

## AN ANALYTIC SOLUTION FOR ONE-DIMENSIONAL DISSIPATIONAL STRAIN-GRADIENT PLASTICITY

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### Abstract

An analytic solution is developed for the one-dimensional dissipational slip gradient equation first described by Gurtin [“On the plasticity of single crystals: free energy, microforces, plastic strain-gradients”, *J. Mech. Phys. Solids* **48** (2000) 989–1036] and then investigated numerically by Anand *et al.* [“A one-dimensional theory of strain-gradient plasticity: formulation, analysis, numerical results”, *J. Mech. Phys. Solids* **53** (2005) 1798–1826]. However we find that the analytic solution is incompatible with the zero-sliprate boundary condition (“clamped boundary condition”) postulated by these authors, and is in fact excluded by the theory. As a consequence the analytic solution agrees with the numerical results except near the boundary. The equation also admits a series of higher mode solutions where the numerical result corresponds to (a particular case of) the fundamental mode. Anand *et al.* also established that the one-dimensional dissipational gradients strengthen the material, but this proposition only holds if zero-sliprate boundary conditions can be imposed, which we have shown cannot be done. Hence the possibility remains open that dissipational gradient weakening may also occur.

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### 1. Introduction

In standard plasticity theories, including gradient plasticity with energetic hardening, the (initial) yield strength is specified as a material parameter. In contrast, for dissipational gradient theories (Gurtin *et al.* [3]) the yield level must be obtained as part of the solution. This has been regarded as a difficult problem, and the general approach has been to treat the elastoplastic problem as the limit of a viscoplastic one.

One purpose of this paper is to show that in some cases an analytic solution may be obtained to the dissipational slip gradient problem. We demonstrate this for a one-dimensional model proposed by Anand *et al.* [1] which represents the grain as

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a one-dimensional strip of length  $h$ . A concise derivation of the equation is given in [Appendix A](#). For the purely dissipational problem a complete analytic solution is derived for displacement and slip at any level of applied shear strain (Sections 2 and 3). If energetic and/or isotropic hardening is included then a solution may be obtained by combining the results obtained here for initial yield with a complementary numerical procedure.

As part of the solution process we show that the dissipational yield strength can be computed analytically (through a single integration) as a function of the dimensionless parameter  $a = h/2l$  ( $h$  is the grain size and  $l$  is the dissipational length scale) and boundary data, here represented as a boundary slip gradient angle  $\theta_0$  (Section 3). The yield strength can in fact be interpreted as an eigenvalue for the dissipational gradient equation.

The specification of appropriate boundary conditions for the dissipational gradient problem is of particular interest. Since the analytic solution developed here is a general one, it includes all possible boundary constraints. However Gurtin and others have proposed the concept of *microscopically hard* or *clamped* boundaries where the sliprate is constrained to be zero. In Section 2 we show that the one-dimensional dissipational gradient equation is not compatible with microscopically hard boundary conditions. This has consequences for the dissipation functional introduced by Anand *et al.* [1], and is discussed in Section 4.

Further clarification of this point is made in Section 5 where the analytic solution is compared with plots of the numerical results given by Anand *et al.* [1] assuming a hard boundary constraint. Good quantitative agreement is obtained except near the boundaries where the numerical results can be interpreted as approximating a boundary discontinuity.

The main argument in this paper concerns the *fundamental solution* of the one-dimensional dissipational gradient equation which has also been identified numerically. However the equation also admits higher mode solutions as pointed out in Section 3 with examples presented in Section 6. In Section 7 we discuss the extension of the one-dimensional results to two and three dimensions.

Further discussion in the Conclusions (Section 8) hypothesizes that the dissipational gradient mechanism is intimately connected with slip discontinuities which must occur at the interface between the grain and the grain boundary.

## 2. Solution of the dissipational gradient equation

We first restrict the model to be purely dissipational with no isotropic or energetic hardening (later this restriction will be relaxed). The flow equation for the one-dimensional model is then (see [Appendix A](#))

$$\tilde{\tau} = g \frac{v}{d_p} - l^2 \frac{d}{d\tilde{x}} \left( \frac{g}{d_p} \frac{dv}{d\tilde{x}} \right) \quad (2.1)$$

where  $\tilde{\tau}$  is the (spatially constant) Schmid stress,  $v = \dot{\varepsilon}$  is the sliprate,  $g$  is the coarse-grain yield strength, and

$$d_p = \sqrt{v^2 + l^2(v')^2} \quad (2.2)$$

is the generalized plastic strain rate. The quantity  $\tilde{\tau}$  can be thought of as the *yield strength*  $\tilde{\tau}_Y$  of the material. It will be shown that  $\tilde{\tau}_Y$  cannot be assigned arbitrarily, but is obtained as an eigenvalue of the differential equation in terms of material constants and boundary data.

