Active Slip Band Separation and the Energetics of Slip in Single Crystals

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Abstract

This research supports recent efforts to provide an energetic approach to the prediction of stress-strain relations for single crystals and to give precise formulations of experimentally observed connections between hardening of single crystals and separation of active slip bands. Non–classical, structured deformations in the form of two-level shears permit the formulation of new measures of the active slip-band separation and of the number of lattice cells traversed during slip. A formula is obtained for the Helmholtz free energy per unit volume as a function of the shear without slip, the shear due to slip, and the relative separation of active slip bands in a single crystal.

Key Words: Crystal plasticity, slip bands, energy methods

Shortened title: Active Slip Band Separation in Crystals

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I Experimental Background

The connection between the behavior of single crystals at small length scales and the macroscopic response of a crystal has been the subject of a multitude of experimental studies. Here, we briefly collect experimental evidence that points to a connection between hardening behavior of single crystals and changes in the separation of active slip bands. Although the relation between the structure and separation of both slip bands and of slip lines, on the one hand, and the strain hardening of crystals, on the other hand, is today not well understood (Kubin, 1993, pp. 145-146), the existence of such a relation was already well established by the year 1950 (Hill, 1950, p. 6). Experimental evidence is cited in Barrett (1952), p. 349 for two basic phenomena: (i) in crystals that deform without appreciable hardening, such as lead, cadmium, and mercury, further deformation due to slip continues on existing slip lines, and (ii) in crystals that deform with appreciable hardening, such as aluminium, further deformation due to slip entails the formation of new slip lines (Crussard, 1945, p. 291; Brown, 1952, p. 468). Moreover, in aluminium crystals, a significant number of active slip lines become inactive as deformation progresses (Crussard, 1945, p. 290). In spite of the fact that the average separation of *all* slip lines, i.e., active and inactive together, decreases with deformation in aluminium crystals (Crussard, 1945, p. 291), there is evidence that the separation of *active* slip bands increases with deformation in the f.c.c. alloy Cu_3Au (Salama, *et al*, 1971, p. 402).

The reader will notice that the experimental evidence cited above pertains in part to the distribution of slip lines and in part to the distribution of slip bands. Although some authors carefully maintain a distinction between slip lines and slip bands (Neuhäuser, 1983, p. 323), others appear to use these terms interchangeably. In this paper, we will model *active slip bands* as surfaces in the crystal between which deformation procedes smoothly and across which tangential discontinuities in displacement occur. This conception of active slip bands agrees with the descriptions in Hill, (1950), p. 6, and in Brown, (1952), pp. 434, 436.

II Geometrical measures of slip-band separation and of slip

The geometrical framework that we employ here consists of a specific class of non-classical, structured deformations (Del Piero & Owen, 1993) called "two-level shears" (Choksi, *et al*, 1998). A two-level shear is specified by giving two real numbers μ and γ, along with the following two mappings g and G :

$$\begin{aligned} g(x,y,z) \ &: \ = (x+\mu y, y, z) \\ G(x,y,z) \ &: \ = \begin{pmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{1}$$

The mapping g, called the transplacement for the two-level shear, is a simple shear of the crystal relative to a suitably chosen cartesian coordinate system, and the mapping G, called the deformation without slip, describes the deformation away from slip bands in the crystal. The Approximation Theorem

(Del Piero & Owen, 1993) and the integral-gradient formula for structured deformations (Del Piero & Owen, 1995) imply that there exists a sequence $n \mapsto f_n$ of piecewise smooth mappings such that

$$g(x,y,z) = \lim_{n\to\infty} f_n(x,y,z) \tag{2}$$

$$G(x,y,z) = \lim_{r\to 0}\lim_{n\to\infty} (vol\,\mathcal{B}(x,y,z;r))^{-1} \int\limits_{\mathcal{B}(x,y,z;r)} \nabla f_n \, dV \tag{3}$$

and

$$M(x,y,z) = \lim_{r\to 0}\lim_{n\to\infty} (vol\,\mathcal{B}(x,y,z;r))^{-1} \int\limits_{\Gamma(f_n)\cap\mathcal{B}(x,y,z;r)} [f_n]\otimes\nu \, dA, \tag{4}$$

where

$$M(x,y,z) := \nabla g(x,y,z) - G(x,y,z) = \begin{pmatrix} 0 & \mu-\gamma & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{5}$$

