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A VARIATIONAL PRINCIPLE FOR GRADIENT PLASTICITY

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Abstract—We elaborate on a generalized plasticity model which belongs to the class of gradient models suggested earlier by Aifantis and co-workers. The generalization of the conventional theory of plasticity has been accomplished by the inclusion of higher-order spatial gradients of the equivalent plastic strain in the yield condition. First it is shown how these gradients affect the critical condition for the onset of localization and allow for a wavelength selection analysis leading to estimates for the width and/or spacing of shear bands. Due to the presence of higher-order gradients, additional boundary conditions for the equivalent plastic strain are required. This question and also the associated problem of the formulation and solution of general boundary value problems were left open in the previous work. We demonstrate here that upon assuming a certain type of additional boundary conditions, the structural symmetries of the gradient-dependent constitutive model are such that there exists a variational principle for the displacement rates and the rate of the equivalent plastic strain. The variational principle can serve as a basis for the numerical solution of boundary value problems in the sense of the finite element method. Explicit expressions for the tangent stiffness matrix and the generalized nodal point forces are given.

1. INTRODUCTION

The recent interest in generalized continuum plasticity theories has its origin in certain serious drawbacks of the conventional theory in the case of strain-softening materials. For such materials, critical configurations exist (e.g. at the insertion of shear bands and other bifurcation points) where the governing differential equations change type (e.g. from elliptic to hyperbolic), thus making it impossible to use the same mathematical setting in the post-critical or post-bifurcation regime where the deformation starts to localize along narrow shear or fracture zones.

The absence of any characteristic or internal length from conventional shear band analyses has left the size of the localized strain zone unspecified and has led to a critical dependence of finite element solutions on the employed finite element mesh size. Furthermore, if the material does not have a residual strength, the energy dissipated in the localized zone tends to zero as the mesh is refined, a fact which is physically unreasonable [e.g. Lasry and Belytschko (1988)]. Some of these features have first been documented by numerical examples for simple strain-softening materials by Schreyer and Chen (1984) and Bazant (1984). More details and references on these aspects can be found in the papers by Pijaudier-Cabot *et al.* (1988) and Lasry and Belytschko (1988).

The mathematical model difficulties mentioned above reflect the physical fact that upon localization the limit of the range of validity of the conventional theory is reached. In models without any internal length or higher-order continuum structure, it should be expected that the deformation is homogeneous on the scale of the characteristic volume element of the material. Thus, no matter how small this scale may be, if the material is capable of developing intense deformation zones (e.g. Dirac delta-like deformation regions), it is obvious that the situation cannot be described by such models.

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The physical range of validity of continuum methods can be extended by adopting a generalized continuum approach [see Kröner (ed.) (1968) for examples]. In these theories, internal length scales are introduced by the consideration of higher-order deformation gradients in the constitutive relations [e.g. Mindlin (1965)] or additional degrees of freedom are assumed as in the Cosserat theory [or Mindlin's (1964) generalization of it: see Schaefer (1962) and Herrmann (1972) for reviews on this subject]. It now appears that it is in the region near bifurcation or instability points that these higher-order continuum theories are most useful as they provide the necessary mathematical structure for describing the material's response in the post-instability regime. Moreover, it turns out that such a description is possible by employing relatively-simple and physically-motivated modifications rather than the full and rather complex available generalized theories.

In the case of Cosserat-type theories, this was illustrated in the papers by Mühlhaus (1985, 1986, 1989); Mühlhaus and Aifantis (1989); Mühlhaus and Triantafyllides (1987); Mühlhaus and Vardoulakis (1986, 1987). In particular, it was shown that materials with a regular block structure, as well as layered and granular materials, can be modelled in an easy and elegant way by employing a specific Cosserat plasticity theory. It thus appears that in this case a standard application of the generalized theories would lead to an unnecessary complexity of the model. Similarly, in the case of higher-order gradient theories, it was shown by Aifantis (1984a, b, c, 1985, 1987, 1989) that inclusion of the second gradient of deformation in the expression of strain energy [for hyperelastic materials see Triantafyllidis and Aifantis (1986)] or flow stress (for plastic materials) is sufficient to preserve ellipticity in the governing equilibrium equations in the softening regime and determine, among other things, the width of shear bands. In connection with these gradient theories it is emphasized that their structure is such that it permits an interesting non-linear analysis in the softening or post-localization regime which, among other things, allows one to distinguish between shear-band width and spacing. This distinction is not possible within the classical linear treatment of the subject.

