^{T}, \quad 2\mathbf{\Omega} = \mathbf{L}-\mathbf{L}^{T}$$

are deformation rate and spin rate. The superscript "T" denotes transpose.

The deformation of the crystal is divided into two parts: one is due to lattice distortion, regarded as purely elastic; the other comes from slip and is plastic. So,

$$\mathbf{D} = \mathbf{D}^{p}+\mathbf{D}^{e}, \quad \mathbf{\Omega} = \mathbf{\Omega}^{p}+\mathbf{\Omega}^{e} \tag{2}$$

where superscripts p and e denote plasticity and elasticity, respectively. Assume that there are k slip systems activated, i.e. the resolved shear stresses of the k slip systems, τ^{α}s, are just equal to the yield stresses of their corresponding systems, τ_c^{α}s, $\tau^{\alpha} = \tau_c^{\alpha}$. If the αth slip is on the plane with the normal $\mathbf{m}^{\alpha}$ and in the direction $\mathbf{s}^{\alpha}$, the deformation it causes will be:

$$\mathbf{d}^{\alpha} = \tfrac{1}{2}(\mathbf{m}^{(\alpha)}\mathbf{s}^{(\alpha)}+\mathbf{s}^{(\alpha)}\mathbf{m}^{(\alpha)})\dot{\gamma}^{(\alpha)} = \mathbf{p}^{(\alpha)}\dot{\gamma}^{(\alpha)} \tag{3}$$

$$\omega^{\alpha} = \tfrac{1}{2}(\mathbf{m}^{(\alpha)}\mathbf{s}^{(\alpha)}-\mathbf{s}^{(\alpha)}\mathbf{m}^{(\alpha)})\dot{\gamma}^{(\alpha)} = \mathbf{w}^{(\alpha)}\dot{\gamma}^{(\alpha)} \tag{4}$$

(no sum when indices are in parentheses)

where $\dot{\gamma}^{\alpha}$ is the shear rate of the αth slip system. The plastic deformation due to the k slip systems is:

$$\mathbf{D}^{p} = \sum_{\alpha}^{k}\mathbf{p}^{(\alpha)}\dot{\gamma}^{(\alpha)}; \quad \mathbf{\Omega}^{p} = \sum_{\alpha}^{k}\mathbf{w}^{(\alpha)}\dot{\gamma}^{(\alpha)}. \tag{5}$$

The above equations, together with (2), lead to:

$$\mathbf{D}^e = \mathbf{D} - \Sigma \mathbf{p}^{(\alpha)} \dot{j}^{(\alpha)}; \quad \mathbf{\Omega}^e = \mathbf{\Omega} - \Sigma \mathbf{w}^{(\alpha)} \dot{j}(\alpha). \tag{6}$$

If there is no coupling between elastic and plastic deformations, and $\mathscr{L}$, the elastic modulus, is of the symmetry,

$$\mathscr{L}_{ijkl} = \mathscr{L}_{klij}$$

the following elastic constitutive relation can be assumed,

$$\overset{\nabla}{\sigma}{}^e + \sigma \operatorname{tr}(\mathbf{D}^e) = \mathscr{L} : \mathbf{D} \tag{7}$$

where σ is Cauchy stress tensor, and tr (.) is the trace of the tensor in parentheses. $\overset{\nabla}{\sigma}{}^e$ is the Jaumann rate of stress tensor based on the spin of the lattice, and

$$\overset{\nabla}{\sigma}{}^e = \dot{\sigma} - \mathbf{\Omega}^e \cdot \sigma + \sigma \cdot \mathbf{\Omega}^e. \tag{8}$$

Let $\overset{\nabla}{\sigma}$ denote the Jaumann rate of stress tensor based on the total spin,

$$\overset{\nabla}{\sigma} = \dot{\sigma} - \mathbf{\Omega} \cdot \sigma + \sigma \cdot \mathbf{\Omega}. \tag{9}$$