Next scale  $\tilde{\tau}$  by  $g$  and  $\tilde{x}$  by  $l$  and then set  $y = v'/v$ . Here we assume that  $v$  is nonzero in the interior of the domain, but will admit the possibility of  $v = 0$  on the boundary (approached as a limit). We choose the coordinate origin at the midpoint of the strip, so that the scaled  $x$ -coordinate varies from  $-a$  to  $+a$  and  $a = h/2l$ . Then (2.1) can be written

$$y' = (1 + y^2)(1 - \tau(1 + y^2)^{1/2}).$$

Now substitute  $y = \tan \theta$ . Then

$$\theta' = 1 - \tau \sec \theta. \quad (2.3)$$

The sliprate  $v$  can then be obtained as a function of  $\theta$  according to

$$v = A \exp\left(\int \tan \theta \, dx\right) \quad (2.4)$$

where  $A$  is a constant to be determined. From (2.3)

$$\int \tan \theta \, dx = \int \tan \theta \frac{dx}{d\theta} d\theta = \int \frac{\sin \theta \, d\theta}{\cos \theta - \tau}$$

and hence (2.4) integrates to

$$v = \frac{A}{\tau - \cos \theta}. \quad (2.5)$$

Note that, according to (2.5),  $v$  is always nonzero and symmetric about  $\theta = 0$  where it attains a maximum, and if  $\tau > 1$  it is bounded. The gradient  $v' = dv/dx = v \tan \theta$  is zero at  $\theta = 0$  and infinite at the ends of the range  $\theta = \pm\pi/2$ . Note however that the ends of the strip (at  $x = \pm a$ ) do not necessarily coincide with the full range of  $\theta$ .

A complete solution for the sliprate profile  $v(x)$  is then obtained by first identifying the constant of integration  $A$ , followed by integration of (2.3) to obtain  $\theta(x)$ , and finally determination of the yield level  $\tau$ . The two latter tasks will be completed in the next section.

To determine the constant  $A$  we proceed as follows. First note that after plastic onset we have

$$\tilde{\tau} = \mu(u' - \varepsilon), \quad (2.6)$$

where  $\mu$  is the shear modulus,  $u$  is the displacement and  $\varepsilon$  is the slip. We first rescale the variables and then integrate from  $-a$  to  $a$ . Since  $\tilde{\tau}$  is constant,

$$\Gamma_Y = \Gamma - \frac{1}{2a} \int_{-a}^a \varepsilon dx, \quad (2.7)$$

where  $\Gamma_Y = \tilde{\tau}/\mu$  is the strain at yield, and  $\Gamma$  is the current applied strain (which we may think of as a time variable). Since  $\varepsilon = \int_{\Gamma_Y}^{\Gamma} v d\Gamma$  it follows from (2.7) and (2.5) that

$$\Gamma - \Gamma_Y = \int_{\Gamma_Y}^{\Gamma} A d\Gamma \cdot \frac{1}{2a} \int_{-a}^a \frac{dx}{\tau - \cos \theta}$$

which is satisfied with  $A$  constant and given by

$$A^{-1} = \frac{1}{2a} \int_{-a}^a \frac{dx}{\tau - \cos \theta}. \quad (2.8)$$

Then the slip at any loading is determined as

$$\varepsilon = (\Gamma - \Gamma_Y)v. \quad (2.9)$$

### 3. Sliprate profile and yield strength

The integration in (2.3) may be performed with the result (see Gradshteyn and Ryzhik, [2, Sections 2.553 and 2.554])

$$x = \theta - \frac{2\tau}{\sqrt{\tau^2 - 1}} \tan^{-1} \left\{ \sqrt{\frac{\tau + 1}{\tau - 1}} \tan \left( \frac{\theta}{2} \right) \right\} + x_0, \quad (3.1)$$

where we have assumed  $\tau > 1$  that is *yield strengthening*. In the following, for convenience, we restrict  $x$  to be an odd function of  $\theta$ , in which case the constant of integration  $x_0 = 0$ . More general nonsymmetric solutions may be analysed by the methods of this paper. By inversion, (3.1) with  $x_0 = 0$  defines the function  $\theta(x)$  which may then be substituted in (2.4) to give the *sliprate profile*  $v(x)$ .

