

Guidelines for Constructing Strain Gradient Plasticity Theories

N. A. Fleck*, J. W. Hutchinson** and J.R. Willis***

*Cambridge University Engineering Dept., Trumpington St., Cambridge, CB2 1PZ, UK

** School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA

*** Centre for Mathematical Sciences, Wilberforce Rd., Cambridge, CB3 0WA, UK

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Abstract Issues related to the construction of continuum theories of strain gradient plasticity which have emerged in recent years are reviewed and brought to bear on the formulation of the most basic theories. Elastic loading gaps which can arise at initial yield or under imposition of non-proportional incremental boundary conditions are documented and analytical methods for dealing with them are illustrated. The distinction between unrecoverable (dissipative) and recoverable (energetic) stress quantities is highlighted with respect to elastic loading gaps, and guidelines for eliminating the gaps are presented. An attractive gap-free formulation that generalizes the classical J_2 flow theory is identified and illustrated.

Key words: Strain gradient plasticity, proportional loading, non-proportional loading, elastic loading gaps

1 Introduction

This paper builds on a recent paper by the authors [1] which investigated two classes of rate-independent continuum strain gradient plasticity theories, dubbed incremental and non-incremental. In particular, the earlier paper illustrated markedly different predictions of the two classes of theories for two problems involving non-proportional loading. The first problem is a layer of material stretched in plane strain tension into the plastic range which, then, undergoes surface passivation that blocks further plastic straining at its surfaces as additional stretch is imposed. The incremental theory predicts continued plastic flow following passivation, although reduced by the constraint imposed by surface passivation. The non-incremental theory predicts that plastic flow is interrupted after passivation and does not resume until the layer experiences additional tensile stress which can be substantial. In other words, according to the non-

incremental theory, passivation gives rise to a delay in plastic flow which will be referred to here as an “elastic loading gap”, or more briefly as a “gap”. Similar behavior has been revealed in [2] for the non-incremental theory for a cylindrical wire that is twisted into the plastic range, passivated and then subject to further twist. The second problem considered in [1] is an unpassivated layer in plane strain that is first stretched into the plastic range in tension and then is subject to bending with no further overall stretch. In this case, the incremental theory predicts continued plastic flow over the half of the layer experiencing increasing tensile strain as soon as bending commences, just as in conventional plasticity, but with the plastic flow constrained by gradient effects. By contrast, the non-incremental theory predicts an initial elastic response at the onset of bending followed by slowly developing plastic flow.

The two classes of rate-independent theories are distinguished from one another by the fact that the constitutive law for the non-incremental theory has certain stress variables expressed in terms of strain increments, whereas the other class employs incremental relations between all the stress and the strain variables. The non-incremental stress quantities arise due to a constitutive construction proposed in [3-5] to ensure that stresses associated with dissipative plastic straining (unrecoverable plastic straining in the terminology of this paper) produce non-negative plastic work. This same construction has been employed in the formulation of non-incremental strain gradient plasticity theories for single crystals and similar consequences for problems involving non-proportional loading conditions can be anticipated.

In this paper, conditions under which theories are expected to predict elastic loading gaps will be further explored, including conditions where a gap occurs at initial yield. It will be seen that conditions must be imposed on both incremental and non-incremental theories if a gap at initial yield is to be avoided. The attitude taken in this paper is agnostic as to whether elastic loading gaps should or should not occur. New experiments will be required to establish the validity or invalidity of such behavior. Instead, the approach here is to provide guidance to what aspects of the theories give rise to the gaps and to how they can be excluded in the constitutive formulation if so desired. The discussion is within the context of small strain, rate-independent strain gradient plasticity. The underlying ideas can be extended to a broader class of theories, including those for single crystals.

The starting point in Section 2 is a discussion of a deformation theory of strain gradient plasticity which can generally be invoked to model history-dependent plasticity, at least as an

approximation, for applications where straining is proportional or nearly so. This is a good place to start because the issue of a gap at initial yield arises here in perhaps the simplest context where the formulation is straightforward. The issue is whether plastic flow starts at the conventional initial yield stress or whether there is a delay beyond this stress. The two classes of plasticity theories, incremental and non-incremental, are introduced in Section 3 and discussed as to whether gaps are expected to occur both at initial yield and also subsequently after plastic straining when non-proportional loading occurs due to abrupt changes in the incremental boundary conditions. Section 4 presents a detailed analysis of the onset of plastic flow at initial yield for a layer that is passivated from the start and then stretched into the plastic range. This analysis complements the analysis in [1] for the case where an unpassivated layer is first stretched into the plastic range and then passivated before more stretch occurs. The analysis in Section 4 illustrates the complexity of the solutions in the early stages of yield whether a gap occurs or not. An incremental version of strain gradient plasticity generalizing classical J_2 flow theory constructed such that elastic loading gaps do not occur is presented and discussed in Section 5.

1.1 Notation and general framework for the gradient plasticity

There is an important distinction in this paper between recoverable and unrecoverable plastic strain quantities reflected by the following notation used throughout the paper. Small strain, rate-independent plasticity is considered throughout. With $\dot{\varepsilon}_{ij}^P$ as the plastic strain increment, or rate, and $\varepsilon_{ij}^P = \int \dot{\varepsilon}_{ij}^P$ as the plastic strain, define a recoverable effective plastic strain as $\varepsilon_p = \sqrt{2\varepsilon_{ij}^P \varepsilon_{ij}^P / 3}$ which can increase or decrease. Define the accumulated effective plastic strain used in classical J_2 flow theory as $e_p = \int \dot{e}_p$ where $\dot{e}_p = \sqrt{2\dot{\varepsilon}_{ij}^P \dot{\varepsilon}_{ij}^P / 3}$ which is monotonically increasing. In this paper, e_p will be referred to as the unrecoverable plastic strain. Under monotonic proportional straining, ε_p and e_p coincide. Two analogous measures of the plastic strain gradients used in this paper are $\varepsilon_p^* = \sqrt{2\varepsilon_{ij,k}^P \varepsilon_{ij,k}^P / 3}$ and $e_p^* = \int \dot{e}_p^*$ with $\dot{e}_p^* = \sqrt{2\dot{\varepsilon}_{ij,k}^P \dot{\varepsilon}_{ij,k}^P / 3}$. More general isotropic measures of the strain gradients have been identified in [6], but ε_p^* and e_p^* adequately expose the issues relevant to the present investigation.

Two generalized effective plastic strain quantities will also appear in the sequel which bring in a material length parameter, ℓ . The recoverable measure is $\mathcal{E}_p = \sqrt{\varepsilon_p^2 + \ell_R^2 \varepsilon_p^{*2}}$, and the accumulated, or unrecoverable measure, is $E_p = \int \dot{E}_p$ with $\dot{E}_p = \sqrt{\dot{\varepsilon}_p^2 + \ell_{UR}^2 \dot{\varepsilon}_p^{*2}}$. The two sets of measures coincide when the straining is monotonic and proportional if $\ell_{UR} = \ell_R$, i.e., $(\dot{\varepsilon}_{ij}^P, \dot{\varepsilon}_{ij,k}^P) = \dot{\lambda}(\varepsilon_{ij}^0, \varepsilon_{ij,k}^0)$ with $(\varepsilon_{ij}^0, \varepsilon_{ij,k}^0)$ independent of λ , and λ increasing from zero.

The small strain framework for strain gradient plasticity will be adopted [3-5,6,7,8]. The principle of virtual work is

$$\int_V \{ \sigma_{ij} \delta \varepsilon_{ij}^e + q_{ij} \delta \varepsilon_{ij}^P + \tau_{ijk} \delta \varepsilon_{ij,k}^P \} dV = \int_S (T_i \delta u_i + t_{ij} \delta \varepsilon_{ij}^P) dS \quad (1.1)$$

with volume of the solid V , surface S , displacements u_i , total strains $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$, plastic strains ε_{ij}^P ($\varepsilon_{kk}^P = 0$), and elastic strains $\varepsilon_{ij}^e = \varepsilon_{ij} - \varepsilon_{ij}^P$. The symmetric Cauchy stress is σ_{ij} , and the stress quantities work conjugate to increments of ε_{ij}^P and $\varepsilon_{ij,k}^P$ are q_{ij} ($q_{ij} = q_{ji}$, $q_{kk} = 0$) and τ_{ijk} ($\tau_{ijk} = \tau_{jik}$, $\tau_{jjk} = 0$). The surface tractions are $T_i = \sigma_{ij} n_j$ and $t_{ij} = \tau_{ijk} n_k$ with n_i as the outward unit normal to S . The equilibrium equations are

$$\sigma_{ij,j} = 0, \quad -s_{ij} + q_{ij} - \tau_{ijk,k} = 0 \quad (1.2)$$

with $s_{ij} = \sigma_{ij} - \sigma_{kk} \delta_{ij} / 3$. The effective Cauchy stress is $\sigma_e = \sqrt{3s_{ij}s_{ij} / 2}$.

Elasticity is isotropic with Young's modulus E and Poisson's ratio ν . The initial tensile yield stress is σ_Y with the associated yield strain $\varepsilon_Y = \sigma_Y / E$. Numerical results will be presented for incompressible materials with a uniaxial tensile stress-strain curve

$$\left. \begin{aligned} \varepsilon &= \sigma / E \ \& \ \varepsilon_p = 0, & \quad \sigma \leq \sigma_Y \\ \varepsilon &= \sigma / E + ((\sigma - \sigma_Y) / k)^{1/N}, & \quad \sigma > \sigma_Y \end{aligned} \right\} \quad (1.3)$$

with $0 < N < 1$ such that beyond yield

$$\sigma = \sigma_Y (1 + k \varepsilon_p^N) \quad (1.4)$$

We have deliberately chosen for the input uniaxial stress-strain behavior a curve with continuous slope at yield rather than a curve with a discontinuous slope such as a bi-linear relation. Had an input curve been adopted with a sharp break in slope at yield, gaps at initial yield would be more

clearly delineated, but, as will be seen, gaps are also quite evident with the smooth curve. A continuous slope is more representative of the initial yielding behavior of annealed metals than a curve with a sharp discontinuity. Moreover, as will be seen in the sequel, this choice will enable us to illustrate an important point concerning recoverable contributions of the gradients of plastic strain to the free energy: namely that these contributions are not necessarily quadratic in the gradients quantities, as is usually assumed.