In view of the above discussion we consider here materials where microstructural effects become significant only at the onset of localization. In this connection we take advantage of the already well-established fact that the conventional (without higher-order gradients) theory satisfactorily predicts the orientation of the localized deformation zones. Consequently, in our modification of the conventional theory we leave the elasticity law and the flow rule unaltered and modify only the yield condition. The latter is accomplished by the inclusion of second- and fourth-order gradients of the equivalent plastic strain characterizing the influence of the underlying heterogeneously-evolving microstructure. As mentioned earlier, a theory for rigid plastic materials where only the second gradient was included was first suggested by Aifantis (1984a, b, c, 1987), Zbib and Aifantis (1988) and Coleman and Hodgdon (1985). The consideration of the fourth-order gradient results in a mathematical structure allowing already in a linear stability analysis the study of salient features (e.g. the determination of preferred wavelengths) of the localized deformation pattern. This is not possible if only the second gradient is included in the yield condition [see also Zbib and Aifantis (1988)].

The paper is organized as follows: in Section 2 an outline of the constitutive equations pertaining to the present gradient theory of plasticity is given. For simplicity and without loss of generality for our purposes, infinitesimal deformations are assumed. In Section 3 some of the implications of higher-order gradients are discussed within the scope of linear bifurcation analysis with emphasis being placed on critical conditions for shear banding. In Section 4 it is shown that for certain non-standard boundary conditions the structural symmetries of the constitutive gradient-dependent equation are such that there exists a variational principle for the displacement rates and the equivalent plastic strain rates (which are treated here as independent variables). The variational principle provides a convenient setting for the numerical solution of boundary value problems in the sense of the finite element method. Therefore, for completeness, in Section 5 explicit representations of the effective tangent stiffness matrix and the generalized nodal point forces are derived.

2. GRADIENT-DEPENDENT PLASTICITY

In this section we provide a modification of the classical theory of rate-independent plasticity by incorporating higher-order gradients of the equivalent plastic strain into the yield condition. First, however, we summarize the notation used:

The inner product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted as usual by $\mathbf{a}\cdot\mathbf{b}$, while the dyadic or tensor product is denoted by $\mathbf{a}\otimes\mathbf{b}$ and defined by the relations $(\mathbf{a}\otimes\mathbf{b})\mathbf{u} = \mathbf{a}(\mathbf{b}\cdot\mathbf{u})$ for all vectors $\mathbf{u}$. The inner product of two tensors $\mathbf{A}$ and $\mathbf{B}$ is defined by $\mathbf{A}\cdot\mathbf{B} = \mathrm{tr}(\mathbf{AB}^T)$ where tr denotes trace and T transpose. It then follows that $(\mathbf{a}\otimes\mathbf{b})\cdot(\mathbf{c}\otimes\mathbf{d}) = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d})$. The symbol ∇ denotes the gradient operator, and $\nabla^{2n} = (\nabla\cdot\nabla)^n$. The deviator of the stress tensor $\boldsymbol{\sigma}$ is denoted as $\boldsymbol{\sigma}'$, $\mathbf{u}$ is the displacement vector and we assume $|\nabla\mathbf{u}| \ll 1$. Then the expression $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$ defines the infinitesimal strain tensor. Upon purely elastic deformation we have $\dot{\boldsymbol{\sigma}} = \mathbf{C}[\dot{\boldsymbol{\varepsilon}}]$ where $\mathbf{C}$ is the elasticity tensor. According to the usual practice in infinitesimal elastoplasticity we assume that $\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e+\dot{\boldsymbol{\varepsilon}}^p$. The equivalent stress and plastic strain rate are given respectively by $\tau = \sqrt{\frac{1}{2}\boldsymbol{\sigma}'\cdot\boldsymbol{\sigma}'}$ and $\dot{\gamma} = \sqrt{2\dot{\boldsymbol{\varepsilon}}'^p\cdot\dot{\boldsymbol{\varepsilon}}'^p}$.