Now let us assume that  $\theta = \tan^{-1}(v'/v)$  has some specific value  $\theta_0$  on the boundary  $x = a$ . For this orientation of the  $x$ -axis,  $\theta_0$  varies between  $-\pi/2$  and  $+\pi/2$  but the values from 0 to  $+\pi/2$  correspond to negative sliprates and negative  $\tau$ . Since this gives no new information, the range of  $\theta_0$  may be restricted to  $[-\pi/2, 0]$  with possible exclusion of the endpoints. Equation (3.1) yields

$$a = \theta_0 - \frac{2\tau}{\sqrt{\tau^2 - 1}} \tan^{-1} \left\{ \sqrt{\frac{\tau + 1}{\tau - 1}} \tan \left( \frac{\theta_0}{2} \right) \right\}. \quad (3.2)$$

This defines the *yield strength*  $\tau(a, \theta_0)$  in terms of the grain size parameter  $a$  and the boundary data  $\theta_0$ . Graphical considerations suggest that there is a unique yield

strength for each  $(a, \theta_0)$  pair, so that  $\tau(a, \theta_0)$  may be considered as an *eigenvalue* for (2.1) together with its boundary data. More generally  $\theta_0$  may be specified on the interval  $I_n = [-\pi/2, 0] - 2n\pi$  with  $n = 0, 1, 2, \dots$  and this gives rise to a sequence of eigenvalues  $\tau_n = \tau(\theta_{0n}, a)$  where  $\theta_{0n} \in I_n$ . Note however that the modes  $\theta_{0n} = \theta_0 - 2n\pi$  all correspond to the same boundary value of  $(v'/v)_0 = \tan \theta_0$ . Furthermore each boundary mode  $\theta_{0n}$  gives rise to a sliprate profile mode  $v_n = v(x, \theta_{0n}, a)$ . For the moment we restrict attention to the fundamental mode  $n = 0$ . The amplitude (2.8) may then be evaluated:

$$A^{-1} = -\frac{1}{a(\tau^2 - 1)} \left[ \frac{2}{\sqrt{\tau^2 - 1}} \tan^{-1} \left\{ \sqrt{\frac{\tau + 1}{\tau - 1}} \tan \left( \frac{\theta_0}{2} \right) \right\} + \frac{\tau \sin \theta_0}{\tau - \cos \theta_0} \right]. \quad (3.3)$$

Using (3.2) this expression can be simplified to

$$A^{-1} = \frac{1}{a(\tau^2 - 1)} \left[ \frac{a - \theta_0}{\tau} - \frac{\tau \sin \theta_0}{\tau - \cos \theta_0} \right]$$

or

$$A = \frac{a\tau(\tau^2 - 1)(\tau - \cos \theta_0)}{(a - \theta_0)(\tau - \cos \theta_0) - \tau^2 \sin \theta_0}$$

and the value of  $v$  on the boundary is then

$$v_0(a, \theta_0) = \frac{a\tau(\tau^2 - 1)}{(a - \theta_0)(\tau - \cos \theta_0) - \tau^2 \sin \theta_0} \quad (3.4)$$

where  $\tau(a, \theta_0)$  is obtained from (3.2). Finally we note that the scaled displacement  $u = \tilde{u}/g$  may be obtained from (2.6) in the form

$$u(x) = (\Gamma - \Gamma_Y) \frac{A(\theta_0)a}{A(\theta)} + \Gamma_Y x + \Gamma a \quad (3.5)$$

where  $A(\theta)$  is given by (3.3) with  $\theta_0$  replaced by  $\theta$ , and  $\Gamma_Y = \alpha\tau$  where  $\alpha = g/\mu$ . In (3.5)  $\theta$  can be written as a function of  $x$  by inverting (3.1) (with  $x_0 = 0$ ). Note that (3.5) satisfies the displacement boundary conditions  $u(a) = 2a\Gamma$ ,  $u(-a) = 0$ ; and at yield onset  $u(x) = \Gamma_Y(x + a)$ , which is therefore continuous with the elastic displacement prior to yield.

Figure 1 exhibits the relation between boundary sliprate  $v_0$  and boundary gradient angle  $\theta_0 = \tan^{-1}(v'/v)$  for fixed grain size  $a = 1$ . This figure shows that the range of possible boundary sliprates is constrained to a small subset of the half-line with an internal maximum. Furthermore, for some sliprates there are two boundary gradient angles and it is not clear which is physically relevant. In contrast the boundary gradients cover the full range apart from the limit point at  $\theta_0 = -\pi/2$ . When the higher modes are included  $\theta_0$  extends over the entire negative real axis apart from excluded limit points at  $\theta_0 = -\pi/2 - 2n\pi$  (the positive real axis corresponds to a reversal in orientation of the  $x$ -coordinate). For this reason it appears that the one-dimensional