2 Deformation theories and the onset of plastic flow

The deformation theories under consideration characterize small strain, nonlinear elastic solids with a strain energy density of the form

$$\psi = \frac{1}{2} L_{ijkl} \varepsilon_{ij}^e \varepsilon_{kl}^e + \psi_p(\varepsilon_p, \varepsilon_p^*) \quad (2.1)$$

with isotropic moduli, L_{ijkl} , and ψ_p as the “plastic” contribution. The associated stresses are

$$\left. \begin{aligned} \sigma_{ij} &= \frac{\partial \psi}{\partial \varepsilon_{ij}^e} = L_{ijkl} \varepsilon_{kl}^e \\ q_{ij} &= \frac{\partial \psi_p}{\partial \varepsilon_{ij}^p} = \frac{\partial \psi_p}{\partial \varepsilon_p} \frac{2\varepsilon_{ij}^p}{3\varepsilon_p}, \quad \tau_{ijk} = \frac{\partial \psi_p}{\partial \varepsilon_{ij,k}^p} = \frac{\partial \psi_p}{\partial \varepsilon_p^*} \frac{2\varepsilon_{ij,k}^p}{3\varepsilon_p^*} \end{aligned} \right\} \quad (2.2)$$

The potential energy of a body is regarded as a functional of u_i and ε_{ij}^p :

$$F(u_i, \varepsilon_{ij}^p) = \int_V \psi dV - \int_{S_T} (T_i u_i + t_{ij} \varepsilon_{ij}^p) dS \quad (2.3)$$

with prescribed T_i and t_{ij} on portions of the surface, S_T , and with u_i and ε_{ij}^p prescribed on the remaining surface S_U . The solution to the boundary value problem minimizes the potential energy among admissible u_i and ε_{ij}^p .

Continuity of the stress variables (q_{ij}, τ_{ijk}) under continuing overall deformation lies at the heart of the issues being addressed in this paper. If the strain variables vary continuously and if $\partial \psi_p / \partial \varepsilon_p$ and $\partial \psi_p / \partial \varepsilon_p^*$ are continuous functions of ε_p and ε_p^* , then the stresses given by (2.2) will vary continuously except possibly when ε_p and/or ε_p^* vanish. Within the linear elastic range, $(\varepsilon_p, \varepsilon_p^*)$ vanish and (q_{ij}, τ_{ijk}) are not defined by (2.2) for the deformation theory. The

onset of yield is where the possible existence of a delay in yielding depends in a critical way on the behavior of ψ_p for small ε_p and ε_p^* . Two distinct behaviors will be illustrated with the following choices for ψ_p , each of which reduces to (1.4) in uniaxial tension:

$$\psi_p = \sigma_Y \left[\mathcal{E}_p + (k / (N + 1)) \mathcal{E}_p^{N+1} \right] \quad (2.4)$$

$$\psi_p = \sigma_Y \left[\varepsilon_p + (k / (N + 1)) \varepsilon_p^{N+1} \right] \quad (2.5)$$

The first choice (2.4) follows the proposal in [6] by replacing ε_p everywhere in the energy density of the classical theory by $\mathcal{E}_p = \sqrt{\varepsilon_p^2 + \ell_R^2 \varepsilon_p^{*2}}$, while the second choice (2.5) retains ε_p in the lowest order contribution.

The overall stress-strain curve for the tensile stretching in plane strain of a layer of thickness $2h$ whose surfaces are passivated from the start is plotted in Fig. 1 for the two choices, (2.4) and (2.5), for $N = 0.2$, $p = k\varepsilon_Y^N = 0.5$ and $\ell_R / h = 1$. The classical limit with no gradient effect corresponding to $\ell_R / h = 0$ is also shown. A passivated surface is assumed to block dislocations requiring zero plastic strain to be imposed at the surfaces of the layer in the continuum model. From an analytical perspective, deformation theory problems are attractive because solutions can be produced at any load without recourse to prior history. For the second choice (2.5) there is no elastic loading gap at the onset of yield and plastic flow initiates when $\sigma_e = \sigma_Y$ (at $\sigma_{11} = \sqrt{3}\sigma_Y / 2$ in plane strain tension). By contrast, there is a substantial gap for choice (2.4) and the plastic flow delayed to $\sigma_e = 1.825\sigma_Y$. For (2.4), the gap depends on ℓ_R / h ; it is plotted in Fig. 2. This is precisely the same elastic loading gap identified in [1] for a particular family of non-incremental theories for the case when passivation is imposed after the layer has been stretched into the plastic range.

The question as to why one form of the deformation theory produces a gap and the other does not is now addressed for the case of initial yield. In the current state with no prior plastic straining, assume σ_{ij} is an equilibrium state of stress ($\sigma_{ij,j} = 0$) such that on the boundary with outward normal n_i , $T_i = \sigma_{ij}n_j$. Let ε_{ij}^P be an admissible trial field associated with the onset of yield and assume that the boundary conditions are such that either $t_{ij} = 0$ or $\varepsilon_{ij}^P = 0$ such that

$t_{ij}\varepsilon_{ij}^p = 0$ on the boundary. Minimization of F in (2.3) requires $\delta F = 0$. At the onset of yield, for arbitrary small variations with $\delta\varepsilon_{ij}^p = \varepsilon_{ij}^p$ and $\delta\varepsilon_{ij}^e = 0$, δF can be obtained as

$$\delta F = \int_V \left(\frac{\partial \psi_p}{\partial \varepsilon_p} \varepsilon_p + \frac{\partial \psi_p}{\partial \varepsilon_p^*} \varepsilon_p^* - \sigma_{ij} \varepsilon_{ij}^p \right) dV = 0 \quad (2.6)$$

where the derivatives of ψ_p are evaluated at $\varepsilon_p = \varepsilon_p^* = 0$. The boundary conditions are homogeneous with either unconstrained ε_{ij}^p or $\varepsilon_{ij}^p = 0$. This is an eigenvalue problem for the stress σ_{ij} at the onset of yield and the non-zero associated eigenfield ε_{ij}^p .

First consider the case where σ_{ij} is uniform. If the lowest order contribution to ψ_p is $\sigma_Y \varepsilon_p$, as in (2.5), (2.6) becomes $\int_V (\sigma_Y \varepsilon_p - \sigma_{ij} \varepsilon_{ij}^p) dV = 0$. This has no dependence on the gradients of plastic strain and no penalty for satisfying $\varepsilon_{ij}^p = 0$ on the boundary. For either set of boundary conditions the eigen solution is $\sigma_e \equiv \sqrt{3s_{ij}s_{ij}/2} = \sigma_Y$ with $\varepsilon_{ij}^p / \varepsilon_p = 3s_{ij}/2\sigma_Y$ such that, by (2.2), $q_{ij} = s_{ij}$ and $\tau_{ijk} = 0$. There is no gap at initial yield in this case. On the other hand, for the choice (2.4), (2.6) becomes $\int_V (\sigma_Y \varepsilon_p^e - \sigma_{ij} \varepsilon_{ij}^p) dV = 0$ which does bring in a dependence on the plastic strain gradients. If zero plastic strain on the boundary is required, there must be non-zero gradients for any non-zero solution and, thus, $\varepsilon_p^e > \varepsilon_p$ over some portion of the body. It follows that any eigen stress associated with the onset of yield must satisfy $\sigma_e > \sigma_Y$. The eigenvalue functional governing the delay in yielding for (2.4) also arises for problems based on the non-incremental theories, as first noted in [1], as will be discussed further in Section 4.

For the deformation theory (2.1), initial yield will occur in a uniformly stressed body when $\sigma_e = \sigma_Y$ if, at $\varepsilon_p = 0$ and $\varepsilon_p^* = 0$, $\partial \psi_p / \partial \varepsilon_p = \sigma_Y$ and $\partial \psi_p / \partial \varepsilon_p^* = 0$. This is tantamount to the requirement $q_{ij} \rightarrow s_{ij}$ and $\tau_{ijk} \rightarrow 0$ as ε_p and ε_p^* approach zero. While according to (2.2), q_{ij} and τ_{ijk} are indeterminate when ε_p and ε_p^* are zero, the assignment $q_{ij} = s_{ij}$ and $\tau_{ijk} = 0$ within the linear elastic range ensures that all the stress variables will vary continuously at yield for materials meeting the above conditions on the first partial derivatives. This assignment is consistent with the second of equilibrium equations (1.2).

Now consider situations where the body, or a sub-region of the body, has not yet yielded and σ_{ij} in (2.6) is not uniform. Assume ψ_p meets $\partial\psi_p / \partial\varepsilon_p = \sigma_Y$ and $\partial\psi_p / \partial\varepsilon_p^* = 0$ when $\varepsilon_p = \varepsilon_p^* = 0$. Plastic yield must begin locally at any location where $\sigma_e = \sigma_Y$. This can be seen from the fact that at this location the integrand of (2.6) is $(\sigma_Y\varepsilon_p - \sigma_{ij}\varepsilon_{ij}^P)$, which is non-negative for all ε_{ij}^P if $\sigma_e \leq \sigma_Y$ and is negative for $\varepsilon_{ij}^P / \varepsilon_p = 3s_{ij} / 2\sigma_Y$ if $\sigma_e > \sigma_Y$. Thus, because there is no local dependence on the gradient and no restriction on continuity of ε_{ij}^P at the onset of yield, plastic flow in the form $\varepsilon_{ij}^P / \varepsilon_p = 3s_{ij} / 2\sigma_Y$ at any location where $\sigma_e > \sigma_Y$ will lead to smaller values of F than if no flow occurred.

In summary, for deformation theory materials satisfying $\partial\psi_p / \partial\varepsilon_p = \sigma_Y$ and $\partial\psi_p / \partial\varepsilon_p^* = 0$ at $\varepsilon_p = 0$ and $\varepsilon_p^* = 0$, the onset of plastic flow is a local condition met where $\sigma_e = \sigma_Y$. For materials not satisfying this condition, the onset of plastic flow is generally governed by a non-local condition and an elastic loading gap beyond $\sigma_e = \sigma_Y$ should be expected. The material specified by (2.4) has $\partial\psi_p / \partial\varepsilon_p = \sigma_Y\varepsilon_p / \mathcal{E}_p$ and $\partial\psi_p / \partial\varepsilon_p^* = \sigma_Y l_R^2 \varepsilon_p^* / \mathcal{E}_p$ which do not satisfy the requirement for no gap at initial yield.

3 Theories of strain gradient plasticity with guidance as to whether they generate elastic loading gaps

A fairly general set of theories will be considered, but special cases that have appeared in the literature will be discussed. The theory laid out is non-incremental but it will be specialized to a class of incremental theories. The general thermodynamic framework is consistent with that developed in [3-5], but here specifically for rate-independent plasticity. The free energy of the solid ψ has the form given by (2.1) with recoverable stresses (energetic stresses in the terminology of [3-5]):

$$\sigma_{ij} = L_{ijkl}\varepsilon_{kl}^e, \quad q_{ij}^R = \frac{\partial\psi_p}{\partial\varepsilon_{ij}^P} = \frac{\partial\psi_p}{\partial\varepsilon_p} \frac{2\varepsilon_{ij}^P}{3\varepsilon_p}, \quad \tau_{ijk}^R = \frac{\partial\psi_p}{\partial\varepsilon_{ij,k}^P} = \frac{\partial\psi_p}{\partial\varepsilon_p^*} \frac{2\varepsilon_{ij,k}^P}{3\varepsilon_p^*} \quad (3.1)$$

A non-negative dissipation function $\varphi(e_p, e_p^*, \dot{e}_p, \dot{e}_p^*)$ is assumed that is homogeneous of degree one in \dot{e}_p and \dot{e}_p^* . Two examples which reduce to (1.4) in uniaxial tension are

$$\varphi = \sigma_Y \left[(1 + k e_p^N) \dot{e}_p + k (\ell_{UR} e_p^*)^N \ell_{UR} \dot{e}_p^* \right] \quad (3.2)$$

and the coupled form using E_p adopted in [8]

$$\varphi = \sigma_Y (1 + k E_p^N) \dot{E}_p \quad (3.3)$$

The dissipation potential φ generates the unrecoverable stresses (dissipative stresses):

$$q_{ij}^{UR} = \frac{\partial \varphi}{\partial \dot{\varepsilon}_{ij}^P} = \frac{\partial \varphi}{\partial \dot{e}_p} \frac{2 \dot{\varepsilon}_{ij}^P}{3 \dot{e}_p}, \quad \tau_{ijk}^{UR} = \frac{\partial \varphi}{\partial \dot{\varepsilon}_{ij,k}^P} = \frac{\partial \varphi}{\partial \dot{e}_p} \frac{2 \dot{\varepsilon}_{ij,k}^P}{3 \dot{e}_p} \quad (3.4)$$

Homogeneity of φ gives

$$q_{ij}^{UR} \dot{\varepsilon}_{ij}^P + \tau_{ijk}^{UR} \dot{\varepsilon}_{ij,k}^P = (\partial \varphi / \partial \dot{e}_p) \dot{e}_p + (\partial \varphi / \partial \dot{e}_p^*) \dot{e}_p^* = \varphi \quad (3.5)$$

ensuring that the work rate of the unrecoverable stresses is non-negative if φ is non-negative. It follows that $(\partial \varphi / \partial \dot{e}_p)$ and $(\partial \varphi / \partial \dot{e}_p^*)$ must also be non-negative. The general form (3.4) derives from the constitutive construction proposed in [3-5] to ensure positive plastic dissipation of the unrecoverable stresses.