Then, by combining eqns (6) to (9), the constitutive relation may be obtained as,

$$\overset{\nabla}{\sigma} + \sigma \operatorname{tr}(\mathbf{D}) = \mathscr{L} : (\mathbf{D} - \mathbf{p}^*) \tag{10}$$

in which

$$\mathbf{p}^* = \sum^{k} [\mathbf{p}(\alpha) + \mathscr{L}^{-1} : (\mathbf{w}^{(\alpha)} \cdot \sigma - \sigma \cdot \mathbf{w}^{(\alpha)})] \dot{j}^{(\alpha)}. \tag{11}$$

The above equations are complete if the hardening law is supplied. Crystal hardening is a complicated subject, and a detailed account could be found in Asaro (1983). Here we choose a simple rule.

Obviously, the shear stress on the αth slip system is:

$$\tau^\alpha = \mathbf{m}^{(\alpha)} \cdot \sigma \cdot \mathbf{s}^{(\alpha)}.$$

Define,

$$\dot{\mathbf{s}}^{(\alpha)} = \mathbf{\Omega}^e \cdot \mathbf{s}^\alpha, \quad \dot{\mathbf{m}}^\alpha = \mathbf{\Omega}^e \cdot \mathbf{m}^\alpha,$$

and the hardening rule of critical systems is assumed to be:

$$\dot{\tau}^\alpha = \dot{\tau}_c^\alpha = \Sigma h_{\alpha(\beta)} \dot{j}^{(\beta)} \quad \dot{j}^\beta > 0, \tag{12}$$

or for an inactive critical system,

$$\dot{\tau}^\alpha \leqslant \dot{\tau}_c^\alpha = \Sigma h_{\alpha(\beta)} \dot{j}^{(\beta)} \quad \dot{j}^\beta = 0. \tag{13}$$

2.2. *The plane model and constitutive relations*

In this section, we only discuss face-centered-cubic crystals. The conclusions can be extended to body-centered-cubic crystals.

Assume that a crystal is undergoing conjugate double slip in the slip system $(111)\,[\bar{1}01]$ and $(\bar{1}\bar{1}1)\,[011]$. Establish coordinates in the following way. Let axis y be the intersection of the two slip planes, z is normal to y and makes an equal angle with the two planes, and x is added to form a right-handed coordinate system. Then, when one observes in the y direction, the conjugate double slip is symmetric in the x–z plane, with the projections of the two slip line intersecting the z-axis at an equal angle of about $35^\circ 16'$. Asaro (1979) pointed out that conjugate double slip in three dimensions could be approximated by a plane model in the x–z plane, and he used this model to analyze the shear bands in specimens of conjugate double slip successfully. Recently, Iwakuma and Nemat-Nasser (1984) used the same model in polycrystalline plasticity calculations. Here, we will use this approximation to provide the constitutive equations for our analysis.

The constitutive equations for the conjugate double slip. In our model, crystal in the shear band is undergoing conjugate double slip. As is shown in Fig. 1, we have the following relations for the case:

$$\mathbf{m}^1 = \begin{pmatrix} -\cos\phi \\ \sin\phi \end{pmatrix} \quad \mathbf{s}^1 = \begin{pmatrix} \sin\phi \\ \cos\phi \end{pmatrix}$$

$$\mathbf{m}^2 = \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix} \quad \mathbf{s}^2 = \begin{pmatrix} -\sin\phi \\ \cos\phi \end{pmatrix}.$$

The specimen is assumed to be loaded uniformly by tensile or compressive force σ per unit area, as shown in Fig. 3, so,

$$\boldsymbol{\sigma} = \begin{pmatrix} 0 & 0 \\ 0 & \sigma \end{pmatrix}$$

After some manipulation, using the formulas in Section 2.1, we get,

$$\overset{\vee}{\sigma}_{22} - \overset{\vee}{\sigma}_{11} = \frac{2G(h+h_1)}{(h+h_1)+2G\sin^2 2\phi}(D_{22}-D_{11}) \tag{14}$$

$$\overset{\vee}{\sigma}_{12} = \frac{2G[(h-h_1)+\sigma\cos 2\phi]}{(h-h_1)+2G\cos^2 2\phi}. \tag{15}$$