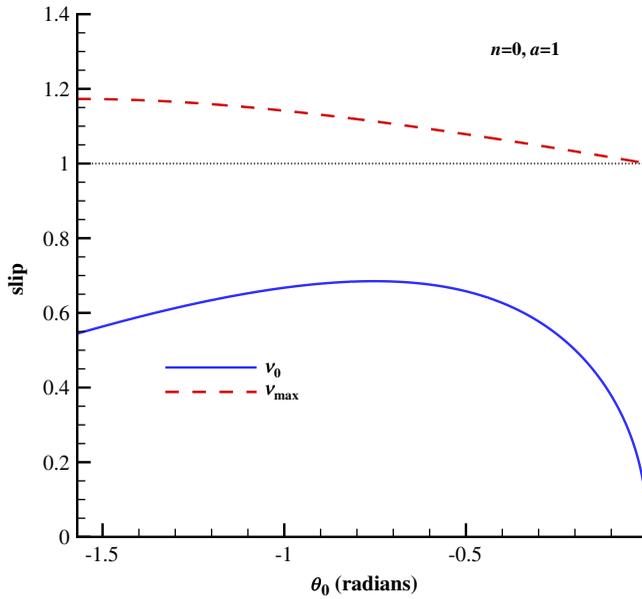


FIGURE 1. Boundary slip and maximum slip against boundary gradient angle for the fundamental mode.

TABLE 1. Asymptotic values.

$\tau$	$a$	$v_{\max}$	$v_0$
1	$\infty$	2	0
$\infty$	0	1	1

dissipational gradient equation is more properly characterized as a type of Neumann boundary problem (for log  $v$ ) rather than as a Dirichlet boundary problem.

The maximum value of  $v$  is at  $\theta = 0$  (see Figure 2) and is given by

$$v_{\max}(a, \theta_0) = \frac{a\tau(\tau + 1)(\tau - \cos \theta_0)}{(a - \theta_0)(\tau - \cos \theta_0) - \tau^2 \sin \theta_0}$$

and is shown in Figure 1 as a function of  $\theta_0$  for  $a = 1$ . As  $\tau \rightarrow 1$  then  $a \rightarrow \infty$  and hence the amplitude  $A \rightarrow 0$ . Conversely as  $\tau \rightarrow \infty$  then  $a \sim -\tau^{-1} \sin \theta_0$  and then  $A \sim \tau$ . The asymptotic values are presented in Table 1. Note that the asymptotic values are all independent of  $\theta_0$ .

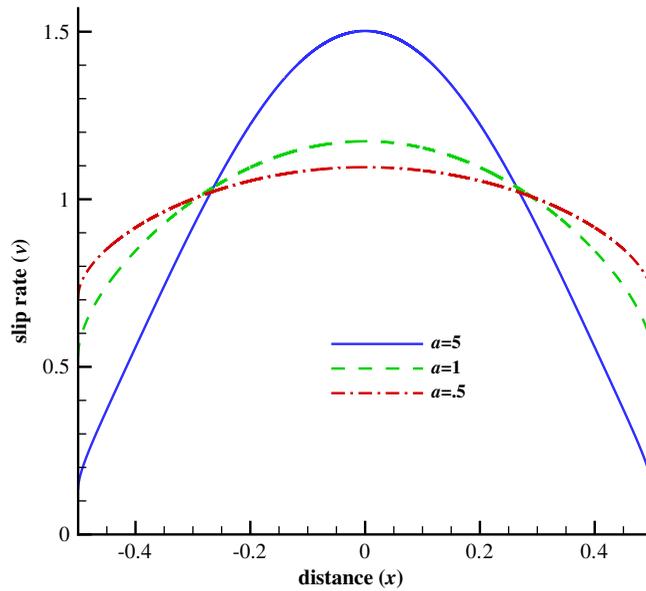


FIGURE 2. Sliprate profiles for several grain sizes. Compare with Figure 3(b) of Anand *et al.* [1].

#### 4. Yield strengthening and weakening

After multiplying (2.1) by  $v$  and integrating over the range of  $x$  we get an expression for the yield stress

$$\tau = \frac{1}{2a} \int_{-a}^a d_p dx - \left. \frac{vv'}{2ad_p} \right|_{-a}^a \tag{4.1}$$

(assuming the normalization  $(1/2a) \int_{-a}^a v dx = 1$  which is implied by (2.8) above).

Anand *et al.* [1] assume that  $v = 0$  on the boundary (“clamped boundary conditions”) and so the second term on the right vanishes. However we have seen that such a boundary condition is incompatible with (2.1). The correct expression in this case is

$$\tau = \frac{1}{2a} \int_{-a}^a d_p dx - \frac{v_0}{a} \sin \theta_0. \tag{4.2}$$

Anand *et al.* [1] use (4.1) without the boundary term to deduce that  $\tau > 1$ , that is, the dissipational gradients *strengthen* the material. However this result cannot be deduced from (4.1) when the boundary term is present (recall that  $\theta_0$  is negative), and it seems possible that *weakening* solutions (with  $\tau < 1$ ) may also be obtainable. For example, if  $\tau < 1$  then (2.5) is unbounded for some value of  $\theta$ , and this may represent rupture, or failure, of the weakening material. However this case must be investigated separately because many expressions used here (for example (3.1)) are only valid when  $\tau > 1$ .