The stresses are the sum of the recoverable and unrecoverable contributions, i.e., σ_{ij} , $q_{ij} = q_{ij}^R + q_{ij}^{UR}$ and $\tau_{ijk} = \tau_{ijk}^R + \tau_{ijk}^{UR}$. An important distinction between the recoverable and unrecoverable stresses, which has implications related to the elastic loading gaps, is that the recoverable stresses (3.1) are known and fixed in the current state while generally the unrecoverable stresses are not. The unrecoverable stresses in (3.4) depend on the plastic strain rate and its gradient and thus are not known in the current state—they depend on the boundary conditions imposed for the incremental problem. The unrecoverable stresses can change discontinuously [8,9] from one increment of loading to another if boundary conditions for the incremental problem change abruptly. It is this feature that motivated the designation “non-incremental” for theories with such stresses in [1]. Alternative formulations which introduce extra gradient-like variables to meet the requirement of positive plastic dissipation have been considered in a broad overview of strain gradient plasticity in [10], but they will not be considered here.

When unrecoverable stresses are present, the second equilibrium equation in (1.2) becomes an equation for the plastic strain rates, and the following minimum principle I was

devised in [8] to satisfy this equation. In the current state with known distributions of σ_{ij} , ε_{ij}^P , e_p and e_p^* , a functional homogenous of degree one in $\dot{\varepsilon}_{ij}^P$ is defined as

$$\Phi_I = \int_V (\varphi + \dot{\psi}_P - s_{ij} \dot{\varepsilon}_{ij}^P) dV \quad (3.6)$$

noting that $\varphi = q_{ij}^{UR} \dot{\varepsilon}_{ij}^P + \tau_{ijk}^{UR} \dot{\varepsilon}_{ij,k}^P$ and $\dot{\psi}_P = q_{ij}^R \dot{\varepsilon}_{ij}^P + \tau_{ijk}^R \dot{\varepsilon}_{ij,k}^P$. In arriving at (3.6), for all cases considered in this paper, it has been assumed that the boundary conditions on the surface and on any internal elastic-plastic boundary are either $t_{ij} = 0$ or $\dot{\varepsilon}_{ij}^P = 0$. Among all non-zero admissible fields $\dot{\varepsilon}_{ij}^P$, the field that minimizes Φ_I satisfies the second equilibrium equation in (1.2). Due to the homogeneous nature of Φ_I and the boundary conditions under consideration, the minimum has $\Phi_I = 0$ and $\dot{\varepsilon}_{ij}^P$ is determined only to within an amplitude factor, or to within multiple amplitude factors if there are multiple disconnected regions of ongoing plastic straining.

A second minimum principle [8] closely resembles the classical principle for an incremental problem, and it provides the amplitudes of the eigenfields $\dot{\varepsilon}_{ij}^P$ and the displacement rate field. Principle II minimizes

$$\Phi_{II} = \frac{1}{2} \int_V (\dot{\sigma}_{ij} \dot{\varepsilon}_{ij}^e + \dot{q}_{ij} \dot{\varepsilon}_{ij}^P + \dot{\tau}_{ijk} \dot{\varepsilon}_{ij,k}^P) dV - \int_{S_T} (\dot{T}_i \dot{u}_i) dS \quad (3.7)$$

where

$$\begin{aligned} \dot{\sigma}_{ij} \dot{\varepsilon}_{ij}^e + \dot{q}_{ij} \dot{\varepsilon}_{ij}^P + \dot{\tau}_{ijk} \dot{\varepsilon}_{ij,k}^P &= L_{ijkl} (\dot{\varepsilon}_{ij} - \dot{\varepsilon}_{ij}^P) (\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^P) + \frac{\partial \varphi}{\partial e_p} \dot{e}_p + \frac{\partial \varphi}{\partial e_p^*} \dot{e}_p^* \\ &+ \frac{\partial^2 \psi_P}{\partial^2 \varepsilon_p} \dot{\varepsilon}_p^2 + 2 \frac{\partial^2 \psi_P}{\partial \varepsilon_p \partial \varepsilon_p^*} \dot{\varepsilon}_p \dot{\varepsilon}_p^* + \frac{\partial^2 \psi_P}{\partial^2 \varepsilon_p^*} \dot{\varepsilon}_p^{*2} + \frac{1}{\varepsilon_p} \frac{\partial \psi_P}{\partial \varepsilon_p} (\dot{e}_p^2 - \dot{\varepsilon}_p^2) + \frac{1}{\varepsilon_p^*} \frac{\partial \psi_P}{\partial \varepsilon_p^*} (\dot{e}_p^{*2} - \dot{\varepsilon}_p^{*2}) \end{aligned} \quad (3.8)$$

Traction rates \dot{T}_i are prescribed on S_T while on the remainder of the surface \dot{u}_i are prescribed, and attention here is restricted to either $\dot{t}_{ij} = 0$ or $\dot{\varepsilon}_{ij}^P = 0$ on S . For the issues at hand it should be noted that, if φ has no dependence on the strain gradients, i.e., if $\varphi = g(e_p) \dot{e}_p$, minimum principle I based on (3.6) is identically satisfied because all the stress quantities are known and fixed in the current equilibrium state, i.e., $\tau_{ijk}^{UR} = 0$ and, from (1.2), $q_{ij}^{UR} = s_{ij} - q_{ij}^R + \tau_{ijk}^R$. Thus, when the unrecoverable contributions do not involve the plastic strain gradients, q_{ij}^{UR} is known in the current state and the entire incremental field is delivered by minimum principle II. This is an important class of incremental theories discussed later.

Minimum principle I based on (3.6) and the associated homogeneous boundary conditions can be thought of as an eigenvalue problem for s_{ij} , similar to that discussed in the previous section. The solution $\dot{\varepsilon}_{ij}^P = 0$ is always available, although it may not provide the minimum to principle II. If a body is deformed plastically under a sequence of boundary loads which change smoothly, then one can anticipate that at each incremental step the stresses and the associated strain rates will vary continuously. In other words, under a sufficiently smooth loading history, when plastic straining starts, a non-zero solution to minimum principle I is expected to exist at each step with the stresses and strain rates varying continuously. What will happen, however, if there is an abrupt change in the incremental boundary conditions? As such an example, consider the stretch passivation problem in [1] where a layer is stretched into the plastic range with plasticity unconstrained on its surfaces ($t_{ij} = 0$) and then passivated such that for subsequent increments $\dot{\varepsilon}_{ij}^P = 0$ on the surfaces. The abrupt imposition of the constraint on plastic flow at the surfaces results in the fact that the only solution to the minimum problem for (3.6) for the case considered in [1] is $\dot{\varepsilon}_{ij}^P = 0$ for a finite range of stress above the stress at passivation. In this case, the abrupt change in the boundary condition is the origin of the elastic loading gap.

3.1 Conditions for eliminating an elastic gap at initial yield

Conditions on φ and ψ to eliminate a gap at initial yield for the theory in this section are first derived, after which conditions at every stage of loading will be addressed. The condition at initial yield to ensure that a non-zero solution exists in minimizing Φ_I for any s_{ij} satisfying $\sigma_e = \sigma_Y$ is derived in a manner similar to that for the deformation theory. Let the current deviator stress distribution be s_{ij} with all the plastic strain quantities zero. In any region where the first increment of plastic strain occurs, $\dot{\varepsilon}_p = \dot{e}_p$ and $\dot{\varepsilon}_p^* = \dot{e}_p^*$, such that (3.6) becomes

$$\Phi_I = \int_V \left(\left(\frac{\partial \varphi}{\partial \dot{e}_p} + \frac{\partial \psi_p}{\partial \dot{\varepsilon}_p} \right) \dot{\varepsilon}_p + \left(\frac{\partial \varphi}{\partial \dot{e}_p^*} + \frac{\partial \psi_p}{\partial \dot{\varepsilon}_p^*} \right) \dot{\varepsilon}_p^* - s_{ij} \dot{\varepsilon}_{ij}^P \right) dV \quad (3.9)$$

with the partial derivatives evaluated at zero plastic strain. Suppose these derivatives have $\partial \varphi / \partial \dot{e}_p = \alpha \sigma_Y$, $\partial \psi_p / \partial \dot{\varepsilon}_p = (1 - \alpha) \sigma_Y$ with $0 \leq \alpha \leq 1$, $\partial \varphi / \partial \dot{e}_p^* = 0$ and $\partial \psi_p / \partial \dot{\varepsilon}_p^* = 0$. Then,

(3.9) reduces to $\Phi_I = \int_V (\sigma_Y \dot{\epsilon}_p - s_{ij} \dot{\epsilon}_{ij}^p) dV = 0$, which is the same eigenvalue functional discussed in the previous section. For such materials, initial yield occurs at $\sigma_e = \sigma_Y$ with $q_{ij} = s_{ij}$ and $\tau_{ijk} = 0$. These conditions on φ and ψ_p eliminate the roles of $\dot{\epsilon}_p^*$ and the material length parameters at the onset of yield. Conversely, if the partial derivatives of φ and ψ_p with respect to \dot{e}_p^* and $\dot{\epsilon}_p^*$ in (19) are not zero, a delay in initial yielding beyond $\sigma_e = \sigma_Y$ must be anticipated. These guidelines are consistent with the numerical examples generated in [11] for a variety of theories, some of which have gaps at initial yield and others which do not.