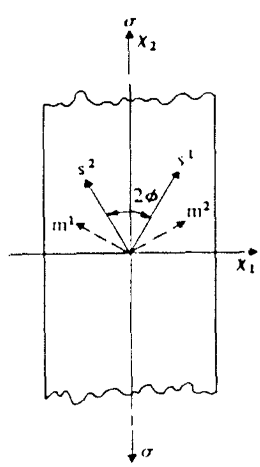

Fig. 1. Conjugate double slip.

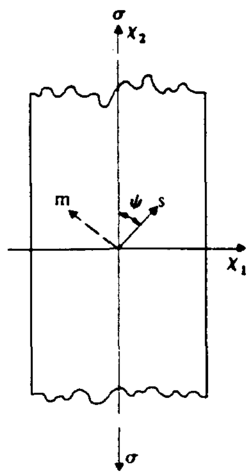

Fig. 2. Single slip.

In obtaining the above formulae, the isotropy and incompressibility of the crystal have been assumed, and $h_{11} = h_{22} = h$, $h_{12} = h_{21} = h_1$.

The constitutive equations for single slip. The crystals outside of the shear band are undergoing single slip in the primary system, whose projection on the x–z plane is shown in Fig. 2. The single slip is also discussed in terms of a plane model. It is easy to obtain:

$$\mathbf{m} = \begin{pmatrix} -\cos\psi \\ \sin\psi \end{pmatrix}, \quad \mathbf{s} = \begin{pmatrix} \sin\psi \\ \cos\psi \end{pmatrix}.$$

Following the same procedure as for the conjugate double slip, and with the same loading as there, we have,

$$\overset{\triangledown}{\sigma}_{16} = 2GD_{11} + G\sin 2\psi\, j \tag{16}$$

$$\overset{\triangledown}{\sigma}_{22} = 2GD_{22} - G\sin 2\psi\, j \tag{17}$$

$$\overset{\triangledown}{\sigma}_{12} = 2GD_{12} - (\sigma/2 - G\cos 2\psi)\, j \tag{18}$$

$$j = \frac{G}{G+h^*}[\sin 2\psi \cdot (D_{22} - D_{11}) - 2\cos 2\psi D_{12}] \tag{19}$$

where h^* is the hardening parameter for the single slip.

3. CONDITIONS FOR THE FORMATION OF SHEAR BANDS

There are numerous works about the formation of shear bands, but most of them were concentrating on cases where material properties are the same both inside and outside the band (Rice, 1977). Since we assume different slips inside and outside the band in our model, we intend to make another deduction here. For simplicity, we adopt the assumption of incompressibility and follow the scheme of Hill and Hutchinson (1974).

We emphasize that our model of a shear band, assuming conjugate double slip inside the band and single slip outside, is only the case where imperfections resist in a homogeneous specimen. To solve a problem like this, the conventional procedure is to follow deformation history, the so-called M–K method (Marciniak and Kuczynski, 1967). Our approach is

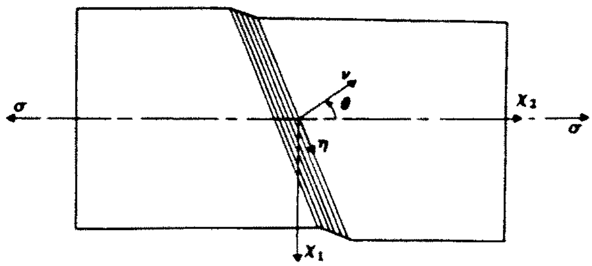

Fig. 3. Shear band.

different in that we first analyze the formation of a shear band in the imperfect layers and then seek the compatibility conditions which define the deformations outside.