In eqns (3) and (4), $\mathcal{B}(x,y,z;r)$ is the ball of radius r centered at (x,y,z), ∇f_n is the usual gradient computed away from any discontinuities of f_n, $[f_n]$ is the jump in the mapping f_n, $\Gamma(f_n)$ is the set of surfaces on which f_n is discontinuous, and ν is the unit normal to $\Gamma(f_n)$. Thus, $G(x,y,z)$ represents a volume average of deformation gradients computed away from jump sites, and $M(x,y,z) = \nabla g(x,y,z) - G(x,y,z)$ measures jumps in deformation per unit volume. The sequence $n \mapsto f_n$ is called a determining sequence for the given two-level shear. The specific example of a determining sequence given in Choksi, *et al*, (1998), eqn 21, shows that $\Gamma(f_n)$ can be taken to be a family of planes, each with normal ν in the y direction, $[f_n]$ can be taken in the

x-direction, and ∇f_n has the same form as G:

$$\nabla f_n = \begin{pmatrix} 1 & (\nabla f_n)_{xy} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{6}$$

We interpret each plane in the family $\Gamma(f_n)$ as an individual, active slip band in the crystal and each tangential jump $[f_n]$ as the slip experienced by the crystal across that slip band. This interpretation and eqns (1), (3)-(5) permit us to call the number γ the *shear without slip* and the number $\mu-\gamma$ the *shear due to slip.* Moreover, we may view each piecewise smooth mapping f_n as a mesolevel view of smooth lattice deformations and discontinuous slips associated with the two-level shear.

We consider henceforth only determining sequences $n \mapsto f_n$ such that $\Gamma(f_n)$ can be taken to be a family of planes, each with normal ν in the y direction, and $[f_n]$ points in the x-direction. For these determining sequences, eqn (5) can be written in the scalar form

$$\mu - \gamma = \lim_{r \to 0} \lim_{n \to \infty} \; s_n(x, y, z; r), \tag{7}$$

where the dimensionless quantity

$$s_n(x, y, z; r) := (vol\, \mathcal{B}(x, y, z; r))^{-1} \int\limits_{\Gamma(f_n) \cap \mathcal{B}(x,y,z;r)} [f_n]_x \, dA \tag{8}$$

is the *amount of tangential jump per unit volume* within the ball $\mathcal{B}(x, y, z; r)$ and where $[f_n]_x$ is the x-component of the jump $[f_n]$. Because the numbers μ and γ are part of the specification of the two-level shear, the limit $\lim\limits_{r \to 0} \lim\limits_{n \to \infty} \; s_n(x, y, z; r)$ is independent of the choice of determining sequence for the given two-level shear, even though each term $s_n(x, y, z; r)$ need not be.

Analogues for the shear without slip γ of eqns (7) and (8) are obtained from eqns (3) and (6):

$$\gamma = \lim_{r\to 0}\lim_{n\to\infty} \gamma_n(x, y, z; r), \tag{9}$$

where the dimensionless quantity

$$\gamma_n(x, y, z; r) := (vol\,\mathcal{B}(x, y, z; r))^{-1} \int\limits_{\mathcal{B}(x,y,z;r)} (\nabla f_n)_{xy}\, dV \tag{10}$$

is the average lattice shear within the ball $\mathcal{B}(x, y, z; r)$. Again, the limit $\gamma = \lim\limits_{r\to 0}\lim\limits_{n\to\infty} \gamma_n(x, y, z; r)$ is independent of the choice of determining sequence, whereas each term $\gamma_n(x, y, z; r)$ need not be.

It is useful to specify for each index n a level of magnification in terms of which we may view the deformation f_n for various determining sequences. We employ as a measure of this magnification a positive number c_n, the *cell-size of the crystal lattice* in the level of magnification for the index n.

We now fix our attention not only on a given two-level shear but also on a given sequence $n \mapsto c_n$. For each determining sequence $n \mapsto f_n$ we define a sequence $(r, n) \mapsto d_n(x, y, z; r)$ of positive numbers through the formula

$$d_n(x, y, z; r) := \frac{1}{c_n}\frac{vol\,\mathcal{B}(x, y, z; r)}{area(\Gamma(f_n) \cap \mathcal{B}(x, y, z; r))}. \tag{11}$$