3.2 Conditions for eliminating an elastic loading gap after plastic deformation has occurred

Now suppose the body has been deformed into the plastic range and inquire whether an abrupt change in boundary conditions for the incremental problem is likely to produce an elastic loading gap where a plastic response would otherwise be predicted by conventional theory. We begin by illustrating with a specific example the assertion that any non-incremental version which has unrecoverable stresses generated by (3.4) with $\tau_{ijk}^{UR} \neq 0$, will necessarily have such gaps for some problems. Consider the two non-incremental versions with dissipation potential specified by (3.2) and (3.3) and take $\psi_p = 0$ which is not essential to the discussion. For the problem considered in [1], where a layer is first stretched into the plastic range and then undergoes passivation followed by further stretch, (3.3) was employed, i.e., $\varphi = \sigma_Y (1 + k E_p^N) \dot{E}_p$. This choice gave rise to the elastic gap alluded to earlier. Had the choice (3.2) been made, i.e., $\varphi = \sigma_Y \left[(1 + k e_p^N) \dot{e}_p + k (\ell_{UR} e_p^*)^N \ell_{UR} \dot{e}_p^* \right]$, no gap would have occurred, as will be discussed further in Section 4. The difference between the two choices for this problem is that (3.3) has a non-zero contribution of order \dot{e}_p^* at the onset of the gap while the corresponding contribution from (3.2) is zero because the current plastic strain is uniform with $e_p^* = 0$.

Suppose, however, if instead of stretching the problem is pure bending into the plastic range with no surface constraint followed by surface passivation and continued bending. Then, because of the existence of a gradient of plastic strain at passivation, there will be a non-zero contribution of order \dot{e}_p^* from both (3.2) and (3.3), and, indeed, from any dissipation potential φ with a dependence on the strain gradients. Fig. 3a presents the moment-curvature relation for

pure bending in plane strain for a specific example computed using (3.2) in the same manner as in [1]. A distinct elastic loading gap is evident. The gap, as measured by the curvature change $\Delta\kappa$ after passivation without any plastic deformation, has been computed based on a numerical implementation of minimum principle I in (3.9) and plotted in Fig. 3b. As in the stretch-passivation examples, the gap can be large corresponding to elastic strain increases on the order of 50% of the yield strain or more. The torsion problem in [2] is another example which will generate a gap following passivation for any non-incremental formulation with dissipation dependent on the gradients of plastic strain.

In conclusion, these examples illustrate the fact that non-incremental theories with unrecoverable stress quantities τ_{ijk}^{UR} will always generate elastic loading gaps for some problems. In the remainder of this section, we present what we believe to be an attractive incremental specialization of the theories considered above with no dependence of e_p^* and no elastic loading gaps either at initial yield or under continued plastic straining.

3.3 A basic incremental theory extension of J_2 flow theory with no elastic loading gaps

For this theory, equations (3.1), (3.4) and (3.5) defining the constitutive relation continue to apply, but the work-rate of the plastic strain rate is partitioned between non-recoverable and recoverable contributions using a factor α in the range $0 \leq \alpha \leq 1$. The dissipation potential is taken as $\varphi = \alpha\sigma_0(e_p)\dot{e}_p$ where $\sigma_0(e_p)$ is the relation of stress to effective plastic strain in uniaxial tension with $\sigma_0(0) \equiv \sigma_Y$. The free energy is taken to be

$$\psi = \frac{1}{2} L_{ijkl} \varepsilon_{ij}^e \varepsilon_{kl}^e + (1 - \alpha) \int_0^{\varepsilon_p} \sigma_0(\varepsilon_p) \varepsilon_p + f(\varepsilon_p^*) \quad (3.10)$$

As in classical J_2 flow theory, the conventional accumulated effective plastic strain e_p is unrecoverable. The limit $\alpha = 0$ is a deformation theory, but the concern here is with $0 < \alpha \leq 1$, including the limit $\alpha = 1$ for which $q_{ij}^R = 0$. As the guidelines in Section 3.1 indicate, gaps at initial yield will be eliminated if $f = df / d\varepsilon_p^* = 0$ at $\varepsilon_p^* = 0$. As noted earlier, this theory is incremental with $q_{ij}^{UR} = s_{ij} - q_{ij}^R + \tau_{ijk,k}^R$ known in the current state. Rather than an equation for q_{ij}^{UR} in terms of the plastic strain rate, the first equation in (3.4) now becomes a constraint on the plastic strain rate. The plastic strain rate must satisfy the normality condition

$$\dot{\varepsilon}_{ij}^P = \frac{3}{2} \alpha \dot{e}_p \frac{q_{ij}^{UR}}{\sigma_0(e_p)}, \quad \dot{e}_p \geq 0 \quad (3.11)$$

With $q_e^{UR} = \sqrt{3q_{ij}^{UR}q_{ij}^{UR}/2}$, q_{ij}^{UR} is on the surface $q_e^{UR} = \alpha\sigma_0(e_p)$ and $\dot{\varepsilon}_{ij}^P$ is normal to this surface. For elastic responses ($\dot{e}_p = 0$) with $q_e^{UR} < \alpha\sigma_0(e_p)$, we define changes in q_{ij}^{UR} by $\dot{q}_{ij}^{UR} = \dot{s}_{ij}$ and take $q_{ij}^{UR} = 0$ prior to any plastic deformation. With this extended definition of q_{ij}^{UR} , the second equilibrium equation in (1.2) is always satisfied. Plastic re-loading occurs when q_e^{UR} returns to the yield surface.

Minimum principle I has no role in this theory. The distributions of \dot{u}_i and \dot{e}_p are given by minimizing Φ_{II} in (3.7) whose integrand (3.8) becomes

$$\begin{aligned} \dot{\sigma}_{ij}\dot{\varepsilon}_{ij}^e + \dot{q}_{ij}\dot{\varepsilon}_{ij}^P + \dot{\tau}_{ijk}\dot{\varepsilon}_{ij,k}^P &= L_{ijkl}(\dot{\varepsilon}_{ij} - \dot{\varepsilon}_{ij}^P)(\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^P) + \alpha \frac{d\sigma_0(e_p)}{de_p} \dot{e}_p^2 \\ &+ (1-\alpha) \left(\frac{d\sigma_0(\varepsilon_p)}{d\varepsilon_p} \dot{\varepsilon}_p^2 + \frac{1}{\varepsilon_p} \sigma_0(\varepsilon_p) (\dot{e}_p^2 - \dot{\varepsilon}_p^2) \right) + \frac{d^2 f(\varepsilon_p^*)}{d^2 \varepsilon_p^*} \varepsilon_p^{*2} + \frac{1}{\varepsilon_p^*} \frac{df(\varepsilon_p^*)}{d\varepsilon_p^*} (\dot{e}_p^{*2} - \dot{\varepsilon}_p^{*2}) \end{aligned} \quad (3.12)$$

By (3.11), $\dot{\varepsilon}_p = \alpha \dot{e}_p q_{ij}^{UR} \varepsilon_{ij}^P / (\sigma_0(e_p) \varepsilon_p)$ and $\dot{\varepsilon}_p^* = \alpha (\dot{e}_p q_{ij}^{UR} / \sigma_0(e_p))_{,k} \varepsilon_{ij,k}^P / (\varepsilon_p^*)$.

Further discussion of this theory and illustrative solutions are presented in Section 5.

4 Analysis of the first increment of plastic strain for a passivated layer in plane strain stretch

4.1 Basics

For the purpose of this section, define \dot{e}_p to be any positive, positively homogeneous function of degree 1 of $\dot{\varepsilon}_{ij}^P$, and \dot{E}_p to be any positive, positively homogeneous function of degree 1 in $\dot{\varepsilon}_{ij}^P$ and $\ell_{UR} \dot{\varepsilon}_{ij,k}^P$. The free energy ψ has the general form

$$\psi(\varepsilon^e, \varepsilon^P, \nabla \varepsilon^P) = \frac{1}{2} \varepsilon_{ij}^e L_{ijkl} \varepsilon_{ij}^e + U_p(\varepsilon_{ij}^P, \varepsilon_{ij,k}^P) \quad (4.1)$$

and the dissipation potential φ is taken to have the form

$$\varphi(\dot{\varepsilon}^P, \nabla \dot{\varepsilon}^P) = \sigma_1(e_p) \dot{e}_p + \sigma_2(E_p) \dot{E}_p. \quad (4.2)$$

The constitutive relations are

$$\sigma_{ij} = \frac{\partial \psi}{\partial \varepsilon_{ij}^e}, \quad q_{ij}^R = \frac{\partial \psi}{\partial \varepsilon_{ij}^p}, \quad \tau_{ijk}^R = \frac{\partial \psi}{\partial \varepsilon_{ij,k}^p},$$

$$q_{ij}^{UR} = \frac{\partial \varphi}{\partial \dot{\varepsilon}_{ij}^p} = \sigma_1(e_p) \frac{\partial \dot{e}_p}{\partial \dot{\varepsilon}_{ij}^p} + \sigma_2(E_p) \frac{\partial \dot{E}_p}{\partial \dot{\varepsilon}_{ij}^p}, \quad \tau_{ijk}^{UR} = \frac{\partial \varphi}{\partial \dot{\varepsilon}_{ij,k}^p} = \sigma_2(E_p) \frac{\partial \dot{E}_p}{\partial \dot{\varepsilon}_{ij,k}^p}. \quad (4.3)$$

(The formulae for the latter two apply when \dot{e}^p and \dot{E}_p are positive; when either one is zero, the derivatives must be replaced by sub-gradients.)

For later use, introduce the potentials $V_1(e_p)$ and $V_2(E_p)$ such that

$$\sigma_1(e_p) = V_1'(e_p), \quad \sigma_2(E_p) = V_2'(E_p). \quad (4.4)$$

4.2 Variational formulation for an increment

An incremental formulation will be adopted, for which the solution is sought at discrete times $t_k = t_0 + k\Delta t$. Correspondingly, the value of any function $f(t)$ at time t_k is denoted $f(t_k) = f_k$. The finite difference $f_{k+1} - f_k$ gives $\Delta t \dot{f}(t_\gamma)$ at some time $t_\gamma = t_k + \gamma\Delta t$ with $0 < \gamma < 1$, at which time $f(t_\gamma)$ itself equals $f_\lambda = f_k + \lambda(f_{k+1} - f_k)$ with $0 < \lambda < 1$. The values of the parameters γ and λ are generally not known but still it will prove convenient to present the formulation as though they were¹. To see what happens next, note that $(q_{ij}^{UR})_\gamma$, with $\dot{\varepsilon}_{ij}^p(t_\gamma)$ given by its finite difference and e_p at time t_γ expressed by linear interpolation like that employed for ε_{ij}^p , can be expressed as

$$q_{ij}^{UR} = \frac{\partial \{V_1((e_p)_\lambda) + V_2((E_p)_\lambda)\}}{\lambda \partial (\varepsilon_{ij}^p)_{k+1}} \quad (4.5)$$

where, for example, $(e_p)_\lambda = (e_p)_k + \lambda\Delta t \dot{e}_p(t_\gamma)$. The higher-order traction τ_{ijk}^{UR} may be expressed similarly. Now consider, for a body occupying a domain V , the variational statement

$$\delta \int_V \left\{ \psi(\varepsilon_\gamma - \varepsilon_\lambda^p, \varepsilon_\lambda^p, \nabla \varepsilon_\lambda^p) + V_1((e_p)_\lambda) + V_2((E_p)_\lambda) - \sigma_{ij}^0(\varepsilon_{ij})_\gamma - \tau_{ijk}^0(\varepsilon_{ij}^p)_\lambda \right\} = 0, \quad (4.6)$$

the variation being taken with respect to ε_{k+1} and ε_{k+1}^p . Assuming that $\gamma > 0$, the variation with respect to ε_{k+1} provides the equation of equilibrium for the Cauchy stress over the domain V , and any associated

¹ The forward difference approximation would take $\gamma = \lambda = 0$. For the backward difference approximation, $\gamma = \lambda = 1$. Both have an error of order Δt . The central difference approximation is defined by $\gamma = \lambda = 1/2$ and has an error of order $(\Delta t)^2$.

traction boundary conditions on the boundary S , at time t_γ . Assuming that $\lambda > 0$, the variation with respect to ε_{k+1}^p yields the second equation of equilibrium in (1.2) and any higher-order traction condition at time t_γ . The fields σ_{ij}^0 , $q_{ij}^0 \equiv 0$ and τ_{ijk}^0 are required to satisfy the equations of equilibrium and any given traction boundary conditions but are otherwise arbitrary. (A similar incremental variational formulation can be developed for rate-dependent material response but this is not required in the present work.)