Figure 3 shows the shear band formed in a slab loaded by stress σ. Let $\boldsymbol{\eta}$ be the direction of shear band, and $\boldsymbol{\nu}$ the normal to it. According to Hill (1961), there are discontinuities in velocity fields when crossing the band. Denote the velocity of the homogeneous deformation outside of the band by $\overset{(1)}{\mathbf{v}}$, and that of inside $\overset{(2)}{\mathbf{v}}$.

$$\overset{(2)}{v}_\beta = \eta_\beta f(\nu_\gamma \chi_\gamma) + \overset{(1)}{v}_\beta \tag{20}$$

$$\overset{(2)}{v}_{\beta,\alpha} = \eta_\beta \nu_\alpha f(\nu_\gamma \chi_\gamma) + \overset{(1)}{v}_{\beta,\alpha}. \tag{21}$$

The incompressibility of the material demands,

$$\overset{(2)}{v}_{\beta,\beta} = \eta_\beta \nu_\beta f + \overset{(1)}{v}_{\beta,\beta} = \eta_\beta \nu_\beta f = 0 \Rightarrow (\eta_1, \eta_2) = (-\nu_2, \nu_1) \tag{22}$$

so, $\boldsymbol{\eta}$ and $\boldsymbol{\nu}$ are orthogonal.

Use $\gamma = 1, 2$ over a quantity to note that the quantity is one outside or inside the shear band, respectively, and $\mathbf{n}$ to denote the first Piola–Kirchhoff stress. The constitutive equations are then

$$\overset{(\gamma)}{\dot{n}}_{\alpha\beta} = \overset{(\gamma)}{c}_{\alpha\beta\lambda\mu} \overset{(\gamma)}{v}_{\mu,\lambda} + \overset{(\gamma)}{\dot{g}} \delta_{\alpha\beta}, \tag{23}$$

where $\overset{(\gamma)}{c}_{\alpha\beta\lambda\mu}$ is the current material modulus including both elastic and plastic parts, and $\overset{(\gamma)}{g}$ is the hydrostatic compression.

The equilibrium across the shear band demands (Rice, 1977),

$$\nu_\gamma \dot{n}_{\alpha\gamma,\alpha} = 0 \Rightarrow \nu_\gamma \overset{(1)}{\dot{n}}_{\alpha\gamma} = \nu_\gamma \overset{(2)}{\dot{n}}_{\alpha\gamma}. \tag{24}$$

By combining (21), (23) and (24), we get,

$$\nu_\gamma \eta_\mu \nu_\lambda \overset{(2)}{c}_{\alpha\gamma\lambda\mu} f = \nu_\gamma [\overset{(2)}{c}_{\alpha\gamma\lambda\mu} - \overset{(1)}{v}_{\alpha\gamma\lambda\mu}] \overset{(1)}{v}_{\mu,\lambda} + \nu_\gamma (\overset{(2)}{\dot{g}} - \overset{(1)}{\dot{g}}) \delta_{\alpha\gamma}. \tag{25}$$

When the above equation is multiplied on both sides by η_α, and summed over α, it yields, by way of the orthogonal condition (22),

$$\eta_\alpha \nu_\gamma \eta_\mu \nu_\lambda \overset{(2)}{c}_{\alpha\gamma\lambda\mu} f = \nu_\gamma \eta_\alpha [\overset{(2)}{c}_{\alpha\gamma\lambda\mu} - \overset{(1)}{c}_{\alpha\gamma\lambda\mu}] \overset{(1)}{v}_{\mu,\lambda}. \tag{26}$$

It may be observed that the equilibrium equation (24) is satisfied everywhere in the specimen. For a specific section within the shear band, the constitutive relations for the two sides of the section are the same by assumption, so, $\overset{(1)}{\mathbf{c}}$ and $\overset{(2)}{\mathbf{c}}$ in the brackets of (26) are the same for the case, and (26) leads to

$$\overset{(2)}{c}_{\alpha\gamma\lambda\mu}\eta_\alpha v_\gamma \eta_\lambda v_\mu = 0. \tag{27}$$

This is the formation condition of a shear band. Substituting it back into (26), and considering the two sides of the section which separate the shear band from the outside homogeneous deformation, we get the compatibility condition,

$$v_\gamma \eta_\alpha [\overset{(2)}{c}_{\alpha\gamma\lambda\mu} - \overset{(1)}{c}_{\alpha\gamma\lambda\mu}]\overset{(1)}{v}_{\lambda,\mu} = 0 \tag{28}$$

which defines the critical deformation outside of the shear band when the shear band begins to appear.