The second fraction in the right-hand side of this formula is the ratio of the volume of the given ball to the total area of active slip bands within that ball and, thus, measures the average separation of active slip bands within the ball. Consequently, the dimensionless number $d_n(x,y,z;r)$ measures the average separation of active slip bands within the ball, relative to the cell-size of the crystal lattice, or, more briefly, the *average relative separation of active slip bands for the index n.* By eqns (11) and (8) we may write

$$\begin{aligned} j_n(x,y,z;r) \quad &: = d_n(x,y,z;r)\, s_n(x,y,z;r) \\ &= \frac{\int\limits_{\Gamma(f_n)\cap\mathcal{B}(x,y,z;r)} ([f_n]_x / c_n) dA}{area(\Gamma(f_n)\cap\mathcal{B}(x,y,z;r))}, \end{aligned} \tag{12}$$

so that the product $j_n(x,y,z;r)$ of the average relative separation of active slip bands within the ball and the tangential jump per unit volume is the average with respect to area of non-dimensional tangential jumps. Because the non-dimensionalization of the jump in eqn (12) is taken with respect to the cell-size of the crystal lattice, $j_n(x,y,z;r)$ may be called the *average (possibly fractional) number of cells spanned by the tangential jumps for the index n* within the given ball.

As we pointed out in eqn (7), the tangential jump per unit volume $s_n(x,y,z;r)$ approaches the shear due to slip $\mu-\gamma$ as $n\to\infty$ and $r\to 0$, no matter what the choice of determining sequence. However, the condition that $n\mapsto f_n$ is a determining sequence for the two-level shear does not, in itself, guarantee that the relative separation of active slip bands $d_n(x,y,z;r)$ has a limit. We now assume that both the the average separation of active slip bands within the ball $\frac{vol\,\mathcal{B}(x,y,z;r)}{area(\Gamma(f_n)\cap\mathcal{B}(x,y,z;r))}$ and the cell-size of the crystal lattice c_n tend to zero in such a way that $d_n(x,y,z;r)$ does have a limit

$d(x, y, z)$, which we call the *relative separation of active slip bands for the given determining sequence.* Eqn (12) now tells us that $j_n(x, y, z; r)$ has the limit $(\mu - \gamma)d(x, y, z)$,

$$\lim_{r \to 0} \lim_{n \to \infty} j_n(x, y, z; r) = (\mu - \gamma)d(x, y, z), \tag{13}$$

so that the product $(\mu - \gamma)d(x, y, z)$ represents an *average (possibly fractional) number of cells spanned by the tangential jumps for the given determining sequence.* Thus, while $\mu - \gamma$ measures the amount of shear due to slip, the product $(\mu - \gamma)d(x, y, z)$ measures the average number of lattice cells traversed during the shear.

III Helmholtz free energy

Our goal in this section is to obtain a formula for the Helmholtz free energy associated with a two-level shear. We follow the idea proposed and analyzed in Choksi & Fonseca (1997) for determining the form of the Helmholtz free energy of arbitrary structured deformations, although the steps in our implementation of this idea differ in significant ways from those in that analysis. We begin with a two-level shear, a sequence $n \mapsto c_n$ of cell-sizes, and sequences $n \mapsto d_n(x, y, z; r)$ and $n \mapsto s_n(x, y, z; r)$ associated with a determining sequence $n \mapsto f_n$ satisfying the assumptions in Section II. For each index n and positive number r we wish to assign a number that measures the Helmholtz free energy per unit volume of the crystal undergoing the piecewise smooth deformation f_n. We assume that this number is a sum of two other numbers, the first being the *free energy density due to lattice distortion*

$\mathcal{H}^d_{n,r}$ and the second being the *free energy density due to tangential jumps across slip bands* $\mathcal{H}^s_{n,r}$. Because $\gamma_n(x,y,z;r)$ given in eqn (10) measures the deformation of the lattice away from slip bands, we assume

$$\mathcal{H}^d_{n,r} = \tilde{\varphi}(\gamma_n(x,y,z;r)) \tag{14}$$

with $\tilde{\varphi}$ a continuous convex constitutive function determined by the slip-free portions of the crystal.

The Helmholtz free energy $\mathcal{H}^s_{n,r}$ per unit volume due to tangential jumps across slip bands should reflect the fact that a single tangential jump of amount $[f_n]_x = kc_n$, with k an integer and c_n the cell-size at magnification n, cannot be detected geometrically and, hence, should not change the free energy. By eqn (12), such a jump gives the value $j_n(x,y,z;r) = k$, i.e., the number of cells spanned by this jump is k, so that $\mathcal{H}^s_{n,r}$ should be unchanged in jumps $j_n(x,y,z;r) = k$. This leads us to assume

$$\mathcal{H}^s_{n,r} = \tilde{\psi}(j_n(x,y,z;r)) \tag{15}$$

where $\tilde{\psi}$ is continuous and periodic of period 1. The assumed oscillatory nature of the constitutive function $\tilde{\psi}$ reflects the tacit physical assumption that mesolevel control of relative tangential lattice displacements across a slip band would result in recoverable work being performed without dissipation. We note, of course, that corresponding control at the macrolevel can result in dissipation (Choksi, *et al* 1998; Deseri & Owen, 1998).