4.3 Plane-strain tension of a passivated strip

The domain V is now the strip defined by $-\infty < x_1 < \infty$, $-h < x_2 < h$. The material is assumed to be isotropic and incompressible. The only non-zero components of total strain are ε_{11} and $\varepsilon_{22} = -\varepsilon_{11}$ and similarly for the plastic strains: $\varepsilon_{22}^p = -\varepsilon_{11}^p$. These quantities are functions only of x_2 and the time-like variable t . It will be convenient to write ε for ε_{11} and ε^p for ε_{11}^p . The strain ε can be prescribed to be uniform, and is henceforth identified as the time-like variable. The step size Δt becomes $\Delta \varepsilon$ and $\varepsilon_k = \varepsilon_0 + k \Delta \varepsilon$. Since all boundary conditions (apart from those that define ε) are homogeneous, σ_{ij}^0 and τ_{ijk}^0 can be chosen to be zero. With these specializations, the variation in the principle (4.6) is taken only with respect to ε^p and the integration is only over $-h < x_2 < h$.

Attention will be focused on the first increment, $k = 1$, and the notation $y = \varepsilon_1^p - \varepsilon_0^p$ will be employed². For this first increment, the variational functional has no explicit dependence on x_2 , and therefore, writing the integrand in the variational functional as $f(y, y')$, the associated Euler - Lagrange equation has first integral $f(y, y') - y' \partial f / \partial y' = \text{constant}$.

To make progress, some further specialization is necessary. The free energy ψ is taken as

$$\psi(\varepsilon^e, \varepsilon^p, \nabla \varepsilon^p) = \frac{E}{3} \varepsilon_{ij}^e \varepsilon_{ij}^e + (1 - \alpha) \psi_p(\varepsilon_p, \varepsilon_p^*), \quad (4.7)$$

² For the first increment, $\varepsilon_0^p = 0$. Retention of ε_0^p allows the general formula to apply, with re-numbering, to any increment and also to the case of uniform straining with surfaces unpassivated up to a uniform plastic strain ε_0^p , as considered in [1].

with ψ_p given by (2.5), the form (2.4) already having been exposed as “unsatisfactory” in the sense of giving an elastic gap, even for deformation theory; and for the rate theory, in which ψ is identified physically as the free energy, it is not acceptable that q_{ij}^R and τ_{ijk}^R are not uniquely defined when $E_p = 0$. Note that, for the present problem, $\mathcal{E}_p = (2/\sqrt{3})\sqrt{(\varepsilon^p)^2 + \ell_R^2(\varepsilon^{p'})^2}$. The variable \dot{e}_p is taken as equivalent plastic strain-rate, and this becomes, for the present problem, $\dot{e}_p = (2/\sqrt{3})|\dot{\varepsilon}^p|$. The variable \dot{E}_p , in the first instance, will be taken as $\sqrt{\dot{e}_p^2 + \ell_{UR}^2(\dot{e}_p^*)^2}$, with $\dot{e}_p^* = \sqrt{2\dot{\varepsilon}_{ij,k}^p \dot{\varepsilon}_{ij,k}^p} / 3$ which becomes, in the present case, $\dot{e}_p^* = (2/\sqrt{3})|\dot{\varepsilon}^{p'}|$. The potentials V_1 and V_2 are taken as

$$V_1(e_p) = (1 - \alpha + \alpha\beta)\sigma_Y e_p \text{ and } V_2(E_p) = \alpha\sigma_Y \left((1 - \beta)E_p + \frac{k}{N+1}E_p^{N+1} \right)$$

with $\alpha, \beta \in [0, 1]$. The forms (4.7) and (4.8) deliver the basic power-law (1.4) in uniaxial tension, and they generalize the law (3.3).

To make the first integral of the Euler-Lagrange equation for the first increment completely explicit—and of manageable length— ε_0^p will be set to zero, and the definitions

$Y_R = \sqrt{y^2 + \ell_R^2 y'^2}$, $Y_{UR} = \sqrt{y^2 + \ell_{UR}^2 y'^2}$ will be employed. The required first integral is

$$\begin{aligned} & \frac{2E}{3}(\varepsilon_Y - \lambda y)^2 + (1 - \alpha)\sigma_Y \left[\frac{2\lambda y}{\sqrt{3}} - \frac{Nk}{N+1} \left(\frac{2\lambda}{\sqrt{3}} Y_R \right)^{N+1} + k \left(\frac{2\lambda}{\sqrt{3}} \right)^{N+1} y^2 Y_R^{N-1} \right] \\ & + (1 - \alpha + \alpha\beta)\sigma_Y \frac{2\lambda y}{\sqrt{3}} + \alpha\sigma_Y \left[(1 - \beta) \frac{2\lambda y^2}{\sqrt{3} Y_{UR}} - \frac{Nk}{N+1} \left(\frac{2\lambda}{\sqrt{3}} Y_{UR} \right)^{N+1} + k \left(\frac{2\lambda}{\sqrt{3}} \right)^{N+1} y^2 Y_{UR}^{N-1} \right] = c \end{aligned} \quad (4.10)$$

The constant c is fixed from the symmetry requirement that $y'(0) = 0$ which implies that

$Y_R(0) = Y_{UR}(0) = y(0) \equiv y_0$ where y_0 has yet to be determined. Thus,

$$c = \frac{2E}{3}(\varepsilon_Y - \lambda y_0)^2 + \sigma_Y \left[\frac{2\lambda y_0}{\sqrt{3}} + \frac{k}{N+1} \left(\frac{2\lambda y_0}{\sqrt{3}} \right)^{N+1} \right]. \quad (4.11)$$

Before continuing, normalized variables are introduced by defining $\varepsilon_Y = \sigma_Y / E$, and then

$$z = \frac{2\lambda y}{\sqrt{3}\varepsilon_Y}, \quad z_0 = \frac{2\lambda y_0}{\sqrt{3}\varepsilon_Y}, \quad \bar{z} = \frac{z}{z_0}, \quad Z_R = \frac{2\lambda Y_R}{\sqrt{3}}, \quad \bar{Z}_R = \frac{Z_R}{z_0}, \quad Z_{UR} = \frac{2\lambda Y_{UR}}{\sqrt{3}\varepsilon_Y}, \quad \bar{Z}_{UR} = \frac{Z_{UR}}{z_0}. \quad (4.12)$$

Equations (4.10), (4.11) now give

$$\begin{aligned}
& (1-\alpha) \left[\bar{z} - \frac{Nk\varepsilon_Y^N}{N+1} z_0^N \bar{Z}_R^{N+1} + k\varepsilon_Y^N z_0^N \bar{z}^2 \bar{Z}_R^{N-1} \right] \\
& + \alpha \left[(1-\beta) \frac{\bar{z}^2}{\bar{Z}_{UR}} - \frac{Nk\varepsilon_Y^N}{N+1} z_0^N \bar{Z}_{UR}^{N+1} + k\varepsilon_Y^N z_0^N \bar{z}^2 \bar{Z}_{UR}^{N-1} \right] + \alpha\beta\bar{z} \\
& = 1 - R_\gamma(1-\bar{z}) + \frac{1}{2} z_0(1-\bar{z}^2) + \frac{k\varepsilon_Y^N z_0^N}{N+1}, \tag{4.13}
\end{aligned}$$

where

$$R_\gamma = \frac{2\varepsilon_\gamma}{\sqrt{3}\varepsilon_Y}. \tag{4.14}$$

It is expedient now to consider special cases, as follows.

4.3.1 The case $\alpha = 0$

Equation (4.13) becomes

$$k\varepsilon_Y^N z_0^N \left[\frac{N}{N+1} \bar{Z}_R^{N+1} - \bar{z}^2 \bar{Z}_R^{N-1} \right] = (R_\gamma - 1)(1-\bar{z}) - \frac{1}{2} z_0(1-\bar{z}^2) - \frac{k\varepsilon_Y^N z_0^N}{N+1}. \tag{4.15}$$

Once this equation is solved for \bar{Z}_R , the solution of the differential equation to which it is equivalent follows as

$$\frac{x_2}{\ell_R} = \int_{\bar{z}}^1 \frac{d\bar{z}}{\sqrt{\bar{Z}_R^2 - \bar{z}^2}} \tag{4.16}$$

and finally for consistency, the requirement that $\bar{z} = 0$ when $x_2 = h$,

$$\frac{h}{\ell_R} = \int_0^1 \frac{d\bar{z}}{\sqrt{\bar{Z}_R^2 - \bar{z}^2}} \tag{4.17}$$

fixes z_0 .

For the purpose of asymptotic analysis, the term of order z_0 in (4.15) can be neglected to leave the equation

$$\frac{N}{N+1} \bar{Z}_R^{N+1} - \bar{z}^2 \bar{Z}_R^{N-1} = \frac{(R_\gamma - 1)(1-\bar{z})}{k\varepsilon_Y^N z_0^N} - \frac{1}{N+1}. \tag{4.18}$$

This equation cannot be solved in closed form, but substitution of its solution into (4.16) would yield an equation for the parameter $(R_\gamma - 1)/(k\varepsilon_Y^N z_0^N)$, requiring z_0 to be of order $(R_\gamma - 1)^{1/N}$. Thus, R_γ should be

close to 1, implying that $\varepsilon_0 = \varepsilon_Y$. Thus, as expected, there is no “gap” and $z_0 \propto (\Delta\varepsilon)^{1/N}$. Note that the form of dependence of z_0 on $\Delta\varepsilon$ is predicted consistently, for any choice of γ and λ . The constant of proportionality is given correctly by taking $\gamma = N^{N/(1-N)}$ and $\lambda = N^{1/(1-N)}$. Note also that, if the boundary of the strip were not passivated, the increment in plastic strain would have the same dependence on $\Delta\varepsilon$, though with different amplitude.