4. SHEAR BANDS IN RIGID-PLASTIC CRYSTALS

For the purpose of giving some approximate numerical results, a specimen of rigid-plastic crystals is now calculated, using formulae from the two sections above.

Since it is assumed that the specimen undergoes conjugate double slip inside the band and single slip outside, we need both constitutive relations discussed in Section 2.2. The constitutive relation of the conjugate double slip in the rigid-plastic case may be obtained directly by letting G in (14) and (15) approach infinity,

$$\overset{\vee}{\sigma}_{22} - \overset{\vee}{\sigma}_{11} = 2\mu^*(D_{22} - D_{11}) \tag{29}$$

$$\overset{\vee}{\sigma}_{12} = 2\mu D_{12} \tag{30}$$

$$D_{11} + D_{22} = 0 \tag{31}$$

where,

$$2\mu = \frac{h - h_1 + \sigma\cos 2\phi}{\cos^2 2\phi}; \quad 2\mu^* = \frac{h + h_1}{\sin^2 2\phi}.$$

Since letting $G \to \infty$ in formulae (16)-(19) can only lead to

$$D_{11} = -\tfrac{1}{2}\sin 2\psi j \tag{32}$$

$$D_{22} = -D_{11} \tag{33}$$

$$D_{12} = -\tfrac{1}{2}\cos 2\psi j, \tag{34}$$

to have the constitutive relations for the single slip in the rigid-plastic case, another relation between $\overset{\vee}{\sigma}_{\alpha\beta}$ and j must be supplied. This is obtained by eliminating G from the formulae of (16)-(19),

$$j = \frac{1}{2}\,\frac{(\overset{\vee}{\sigma}_{22} - \overset{\vee}{\sigma}_{11})\sin 2\psi - 2\overset{\vee}{\sigma}_{12}\cos 2\psi}{h^* + (\sigma/2)\cos 2\psi}. \tag{35}$$

Actually, for the special case we now discuss, the constitutive relation outside the shear band could also be expressed in the neat form as in (29)-(31). For this purpose, the boundary conditions are used. They are,

$$\dot{n}_{11} = \dot{n}_{12} = \dot{n}_{21} = 0$$

as can easily be read from Fig. 3. By using the formulae (40)–(43) introduced later, we can get the following expressions of the boundary conditions above when the reference configuration is chosen to coincide with the current one so that $\sigma_{\alpha\beta} = n_{\alpha\beta}$.

$$\overset{\nabla}{\sigma}_{11} = 0, \quad \overset{\nabla}{\sigma}_{12} = \overset{\nabla}{\sigma}_{21} = \sigma D_{12}. \tag{36}$$

Since the deformation outside the shear band is homogeneous, eqns (36) will be satisfied everywhere outside the shear band. The constitutive relation for single slip can thus be arranged in the form,

$$\overset{\nabla}{\sigma}_{22} - \overset{\nabla}{\sigma}_{11} = 2\delta^*(D_{22} - D_{11}) \tag{37}$$

$$\overset{\nabla}{\sigma}_{12} = 2\delta D_{12} \tag{38}$$

$$D_{11} + D_{22} = 0, \tag{39}$$

by combining formulae from (32)–(36). In the equations above,

$$2\delta = \sigma, \quad 2\delta^* = \frac{2[h^* + (\sigma/2)\cos 2\psi]}{\sin^2 2\psi} - \sigma \operatorname{ctg}^2 2\psi.$$