Our assumptions on the determining sequence $n \mapsto f_n$ and the continuity of the constitutive functions $\tilde{\varphi}$ and $\tilde{\psi}$ imply that the sum $\mathcal{H}^d_{n,r} + \mathcal{H}^s_{n,r}$ of the volume densities of free energy due to lattice distortion and due to tangential jumps across slip bands has a limit as n tends to infinity and as r tends to zero :

$$\begin{aligned}
\mathcal{H}(x,y,z) \quad : &= \lim_{r\to 0}\lim_{n\to\infty}(\mathcal{H}^d_{n,r}+\mathcal{H}^s_{n,r}) \\
&= \tilde{\varphi}(\lim_{r\to 0}\lim_{n\to\infty}\gamma_n(x,y,z;r))+\tilde{\psi}(\lim_{r\to 0}\lim_{n\to\infty}j_n(x,y,z;r)) \\
&= \tilde{\varphi}(\gamma)+\tilde{\psi}\left((\mu-\gamma)d(x,y,z)\right). \qquad (16)
\end{aligned}$$

The number $\mathcal{H}(x,y,z)$ is the *Helmholtz free energy per unit volume at the point* (x,y,z), and this relation tells us that the $\mathcal{H}(x,y,z)$ is determined by the shear without slip γ, the shear due to slip $\mu-\gamma$, and the relative separation of active slip bands $d(x,y,z)$.

We emphasize that γ and $\mu-\gamma$ depend only on the given two-level shear, whereas $d(x,y,z)$ depends also on the given determining sequence $n\mapsto f_n$ for the two-level shear, so that eqn (16) tells us that the free energy density need not be determined by the two-level shear alone. In spite of the general lack of experimental observations on the separation of active slip bands in single crystals, the reference Salama, *et al*, (1971) cited in Section I suggests that relative separation $d_n(x,y,z;r)$ may be regarded in a particular crystal as an increasing function of the amount of tangential jump per unit volume $s_n(x,y,z;r)$:

$$d_n(x,y,z;r)=\hat{d}\left(s_n(x,y,z;r)\right). \qquad (17)$$

If the constitutive function $\hat{d}$ is continuous, then eqn (7) permits us to pass to the limit in both sides of this relation to obtain

$$d(x,y,z) = \hat{d}(\mu-\gamma), \tag{18}$$

and eqns (16) and (17) yield the following constitutive formula for the free energy density $\mathcal{H}(x,y,z)$:

$$\mathcal{H}(x,y,z) = \tilde{\varphi}(\gamma) + \tilde{\psi}\left((\mu-\gamma)\hat{d}(\mu-\gamma)\right). \tag{19}$$

Of course, this relation tells us not only that the Helmholtz free energy per unit volume is determined by the two-level shear alone, but also that this free energy density is constant throughout a crystal that undergoes the two-level shear. The formula eqn (19), together with the assumption that the derivative of the function $\mu-\gamma \longmapsto (\mu-\gamma)\hat{d}(\mu-\gamma)$ is increasing, is the basis for a model of hardening of single crystals (Deseri & Owen, 1998) that is consistent with observed phenomena such as the Portevin-le Chatelier effect and the existence of a critical resolved shear stress.

Suppose now that a crystal has the property that the separation of active slip bands is independent of deformation. We may then take $\hat{d}$ to be a positive constant d_0, and eqn (19) for $\mathcal{H}(x,y,z)$ becomes

$$\mathcal{H}(x,y,z) = \tilde{\varphi}(\gamma) + \tilde{\psi}\left((\mu-\gamma)d_0\right). \tag{20}$$

In this case, the free energy density due to tangential jumps across slip bands is a periodic function of the shear due to slip $\mu-\gamma$, with period $\frac{1}{d_0}$. According to Hill (1950), d_0 is of the order 10^4 in many crystals, so that the period of the function $\mu-\gamma \longmapsto \tilde{\psi}\left((\mu-\gamma)d_0\right)$ is of the order 10^{-4} (Choksi, *et al*, 1998). Eqn (20) together with smoothness assumptions on $\tilde{\varphi}$ and on $\tilde{\psi}$ is the basis of a model of the response of single crystals (Choksi, *et al*, 1998) that is consistent with the observed yielding, hysteresis, and dissipation in crystals that do not appreciably harden.

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