Note that (4.2) also shows that the dissipational yield stress cannot be identified with the dissipation functional (the integral in (4.2)) as proposed by Anand *et al.* [1].

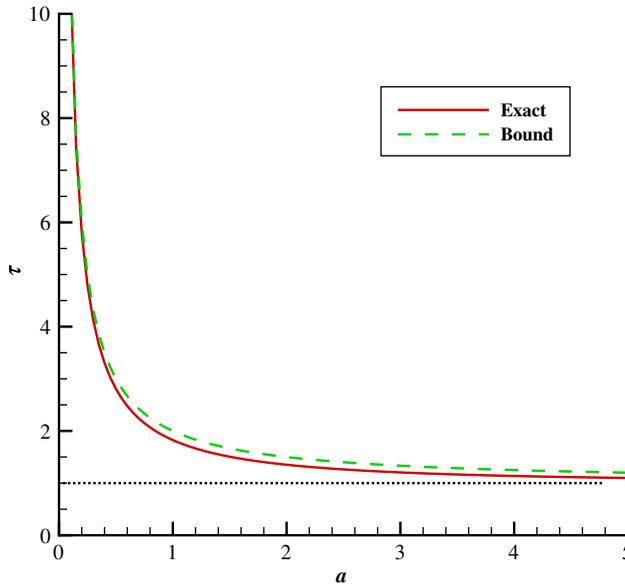


FIGURE 3. Dimensionless yield strength as a function of grain size.

**5. Comparison with numerical results**

If the full range of  $\theta$  extends over the strip then we take  $\theta_0 = -\pi/2$  at  $x = a$ . This is the case considered by Anand *et al.* [1]. When  $\theta_0 = -\pi/2$  the above formulae reduce to

$$a = -\frac{\pi}{2} + \frac{2\tau}{\sqrt{\tau^2 - 1}} \tan^{-1} \left( \sqrt{\frac{\tau + 1}{\tau - 1}} \right), \tag{5.1}$$

$$v_0 = \frac{\tau^2 - 1}{1 + (\tau + \pi/2)/a}, \tag{5.2}$$

$$A = \frac{\tau(\tau^2 - 1)}{1 + (\tau + \pi/2)/a}, \quad v_{\max} = \frac{\tau(\tau + 1)}{1 + (\tau + \pi/2)/a}.$$

Figure 3 summarizes the relation between  $\tau$  and  $a$  as expressed in (5.1). The figure also shows the upper bound  $a = 1/(\tau - 1)$  given by Anand *et al.* [1]. Having found  $\tau$ , the sliprate profile at yield may be computed from (2.4). Note that the calculation of  $\tau$  is identical when isotropic and/or energetic hardening are included since in this case  $\varepsilon = 0$  and  $g$  has its initial value.

Figure 2 shows sliprate profiles  $v(x)$  obtained from (2.5) for several grain sizes. Figure 4 is a magnification, showing the approach to the vertical tangent at the boundary. There is close agreement with Figure 3(b) of Anand *et al.* [1], obtained by finite element methods and in the viscoplastic limit. The values of  $a = 0.5, 1, 5$

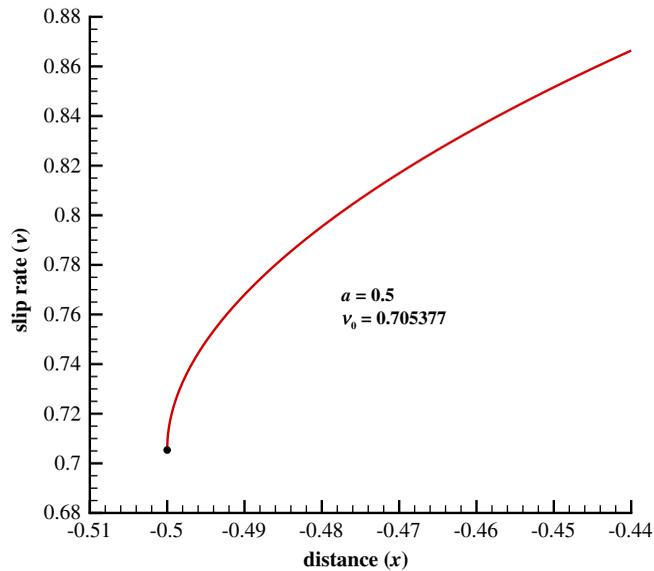


FIGURE 4. Magnification of the sliprate profile near the boundary ( $x = -a$ ) for  $a = 0.5$  showing a vertical tangent. The boundary slip  $v_0 = 0.705377$  is also indicated.