4.3.2 The case $\alpha = 1$

Equation (4.13) becomes

$$\frac{Nk\varepsilon_Y^N z_0^N}{N+1} \bar{Z}_{UR}^{N+2} = \bar{z}^2 \left(1 - \beta + k\varepsilon_Y^N z_0^N \bar{Z}_{UR}^N \right) - a(\bar{z}) \bar{Z}_{UR}, \quad (4.19)$$

where

$$a(\bar{z}) = 1 - \beta \bar{z} - R_\gamma (1 - \bar{z}) + \frac{1}{2} z_0 (1 - \bar{z}^2) + \frac{k\varepsilon_Y^N z_0^N}{N+1}. \quad (4.20)$$

The lowest-order asymptotic solution to (4.19) as $z_0 \rightarrow 0$ is as follows:

$$\bar{Z}_{UR} \sim \left[\left(\frac{N+1}{Nk\varepsilon_Y^N z_0^N} \right) (R_\gamma - 1 - (R_\gamma - \beta) \bar{z}) \right]^{\frac{1}{N+1}} \quad \text{if } 0 \leq \bar{z} < z^*$$

and

$$\bar{Z}_{UR} \sim \bar{z}^2 \left[1 - \left(\frac{R_\gamma - \beta}{1 - \beta} \right) (1 - \bar{z}) \right]^{-1} \quad \text{if } z^* < \bar{z} \leq 1, \quad (4.21)$$

where

$$z^* = \frac{R_\gamma - 1}{R_\gamma - \beta}. \quad (4.22)$$

Substituting the asymptotic forms (4.21) into (4.17) requires the calculation of two integrals:

$$\int_0^{z^*} \frac{d\bar{z}}{\sqrt{\bar{Z}_{UR}^2 - \bar{z}^2}} \sim \int_0^{z^*} \frac{d\bar{z}}{\bar{Z}_{UR}} \sim (k\varepsilon_Y^N)^{1/(N+1)} \left(\frac{(N+1)z_0}{N} \right)^{N/(N+1)} \frac{(R_\gamma - 1)^{N/(N+1)}}{R_\gamma - \beta} \quad (4.23)$$

and³

³ The integral to follow is obtained via the variable transformation $\cos \theta = \bar{z} / [1 - \hat{R}(1 - \bar{z})]$, as in [1].

$$\int_{z^*}^1 \frac{d\bar{z}}{\sqrt{\bar{Z}_{UR}^2 - \bar{z}^2}} \sim \frac{2\hat{R}}{\sqrt{\hat{R}^2 - 1}} \tan^{-1} \left[\left(\frac{\hat{R}+1}{\hat{R}-1} \right)^{1/2} \right] - \frac{\pi}{2}, \quad (4.24)$$

where

$$\hat{R} = \frac{R_\gamma - \beta}{1 - \beta}. \quad (4.25)$$

The integral (4.24) decreases monotonically from $+\infty$ to 0 as \hat{R} increases from 1 to ∞ . It is therefore *impossible* to satisfy equation (4.17) unless \hat{R} is *at least* \hat{R}_c , the value of \hat{R} for which that integral equals h / ℓ_{UR} . Thus, an elastic gap is predicted⁴. Plastic flow does not commence until ε reaches a value $\varepsilon_0 > \varepsilon_Y$, corresponding to the attainment of \hat{R}_c . Now when ε is increased to $\varepsilon_0 + \Delta\varepsilon$, the associated value of z_0 is obtained when the integral (4.23) exactly compensates for the shortfall of (4.24) below h / ℓ_{UR} .

To first order,

$$\int_{z^*}^1 \frac{d\bar{z}}{\sqrt{\bar{Z}_{UR}^2 - \bar{z}^2}} \sim h / \ell_{UR} - \frac{1}{\hat{R}_c(\hat{R}_c^2 - 1)} \left[h / \ell_{UR} + \pi / 2 + \hat{R}_c \right] (\hat{R} - \hat{R}_c). \quad (4.26)$$

Completing the algebra gives the result

$$\frac{2\lambda y_0}{\sqrt{3}\varepsilon_Y} \sim \frac{N+1}{Nk^{1/N}\varepsilon_Y(1-\beta)(\hat{R}_c-1)} \left[\frac{h / \ell_{UR} + \pi / 2 + \hat{R}_c}{\hat{R}_c^2 - 1} \right]^{\frac{N+1}{N}} \left(\frac{2\gamma\Delta\varepsilon}{\sqrt{3}\varepsilon_Y} \right)^{\frac{N+1}{N}}. \quad (4.27)$$

This result is asymptotically exact if $\gamma = (N / (N+1))^N$ and $\lambda = (N / (N+1))^N$. Remarkably, this exact result for y_0 is also produced by the choices $\gamma = \lambda = 1$, corresponding to the use of the (inexact) “backward Euler” approximation.

It should be noted that the derivation given is far from rigorous: the asymptotic approximations (4.21) break down near $\bar{z} = z^*$, and there is also a serious problem in obtaining a good approximation near $\bar{z} = 1$ when $z_0 > 0$. We have, however, performed analysis that shows that terms neglected are of lower order than those retained; these details are omitted here, for the sake of brevity.

4.3.3 The case $\ell_R = \ell_{UR}$

⁴ Strictly, it is necessary to demonstrate that there exist fields q^{UR} and τ^{UR} that do not exceed the yield criterion, when $\hat{R} < \hat{R}_c$. This demonstration was made in a slightly different context in [1]; it is omitted here.

Equation (4.13) becomes

$$\frac{Nk\varepsilon_Y^N z_0^N}{N+1} \bar{Z}_R^{N+2} = \bar{z}^2 \left[\alpha(1-\beta) + k\varepsilon_Y^N z_0^N \bar{Z}_R^N \right] - \left[1 + (1-\alpha + \alpha\beta)\bar{z} - R_\gamma(1-\bar{z}) + \frac{1}{2}(1-\bar{z}^2) + \frac{k\varepsilon_Y^N z_0^N}{N+1} \right] \bar{Z}_R. \quad (4.28)$$

This has exactly the same form as (4.19) and gives the same type of delay, basically induced by the term $\alpha(1-\beta)\bar{z}^2 / \bar{Z}_{UR}$ in (4.13).

4.3.4 The case $\alpha = 1$, $\beta = 1$

The analysis of subsection 4.3.2 becomes non-uniform as β approaches 1. The value R_c of R_γ that corresponds to \hat{R}_c (which is fixed) tends to 1 as $\beta \rightarrow 1$, implying that the elastic gap reduces to zero. Correspondingly, the size of $\Delta\varepsilon$ for which the asymptotic formula has validity tends to zero. Furthermore, when $\beta = 1$, equation (4.19) reduces exactly to (4.18) to leading order, except that ℓ_R is replaced by ℓ_{UR} , so z_0 becomes proportional to $(\Delta\varepsilon)^{1/N}$.

4.3.5 A class of non-recoverable laws that display no gap under stretch-passivation

There does, however, remain a difference between the cases for which the gradient term is recoverable or non-recoverable. The present problem does not show it, but if the strip were subjected to plane-strain tension with unpassivated boundaries, and then strain increased following passivation, as discussed in [1], a gap would still be displayed with the present constitutive law⁵.

Now here is a non-recoverable law that will display no gap under stretch-passivation; it is a slight generalization of the law (3.2). The free energy is unchanged, but E_p is chosen to be $\ell_{UR} e_p^*$ and

$$V_1(e_p) = \sigma_Y \left[e_p + \frac{\alpha k}{N+1} e_p^{N+1} \right], \quad V_2(\ell_{UR} e_p^*) = \alpha \sigma_Y \frac{k^*}{N+1} (\ell_{UR} e_p^*)^{N+1}. \quad (4.29)$$

This leads to the equation

$$(1-\alpha) \left[\frac{N}{N+1} \bar{Z}_R^{N+1} - \bar{z}^2 \bar{Z}_R^{N-1} \right] - \frac{\alpha}{N+1} \bar{z}^{N+1} + \frac{\alpha N(k^*/k)}{N+1} (\ell_{UR} |\bar{z}'|)^{N+1}$$

⁵ We refrain from recording the analysis, in the interest of conciseness.

$$\sim \frac{(R_\gamma - 1)(1 - \bar{z})}{k \varepsilon_Y^N z_0^N} - \frac{1}{N + 1}. \quad (4.30)$$

This is similar in character to (4.18) and displays no gap. In the case $\alpha = 1$ the parameter

$(R_\gamma - 1)/(k \varepsilon_Y^N z_0^N)$ is fixed by the requirement

$$\left(\frac{Nk^*}{k} \right)^{\frac{1}{N+1}} \int_0^1 \left[(N+1) \left(\frac{R_\gamma - 1}{k \varepsilon_Y^N z_0^N} \right) (1 - \bar{z}) - (1 - \bar{z}^{N+1}) \right]^{\frac{1}{N+1}} d\bar{z} = \frac{h}{\ell_{UR}}. \quad (4.31)$$

This is, of course, only one representative of a class of laws. The essential feature is that V_2 should be a function of *any* positively homogeneous function $\ell_{UR} e_P^*$ of degree 1, of $\ell_{UR} \varepsilon_{ij,k}^p$ only, with the additional property that $V_2'(0) = 0$. However, as argued in Section 3.2, such theories will still display gaps for problems in which non-uniform plastic strain is developed prior to passivation.

Still continuing with the case $\alpha = 1$, if there is already a plastic strain ε_0^p , the equation governing the increment is

$$\begin{aligned} \frac{2}{3\varepsilon_Y} [\varepsilon_\gamma - (\varepsilon_0^p + \lambda y)]^2 + \frac{2(\varepsilon_0^p + \lambda y)}{\sqrt{3}} + \frac{k}{N+1} \left(\frac{2(\varepsilon_0^p + \lambda y)}{\sqrt{3}} \right)^{N+1} \\ + \frac{k^*}{N+1} \left(\frac{2\ell_{UR}}{\sqrt{3}} \right)^{N+1} |\varepsilon_0^{p'} + \lambda y'|^N (\varepsilon_0^{p'} - N y') \operatorname{sgn}(\varepsilon_0^{p'} + \lambda y') = c. \end{aligned} \quad (4.32)$$

If the strip is stretched uniformly prior to passivation at plastic strain ε_0^p , then $y'(0) = 0$ and this equation implies

$$\frac{Nk^* \varepsilon_Y^N}{N+1} (\ell_{UR} |z'|)^{N+1} = \left[\frac{2\varepsilon_\gamma}{\sqrt{3}} - \left(1 + k \varepsilon_Y^N \left(\frac{2\lambda \varepsilon_0^p}{\sqrt{3}\varepsilon_Y} \right)^N \right) \right] (z_0 - z) \quad (4.33)$$

which delivers no gap. If, however, ε_0^p depends on x_2 , the presence of $\varepsilon_0^{p'}$ alters this conclusion. The derivation of (4.33) made use of a Taylor expansion, valid for $\Delta\varepsilon \ll \varepsilon_0^p$, which is why it does not reduce exactly to (4.30) (with $\alpha = 1$) when $\varepsilon_0^p \rightarrow 0$.