For the realization of the formation condition (27) and the compatibility condition (28), the following relations are needed (Hill and Hutchinson, 1974),

$$\dot{n}_{11} = \overset{\nabla}{\sigma}_{11} - \sigma_{11} D_{11}; \qquad \dot{n}_{12} = \overset{\nabla}{\sigma}_{12} - \sigma_{22} D_{12} - \sigma_{11}\Omega_{12}$$

$$\dot{n}_{22} = \overset{\nabla}{\sigma}_{22} - \sigma_{22} D_{22}; \qquad \dot{n}_{21} = \dot{\sigma}_{12} - \sigma_{11} D_{12} - \sigma_{22}\Omega_{21}. \tag{40)–(43}$$

By these relations, the constitutive relations listed above, and by the orthogonal condition (22), the formation condition (27) and the compatibility condition (28) could be expressed in the form,

$$[\mu - \tfrac{1}{2}\sigma]v_1^4 + 2(2\mu^* - \mu)v_1^2 v_2^2 + [\mu + \tfrac{1}{2}\sigma]v_2^4 = 0 \tag{44}$$

$$2v_1 v_2[2\mu^* - 2\delta^*] - (v_1^2 - v_2^2)(2\mu - 2\delta)\operatorname{ctg} 2\psi = 0. \tag{45}$$

(44) as an equation of $(v_2/v_1) = \operatorname{ctg}\theta$ could be solved. Here θ is the angle between the normal to shear band and the x_2 axis, as denoted in Fig. 3. The result is,

$$\operatorname{ctg}^2\theta = (v_2/v_1)^2 = \frac{\mu - 2\mu^* \pm (1/2)\cdot\sqrt{16\mu^*(\mu^* - \mu) + \sigma^2}}{\mu + \sigma/2}. \tag{46}$$

If the inequality $\mu > 2\mu^?$ is assumed, the condition that $(v_2 v_1)$ has real roots leads to

$$(h/\sigma) \leqslant \left[\frac{\cos 2\phi + \sin 4\phi/\sqrt{1+q}}{2(q + \cos 4\phi)}\right]\sin^2 2\phi \tag{47}$$

where $q = h_1/h$.

As for the inequality $\mu > 2\mu^*$ itself, and other cases not discussed, a detailed discussion can be found in Asaro (1979).

Table 1. Critical (h/σ) and θ ($\phi = 35°$, ctg $\theta > 0$)

q	0	1	2
$(h/\sigma)_{crit}$	0.065	0.039	0.0285
θ	49°22′	50°07′	50°58′

Table 2. Critical h^*/σ for shear bands

q	ψ 40.00°	42.50°	45.00°	47.50°	50.00°
0	−0.0035	0.0132	0.0368	0.0674	0.1050
1	0.0008	0.0191	0.0442	0.0761	0.1150
2	0.0055	0.0237	0.0484	0.0800	0.1185

Since h/σ is a decreasing function of σ, the maximum of (h/σ) satisfying (47) is the one when equality is established. On the other hand, shear band formation becomes possible only when the relation (47) is satisfied. So the critical (h/σ), $(h/\sigma)_{crit}$, is obtained by establishing the equality in (47). By substituting $(h/\sigma)_{crit}$ back into (46), θ can be obtained.

Table 1 gives the $(h/\sigma)_{crit}$ and θ for several qs. They are obtained by taking the positive root in (46) for ctg θ, and taking $\phi = 35°$ for the f.c.c. crystals.

Now that $(h/\sigma)_{crit}$ and θ are known, the compatibility condition (45) will be used to define the field outside. For the usual "soft" region of "easy glide" within the stereographic triangle (Honeycombe, 1984), ψ ranges from 54° to 35° in the plane model. By taking suitable ψs, (45) leads to the (h^*/σ) when shear bands possibly appear. Some of the results of the calculation are listed in Table 2. We note that $(h^*/\sigma)_{crit}$ is the actual critical quantity which is measured in the experiment.