For isotropic hardening (softening) plasticity, the appropriate von Mises yield condition reads

$$F = \tau - \kappa[\gamma] = 0 \tag{1}$$

where $\gamma = \int \dot{\gamma}\, dt$ and κ is the flow stress with the symbol [ ] being introduced to allow a possible non-local dependence; i.e. κ is, in general, a function of γ. On assuming an associated flow rule [e.g. Hill (1950)] as justified, for example, on the basis of dislocation mechanics (Aifantis, 1987), we can then write

$$\dot{\boldsymbol{\varepsilon}} = \mathbf{C}^{-1}[\dot{\boldsymbol{\sigma}}]+\dot{\gamma}\frac{\boldsymbol{\sigma}'}{2\tau}, \tag{2}$$

where $F \leqslant 0$, $F\dot{\gamma} \equiv 0$ and $\dot{\gamma} \geqslant 0$. The equivalent plastic strain rate $\dot{\gamma}$ is determined from the consistency condition

$$\dot{F} = \dot{\tau} - \dot{\overline{\kappa[\gamma]}} = 0. \tag{3}$$

In the classical theory of plasticity it is usually assumed that the flow stress κ depends on the equivalent plastic strain γ alone. This may be appropriate for nearly homogeneous deformations and specific forms of $\kappa[\gamma]$ are often justified on the basis of homogeneously-evolving microstructures (e.g. dislocations) whose "homogeneous" motion is directly related to the observable "homogeneous" plastic deformation. While for many deformation processes such an assumption of homogeneity holds true, this is not the case with shear banding problems where the deformation localizes in narrow zones and homogeneity is lost at the scale of the element. Naturally, in this case, the hardening/softening function has to be modified to account for the heterogeneous evolution of deformation or the net local flux of microstructures inducing it (Mühlhaus and Aifantis, 1989). Here we accomplish this modification by assuming, as originally suggested by Aifantis (1984a, b, c, 1985), that κ depends on the gradients of γ as well. The gradient terms supplement the conventional model with information on the material's behaviour on the next smaller length scale. For instance, it is well known (Aifantis, 1989; Harren *et al.*, 1988) that macroscopic shear bands are often made up of mini deformation bands which are separated by lamellae of elastically-unloaded material. In this case the internal length scale introduced by the gradient terms is related to the average thickness of the lamellae. In a slightly different context, Kratochvil (1988) has used a non-local hardening model in connection with a dipole drift mechanism to explain the formation of certain dislocation patterns. By expanding the convolution integral of his non-local hardening law in a Taylor series, a model is obtained similar to the one which is considered in this paper.

We suppose further that the dependence of κ on the gradients of γ is linear so that it follows from the assumed isotropy that such a dependence can only involve gradients of even order $\nabla^{2n}\gamma$, $n = 0, 1, \ldots$. Retaining only terms up to $n = 2$, we then have [see also Zbib and Aifantis (1988, 1989a, b)]:

$$\kappa[\gamma] = c_0 + c_1\nabla^2\gamma + c_2\nabla^4\gamma, \tag{4}$$

where $c_i = c_i(\gamma)$. Rigid plastic versions of (1), (2), (4) with $c_2 = 0$ and $c_1 < 0$ have been discussed by Aifantis (1987) and Coleman and Hodgdon (1985) in relation to non-linear shear-band analyses. In passing, we note that the unloading criterion assumed by Coleman and Hodgdon differs from the one used here and by Aifantis. It implies an additional boundary condition for γ, namely $\nabla^2\gamma = 0$, on the rigid/plastic boundary. As already mentioned in the Introduction, we proceed here along different lines and deduce the possible forms of the additionally-required boundary conditions from a variational principle. [In this connection, we point out that the problem of boundary conditions for a related problem dealing with the dynamic stability and the corresponding Lyapunov function of a one-dimensional solid with higher-order gradients and viscosity was recently considered by Kuttler and Aifantis (1989).]