correspond to  $l/h = 1, 0.5, 0.1$  respectively. Note that the exact solution given here does not extend down to  $v = 0$  on the boundary but terminates at some nonzero  $v$  given by (5.2). The numerical “solution” in Anand *et al.* [1] attempts to force the zero-sliprate boundary condition by including what looks like a sliprate discontinuity at the boundary. Note also that the sliprate profile does not tend to the zero-gradient profile ( $v \equiv 1$ ) as  $l \rightarrow 0$ . This is because the boundary conditions  $\theta = \theta_0 = -\pi/2$  do not permit it.

Once the yield strength is known the subsequent solution after yield may be obtained numerically. For pure dissipation the analytic solution given above is available.

## 6. Higher modes

The higher modes  $n = 1, 2, \dots$  for the boundary gradient angles appear to be associated with much smaller sliprate amplitudes, as shown in Figure 5 for  $n = 1$  and grain size  $a = 1$  (compare with Figure 1). Figure 6 shows the corresponding maximum sliprate.

As noted above the higher modes reference the same velocity gradient ( $v'/v$ ) range so the boundary sliprates become multi-valued. The fundamental mode may well be selected on the basis of maximal energy dissipation but this is a topic for further investigation.

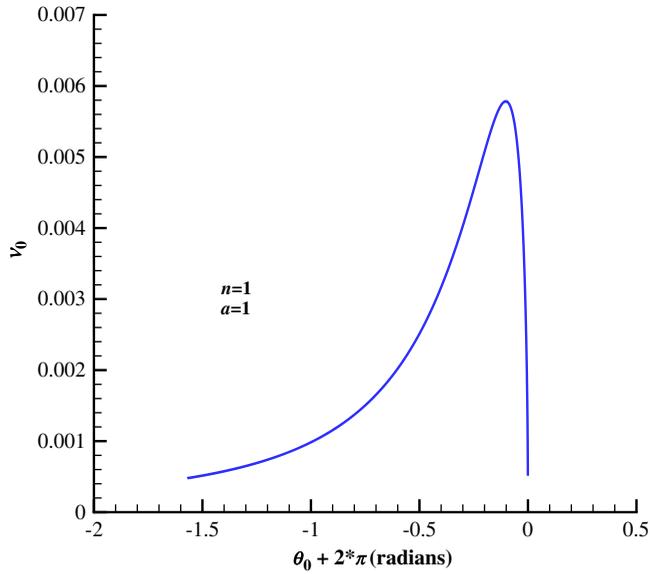


FIGURE 5. Boundary sliprate against boundary gradient for the  $n = 1$  mode.

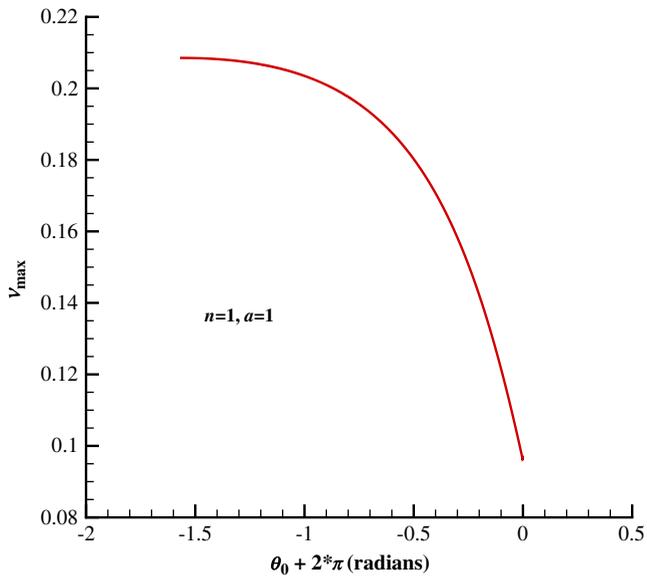


FIGURE 6. Maximum sliprate against boundary gradient angle for the  $n = 1$  mode.