5 A basic gap-free incremental theory

The incremental formulation introduced in Section 3.3 is a gap-free incremental strain gradient plasticity which reduces to classical J_2 flow when the gradients are sufficiently small. It will be implemented to illustrate several aspects of behavior of a stretched layer under passivation. In the examples, the input tensile relation (1.4), $\sigma_0(\varepsilon_p) = \sigma_Y (1 + k\varepsilon_p^N)$, is again used and we take $\alpha = 1$ such that the dissipation function is $\varphi = \sigma_0(e_p)\dot{e}_p$. The contribution of the plastic strain gradients to the free energy in (3.10) is taken to be

$$f(\varepsilon_p^*) = \frac{\sigma_Y k}{N+1} (\ell_R \varepsilon_p^*)^{N+1} \quad \text{with} \quad \tau_{ijk}^R = \frac{2\sigma_Y k \ell_R (\ell_R \varepsilon_p^*)^N}{3} \frac{\varepsilon_{ij,k}^P}{\varepsilon_p^*} \quad (5.1)$$

In making the above choice for $f(\varepsilon_p^*)$, we have followed [12,13] by assuming that geometrically necessary dislocations associated with ε_p^* contribute to the hardening with a functional dependence that is similar to that of the statistically stored dislocations generated by e_p . In this particular case, the stress increase due to e_p is $\sim \sigma_Y k e_p^N$ while the corresponding stress generated by $f(\varepsilon_p^*)$ is $\sim \sigma_Y k (\ell_R \varepsilon_p^*)^N$. We will return to the issue of identifying $f(\varepsilon_p^*)$ shortly.

The average stress as a function of strain for a layer of thickness $2h$ which is passivated from the start and stretched in plane strain tension has been computed for the theory defined above. For this one-dimensional problem, because $\dot{e}_p = \dot{\varepsilon}_p$ and $e_p^* = \varepsilon_p^*$, it is readily shown that the solution is identical to that of the corresponding deformation theory with $\alpha = 0$ in Section 3.3. This correspondence has been exploited in generating the numerical results. The stress-strain behavior is plotted in Fig. 4 with associated results in Fig. 5. Fig. 5a shows the emergence of the plastic strain at the center of the layer after yield, comparing the exact numerical result with an analytical asymptotic result. Fig. 5b plots the distribution of the normalized plastic strain across one half of the layer at a particular imposed strain.

The stress-strain curves in Fig. 4 have no gaps at initial yield yet they reveal substantial increases in flow strength in the early stages of plastic deformation due to strain gradient effects. Thus, the functional form for $f(\varepsilon_p^*)$ adopted in (5.1) gives rise to both early flow strength elevation and subsequent hardening elevation, even though the gradient contributions are entirely recoverable. There are more than a few theories in the literature with aspects in common with the basic theory in this section with unrecoverable contributions to q_{ij} and only recoverable

contributions to τ_{ijk} . Among them are papers on isotropic theories [4,7,11,14] and on single crystal theories [15,16]. To our knowledge, all except [16] have taken $f(\varepsilon_p^*)$, or its equivalent, to have a quadratic dependence on the gradients of plastic strain. A quadratic dependence on gradients does not display the strength elevation seen in Fig. 4, but, instead, it only reveals an increase in linear hardening behavior. Apparently, for this reason, a mistaken notion has taken hold in the literature that recoverable gradient effects contribute to hardening but not to strengthening. The argument for taking $f(\varepsilon_p^*) \sim (\ell_R \varepsilon_p^*)^{N+1}$ with N as the tensile hardening exponent is phenomenological but with some physical basis for metals with well-developed microstructures such as precipitates or dislocation cell structures [12,13]. The single crystal formulation applied to the grain size effect on strength in [16] estimated the free energy of geometrically necessary dislocations using the self-energy of a dilute distribution of dislocations giving a strictly linear dependence of the free energy on the plastic strain gradients. This choice gives a gap at initial yield noted by the authors. Evaluation of $f(\varepsilon_p^*)$ using fundamental dislocation computations is likely to be a fruitful point of contact between continuum theory and discrete dislocation theory. Some preliminary results [17] along these lines for an elementary, non-dilute distribution of geometrically necessary dislocations suggest that $f(\varepsilon_p^*)$ is not quadratic but nearly linear in ε_p^* .

The theory in this section has also been applied to the stretch-passivation problem considered in [1] where an unpassivated layer is first stretched into the plastic range and then passivated followed by further stretch. Prior to passivation the stress and strain distributions are uniform. After passivation the distributions become non-uniform and the problem requires an incremental step-by-step solution procedure. A numerical example is shown in Fig. 6 computed using minimum principle II in (3.7). There is no elastic loading gap after passivation, but there is a short rapid rise in the average stress analogous to that at initial yield. This is due to the fact that the stress contribution of the gradients is proportional to $(\ell_R \varepsilon_p^*)^N$.

6 Conclusions

This paper has focused on identifying, analyzing and possibly eliminating elastic loading gaps which arise in some formulations of strain gradient plasticity at initial yield and under non-

proportional loading histories. While physical arguments against elastic loading gaps can be put forward, the view taken in this paper is that it is premature to prejudge the outcome on this matter until experiments and more fundamental dislocation studies concerning the existence of gaps become available. Discrete dislocation models of boundary value problems of the type analyzed in this paper, if properly formulated and interpreted, should be capable of providing qualitative insight into the existence, or lack thereof, of elastic loading gaps. Also, the insights so gained might assist the design of experiments to test the existence or otherwise of gaps. The approach here has been to identify the features of the continuum constitutive laws which give rise to the gaps and to present a selection of examples which illustrate how to analyze the gaps and the early stage when plastic flow resumes. These problems can be fairly complex with unusual boundary layer behavior. While not exhaustive, the analysis in Section 4 illustrates a variety of behaviors that can arise.

Relatively simple guidelines emerge for ensuring that there are no gaps at initial yield. A general finding is that all non-incremental formulations which contain unrecoverable (dissipative) contributions dependent on the gradients of plastic strain will necessarily produce elastic loading gaps for some problems. To date, it appears no thermodynamically acceptable recipes exist for an incremental formulation with dissipative contributions dependent on the gradients of plastic strain.

An attractive gap-free, generalization of J_2 flow theory incorporating strain gradients has been identified. The theory is incremental with recoverable and unrecoverable contributions and a well-defined yield surface. The contributions from the gradients of plastic strain are entirely recoverable. The examples considered in this work offer some guidance for the interpretation of experiments on passivated layers.

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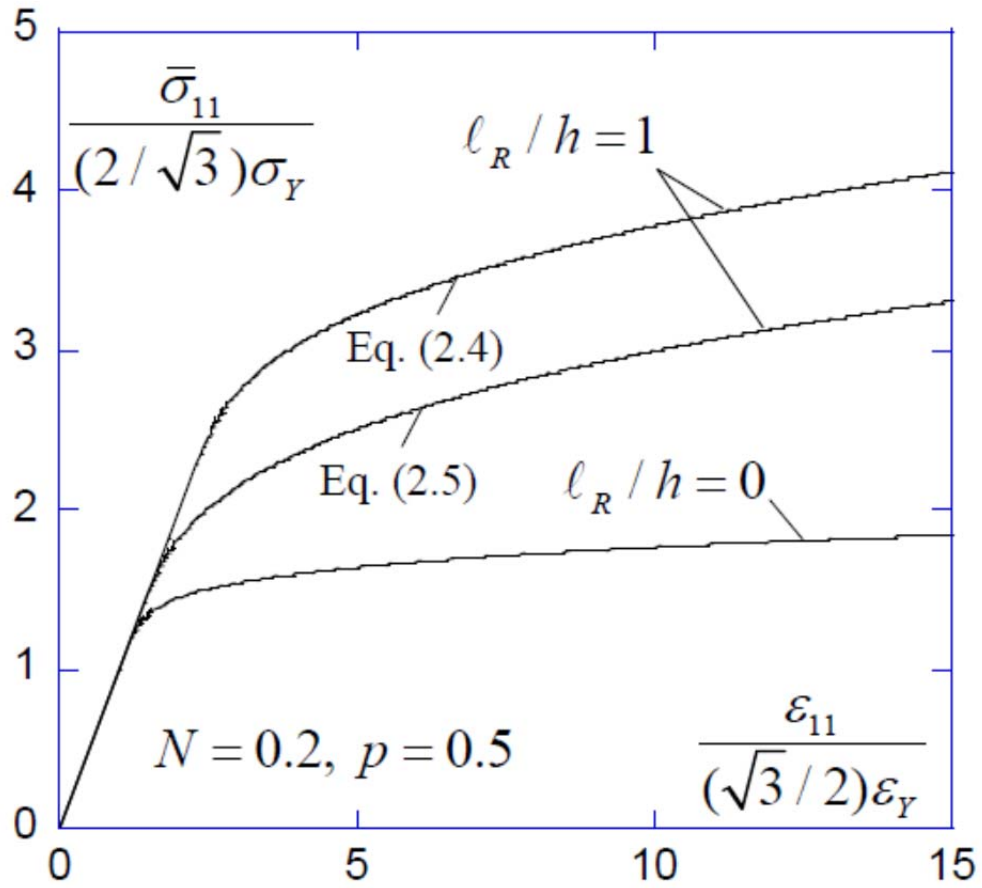


Fig. 1 Comparison overall stress-strain response based of deformation theory for a layer of thickness $2h$ with surfaces passivated from the start and stretched in plane strain. The material is incompressible. The lower curve is applies to an unpassivated layer or, equivalently, a layer with $\ell_R/h = 0$. The upper two curves have $\ell_R/h = 1$. The top curve is based on formulation (2.4), and it has an elastic loading gap on the vertical axis from 1 to 1.825. The middle curve is based on (2.5) and it has no elastic loading gap.

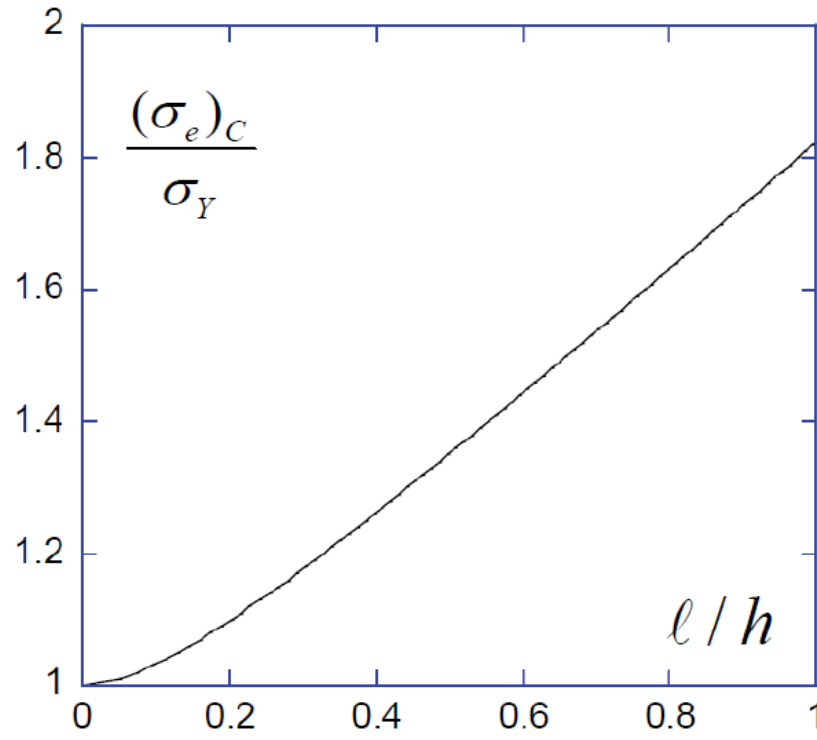


Fig. 2 Elastic loading gap at the onset of yield for a passivated layer in plane strain for the deformation theory based on formulation (2.4) with $\ell = \ell_R$. This same gap arose for the non-incremental theory considered in [1] for a layer stretched into the plastic range and then passivated followed by further stretch with $\ell = \ell_{UR}$.