It is clear from Tables 1 and 2 that shear bands can form in the hardening range of crystal. The directions of the shear bands listed are almost orthogonal to the slip direction. These shear bands are kink bands.

For cases where ctg $\theta < 0$, i.e. when the minus root in (46) is taken, we could obtain shear bands by the same procedure. But now the directions of shear bands are nearly parallel to the slip direction of the specimen, corresponding to coarse slip bands.

5. DISCUSSION

In the present paper we suggest that the shear bands of single crystals undergoing single slip are due to the existence of layers of multiple slip. Layers of conjugate double slip, which are common after some deformation history, can lead to kink bands.

Multiple slip actually is unavoidable in single crystals arranged for single slip, especially after the crystals have had some history of deformation. Their appearance may be due to the possible distortion of the specimen prepared for test, or be induced by the test. As is well known, even well-annealed crystals contain a network of dislocations that every slip plane will be threaded by dislocations and a dislocation moving in the plane will have to intersect the dislocations crossing the slip plane, so-called forest dislocations (Hull and Bacon, 1984). So, when a dislocation moving on the primary slip plane is trapped by the forest dislocations, following dislocations on the same plane will pile-up. These pile-up dislocations could introduce stress fields to trigger slips on other planes, even though the resolved stresses on those slip systems are not critical. So, multiple slip could be a common feature of an experiment of this kind, as Honeycombe (1952) found. We emphasize here that the layers of conjugate double slip which the present paper concentrates on, are particularly easy to be induced by test. Since the crystal lattice is rotating during the test towards a position where conjugate double slip is favored, if the speeds of the layers of the specimen are not the same in going to this position for one reason or another, those which rotate in larger angles and are more severely influenced by the stress fields of the dislocation pile-ups mentioned above, will supply places for kink bands to develop, as hypothesized earlier in the paper. This may be the reason why kink bands are frequently observed in crystals undergoing single slip. The reasoning here is supported by the experimental findings that crystal rotations are more pronounced in kink bands than in the rest of the specimen (Honeycombe, 1952).

Our hypothesis that kink band is possibly caused by multiple slip, particularly conjugate double slip, could account for some common features of kink bands found in experiments. First, we note that shear bands are localizations of deformation, and they appear in those parts of the specimen which are weaker in shear stiffness than the rest of the specimen. If the specimen is undergoing single slip, and there are layers of conjugate double slip, these layers constitute layers of weaker shear stiffness, and kink bands develop. But when the whole specimen is undergoing conjugate double slip, the layers of weaker shear stiffness are no longer the layers of conjugate double slip itself, so kink band will not develop in this case. Shear bands developed in the specimen of conjugate double slip are of other kinds, as discussed by Asaro (1979). Again, pile-up dislocations which trigger multiple slip are easier to break through forest dislocations by cross slip at high temperatures, so, the chances for multiple slip are less and kink bands are sparser at higher temperatures.

Nevertheless our analysis in this paper is rather speculative, and the calculations are rough in several aspects. The plane model adopted reduces an inherent three-dimensional problem to a plane one. This will possibly introduce large errors, especially in the part of the specimen outside of shear band, where deformation by single slip does not possess the neat symmetry of the deformation by conjugate double slip, as is inside the shear band. Also conjugate double slip may occur, under the stress field of pile-up dislocations, well before the crystal rotates to the [001]–[$\bar{1}$11] boundary. If this happens, there should be an angle between the orthogonal symmetry axes of the conjugate double slip and the loading axis. Our calculation does not include this case. So, further experiments or numerical calculations are needed to have a clearer view of the problem. But the rough rigid–plastic calculation of Section 4 gives results which still compare with experimental conclusions positively. This gives us some confidence.

Our analysis also bears the limitation in that shear band possibly appears in purely single slip crystals. But in this case it will probably appear in minus or zero hardening range, or caused by non-Schmid effects as Asaro and Rice (1977) suggested.

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