## 7. Higher dimensional considerations

The generalization of (2.1) to higher dimensions (and more than one slip system) has been given by Gurtin *et al.* [4]. A simple version of the multi-dimensional flow equation excluding energetic effects can be written (in nondimensional form)

$$\tau = \frac{v}{d_p} - \nabla \cdot \frac{\nabla v}{d_p} \quad (7.1)$$

where now  $d_p = \sqrt{v^2 + (\nabla v)^2}$  (see Appendix A for a concise derivation of this equation). Assuming, as above, that  $v$  is nonzero in the interior of the computational domain, (7.1) may be written in terms of  $y_a = \nabla_a \phi = \nabla_a \log(v)$

$$\tau = \frac{1}{\sqrt{1 + y^2}} - D_{ab} \nabla_a \nabla_b \phi,$$

where  $y^2 = y_a y_a$  and the second order operator

$$D_{ab} = (1 + y^2) \delta_{ab} - y_a y_b$$

is strongly elliptic with eigenvalues

$$\begin{aligned} \lambda &= 1 && \text{for } d = 1 \\ \lambda &= 1, 1 + y^2 && \text{for } d = 2 \\ \lambda &= 1, 1 + y^2, 1 + y^2 && \text{for } d = 3 \end{aligned}$$

in  $d = 1, 2, 3$  dimensions. The corresponding eigenvectors are normal to ( $\lambda = 1$ ), or tangential to ( $\lambda = 1 + y^2$ ), the constant  $v$  equipotential surfaces. The spherical part of the operator (the Laplacian) is a direct generalization of the one-dimensional case and the nonspherical part relates to the angular anisotropy. Furthermore, the first order equation (2.3) has a multi-dimensional analogue

$$\frac{d\theta}{ds} = 1 - \tau \sec \theta - \rho \tan \theta,$$

where the arc-length  $s$  replaces the  $x$ -coordinate and we have written  $y_a = |y| n_a$ ,  $|y| = \tan \theta$ ,  $\rho = \nabla_a n_a$ . However, in spite of the intriguing correspondence between the  $d > 1$  and the one-dimensional cases, the solution of the multi-dimensional problem looks to be much more difficult than its one-dimensional counterpart.

## 8. Conclusions

We have shown that a logical scheme is now available to solve the elastoplastic dissipational slip gradient problem, at least in the one-dimensional case. The key to the method is the partial integration of the flow equations followed by evaluation on the boundary, assuming a given value for the sliprate gradient  $v'/v$  there. From this, a

nonzero boundary sliprate is determined, and it has been shown that it is not possible to have  $v = 0$  on the boundary in this simple one-dimensional model. The augmented yield stress (yield strengthening) can be computed and is in general a function of both the material properties and the applied boundary conditions.

The physical significance of these boundary conditions is open to debate. One interpretation is to imagine that the strip consists of a region of lowered yield strength sandwiched between two elastic regions. Then we can consider the situation where the central part has yielded but the two ends remain elastic. In this case the slip is trivially zero in the elastic parts and slip discontinuities given by (2.9) (with  $v = v_0$ ) must be present at the intersections with the plastic zone. The magnitude of the boundary discontinuity will be precisely that determined from (2.9) and (5.2). More generally, if there are two adjoining plastic regions with different yield strengths there will be an internal slip discontinuity at their common interface given by (2.9) and (3.4) with the two values of  $\theta_0$  (on either side of the interface) determined by the material and geometrical parameters. This suggests that dissipational gradient plasticity equation is best thought of as describing plastic flow in the presence of strengthened structures; for example, grain boundaries. In that case the present analysis predicts that internal slip discontinuities must develop at the interface between the grain and the grain boundary.

The case of dissipational gradient yield weakening has been mentioned but not further explored in this note. Consideration of these matters and associated numerical work will be presented in a later paper.

### Appendix A. Derivation of the dissipational slip gradient equation

Plastic-flow equations for the microstructure have been proposed by many authors (see Gurtin *et al.* [4] and references therein) and all involve some degree of arbitrariness. The following is a concise derivation based on thermodynamical principles together with a normality argument and a specific form of the yield function proposed by Reddy *et al.* [5].

The derivation starts with the expression of the mechanical stress-power as a sum of macro and micro contributions

$$\dot{W} = P : \dot{F} + \pi \cdot \dot{\varepsilon} + \Pi \cdot \nabla \dot{\varepsilon} \quad (\text{A.1})$$

where  $F = \nabla x$  is the deformation gradient,  $P$  is a macroscopic stress,  $\varepsilon$  is an internal strain-like variable (slip), and  $\pi$ ,  $\Pi$  are conjugate internal force-like and stress-like variables. We use the tensorial inner-product notation so that if  $A$ ,  $B$  are matrices then  $A : B \equiv \text{tr}(AB^T)$ . Note that the internal variables are generally vectorial, so that the product  $\pi \cdot \dot{\varepsilon}$  actually denotes the sum  $\sum_{\alpha} \pi_{\alpha} \dot{\varepsilon}_{\alpha}$  over the slip systems, and similarly  $\Pi \cdot \nabla \dot{\varepsilon} = \sum_{\alpha} \Pi_{\alpha} \cdot \nabla \dot{\varepsilon}_{\alpha}$ . These summations will be understood in the following.