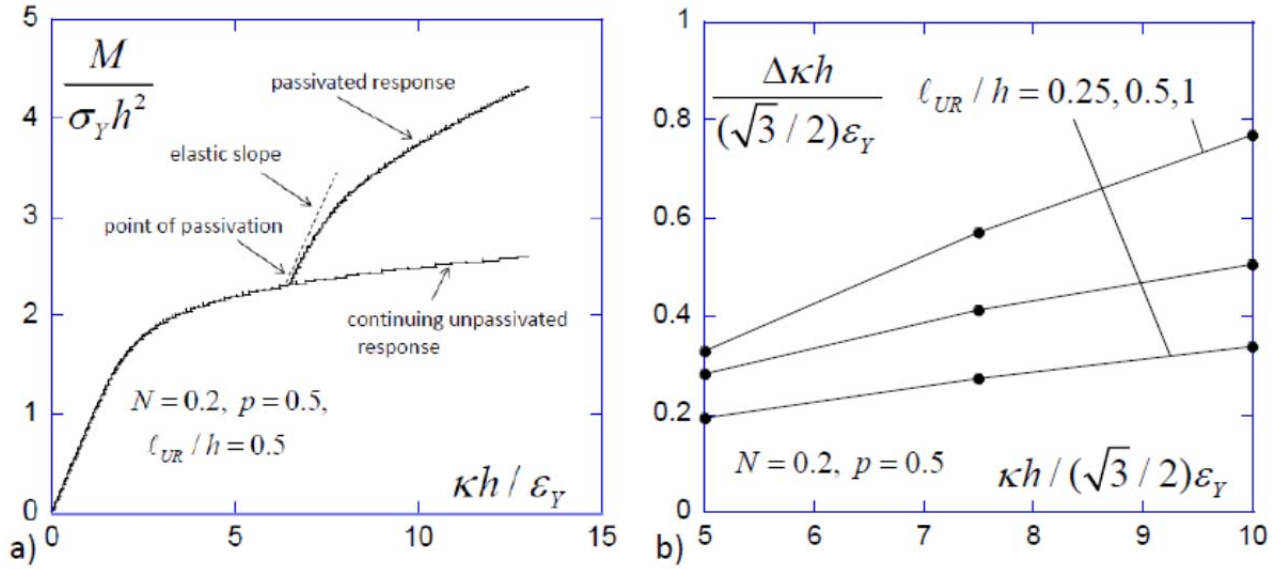


Fig. 3 Pure bending in plane strain with no passivation followed by continued bending with passivation. The constitutive law is specified by a dissipation potential φ given by (3.2) with no recoverable contributions. The material is taken to be incompressible and the computation in a) is carried out using the rate-dependent version with a strain-rate exponent $m = 0.1$, as in [1]. The elastic loading gap as specified by the curvature increase $\Delta\kappa$ after passivation without plastic flow is plotted as a function of the curvature κ at passivation in b). The predictions in b) are based on the rate-independent formulation and minimum principle I (3.9).

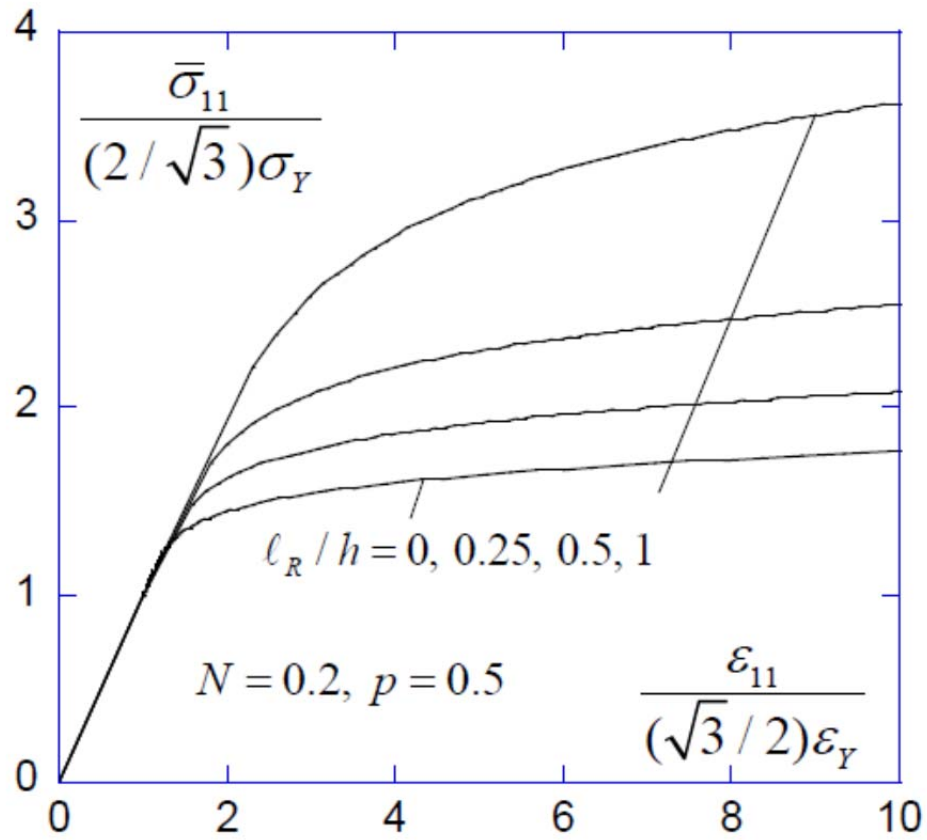


Fig. 4 Average stress versus stretching strain for a passivated layer specified by the gap-free incremental theory defined in Section 5. The material is incompressible and the deformation is plane strain.

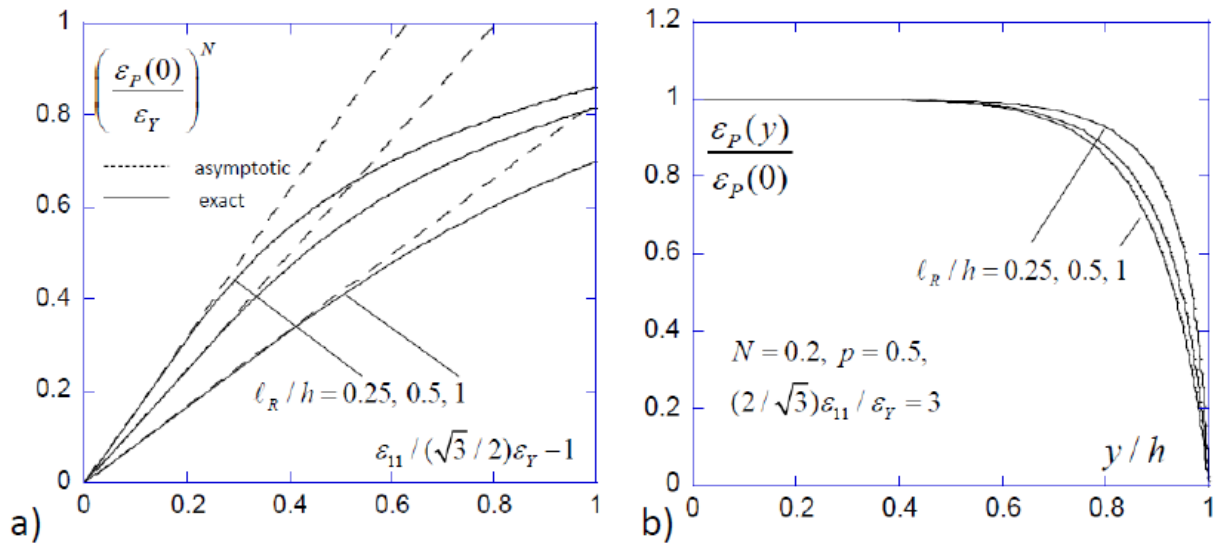


Fig. 5 a) The plastic strain at the center of the passivated layer as a function of the strain imposed on the layer—a comparison between asymptotic and exact results. b) The distribution of the normalized plastic strain across the layer at $2\varepsilon_{11}/\sqrt{3} = 3\varepsilon_Y$. In both parts, for the incompressible, incremental material in Section 5 with $N = 0.2$ and $p = 0.5$.

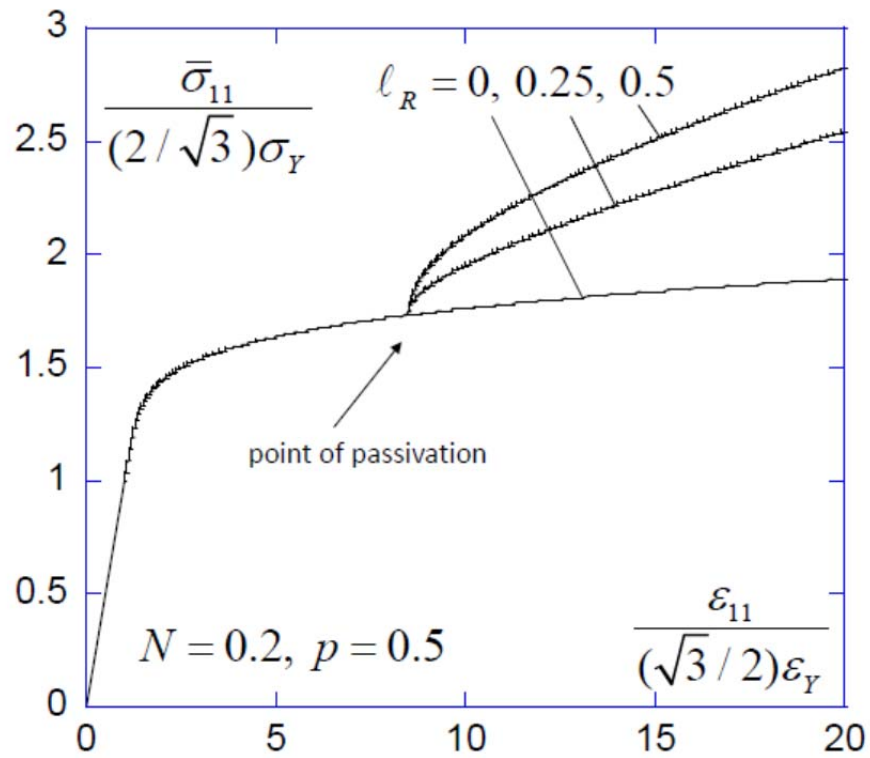


Fig. 6 An unpassivated layer of thickness $2h$ stretched into the plastic range and then passivated followed by additional stretch, as predicted by the incremental theory in Section 5 for an incompressible layer in plane strain.