The stress equilibrium equations associated with (A.1) are

$$\nabla \cdot P = p = 0, \quad (\text{A.2})$$

$$\nabla \cdot \Pi = \pi. \quad (\text{A.3})$$

Note that the right-hand side  $p$  of (A.2) is zero because of momentum conservation. This accounts for the absence of a macro-force term  $p \cdot \dot{x}$  in (A.1). Otherwise there is a complete parallelism between the macro and micro terms.

The macrostructure is connected with the microstructure by representing the deformation gradient as a product of elastic and inelastic factors in a well-known manner

$$F = F_e F_p.$$

The macroscopic stress power may then be formally decomposed into elastic and plastic contributions

$$P : \dot{F} = P_e : \dot{F}_e + M : L_p,$$

where  $L_p = \dot{F}_p F_p^{-1}$  is the plastic velocity gradient,  $P_e = P F_p^{-\top}$  and  $M$  is the Biot stress  $M = F_e^{-\top} P F_p^{-\top}$  for the intermediate configuration.

The second law of thermodynamics is

$$\dot{D} = \dot{W} - \dot{\psi} \geq 0,$$

where  $\dot{D}$  is the dissipation rate,  $\dot{W}$  is the mechanical stress-power, and  $\psi$  is the free energy specified as a function of the deformation gradient, and the internal strain-like variables and their gradients. In the present case this is the set  $\{F, F_p, \varepsilon, \nabla \varepsilon\}$ . In the following we shall assume that the free energy depends on  $F, F_p$  through the combination  $F_e = F F_p^{-1}$ . For clarity we shall also ignore the dependence of the free energy on the internal slips, which means that the corresponding energetic terms will be absent from the flow equation. These terms are additive and it is a simple matter to re-insert them.

Using standard thermodynamical arguments the constitutive equation for the macroscopic (Piola–Kirchhoff) elastic stress is then established

$$P_e = \frac{\partial \psi}{\partial F_e}$$

and the dissipation reduces to

$$\dot{D} = M : L_p + \pi \cdot \dot{\varepsilon} + \Pi \cdot \nabla \dot{\varepsilon}. \quad (\text{A.4})$$

To derive the dissipational gradient flow equation it is convenient to assume a von Mises type yield function (Reddy *et al.* [5]) for each slip system of the form

$$s(M, \pi, \Pi) = \sqrt{(\tau + \pi)^2 + l^{-2} \Pi^2} \quad (\text{A.5})$$

where  $l$  is an internal gradient length scale and  $\tau = M : N$  is the Schmid stress relative to the slip-system dyadic  $N$ . Here both  $\tau$  and  $N$  carry the slip-system index  $\alpha$  so that, in more explicit terms,  $\tau_\alpha = \text{tr}(M N_\alpha^T)$ . A yield law is specified when the von Mises yield function (A.5) is equated to a yield stress level  $g$ , that is

$$s(M, \pi, \Pi) = g \quad \text{at yield}. \quad (\text{A.6})$$

Assuming maximal dissipation of (A.4) under the constraint (A.6) (that is, normality), we derive the flow equations

$$L_p = \sum \dot{\lambda} \frac{\tau + \pi}{s} N, \quad (\text{A.7})$$

$$\dot{\varepsilon} = \dot{\lambda} \frac{\tau + \pi}{s}, \quad (\text{A.8})$$

$$\nabla \dot{\varepsilon} = \dot{\lambda} l^{-2} \frac{\Pi}{s}. \quad (\text{A.9})$$

From (A.8) and (A.9) together with (A.5) we can identify the Lagrange multiplier  $\dot{\lambda} = \sqrt{\dot{\varepsilon}^2 + l^2(\nabla \dot{\varepsilon})^2} \equiv d_p$  as the generalized plastic strain rate. Since  $s = g$  at yield, (A.8) and (A.9) may be re-written

$$\tau + \pi = g \frac{\dot{\varepsilon}}{d_p}, \quad \Pi = g l^2 \frac{\nabla \dot{\varepsilon}}{d_p} \quad (\text{A.10})$$

for each slip system. Combining (A.10) with (A.3) the dissipational gradient equation is obtained in the form

$$\tau + l^2 \nabla \cdot \left( g \frac{\nabla \dot{\varepsilon}}{d_p} \right) = g \cdot \frac{\dot{\varepsilon}}{d_p}.$$

Note also that the plastic velocity gradient (A.7) assumes its usual form when distributed over slip systems  $L_p = \sum \dot{\varepsilon} N$ , and the dissipation rate (A.4) reduces to  $\dot{D} = \sum g \cdot d_p$ , thus identifying  $g$  as conjugate to the generalized plastic strain rate  $d_p$  (on each slip system).

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