In recent papers, Lasry and Belytschko (1988) and Pijaudier-Cabot *et al.* (1988) studied localization phenomena in a rod under uniaxial dynamic loading. In one of the constitutive models considered, the assumption was made that the stress at a position x depends on the average strain within some symmetric neighbourhood of x. This non-local hypothesis [see also Aifantis (1984a, b, c) and Bazant and Lin (1988)] contains the proposed gradient modification and it is instructive to elaborate on this a little more within the present context. Thus on assuming that τ is a function of the average strain $\bar{\gamma}$, we have

$$\tau = g(\bar{\gamma}), \quad \bar{\gamma} = \frac{1}{V_s}\int_{V_s} \gamma(\mathbf{x}+\mathbf{s})\,\mathrm{d}V_s, \tag{5}$$

where, in view of the assumed isotropy, we have $|s| \leqslant R$ and $V_s = \frac{4}{3}\pi R^3$ and where R is an internal characteristic length. The definition $(5)_2$ can be generalized by the inclusion of a weighting function in the integrand (Bazant *et al.*, 1984). To bring out similarities between (4) and (5) we first expand $\gamma(\mathbf{x}+\mathbf{s})$ into a Taylor series about $\mathbf{s} = \mathbf{0}$. We have

$$\gamma(\mathbf{x}+\mathbf{s}) \approx \gamma + \nabla\gamma\cdot\mathbf{S} + \frac{1}{2!}\nabla^{(2)}\gamma\cdot\mathbf{S}^{(2)} + \frac{1}{3!}\nabla^{(3)}\gamma\cdot\mathbf{S}^{(3)} + \frac{1}{4!}\nabla^{(4)}\gamma\cdot\mathbf{S}^{(4)} + \cdots \tag{6}$$

where $\mathbf{S}^{(2)} = \mathbf{s}\otimes\mathbf{s}$, $\mathbf{S}^{(n)} = \mathbf{s}\otimes\ldots n\text{-times}\ldots\otimes\mathbf{s}$ and the dot $\cdot$ again denotes inner product between nth-order tensors. In view of the fact that $\int\nabla^{(2n+1)}\cdot\mathbf{S}^{(2n+1)}\,\mathrm{d}V_s = 0$, it then follows by simple integration that

$$\bar{\gamma} \approx \gamma + \frac{1}{V_s}\left(\frac{1}{2!}\frac{4\pi R^5}{15}\nabla^2\gamma + \frac{1}{4!}\frac{4\pi R^7}{35}\nabla^4\gamma + \cdots\right). \tag{7}$$

Now we either assume that $|\bar{\gamma}-\gamma| \ll 1$ or that $\kappa[\cdot]$ varies sufficiently slowly with $\bar{\gamma}$ so that we can write

$$\tau = \kappa(\gamma) + h(\bar{\gamma}-\gamma), \quad h = \left.\frac{\mathrm{d}\kappa}{\mathrm{d}\bar{\gamma}}\right|_{\bar{\gamma}=\gamma}. \tag{8}$$

Comparing (7), (8) with (4) yields:

$$c_0 = \kappa(\gamma), \quad c_1 = h\frac{R^2}{10}, \quad c_2 = h\frac{R^4}{280}. \tag{9}$$

The model (5) has significantly simplified the problem of calibration of the constitutive parameters entering the gradient-dependent yield condition (4). Instead of the functions $c_1(\gamma)$ and $c_2(\gamma)$, it only remains to determine the parameter R, the radius of the characteristic volume element which, in turn, is directly related to the width of the zone of localized deformation (see Section 3). The simplicity, however, has to be paid for by a possible serious mathematical shortcoming; namely that the associated boundary-value problems are well posed only if $h > 0$ (or $h < 0$) for all values of γ. Otherwise loss of ellipticity takes place (see Section 4). Nevertheless, relations (9) can give a helpful hint for the order of magnitude of c_1, c_2 if one is only interested in the condition of the onset of the loss of homogeneity and the nearby states (provided of course that for these states h is strictly positive or strictly negative). In concluding this section, we emphasize that the average strain approach need not necessarily be adopted for the interpretation of the gradient-dependent constitutive relation (4). In fact, this approach breaks down in the case where one needs to perform a fully non-linear analysis for a deformation regime where the material undergoes both hardening and softening and thus h goes from positive to negative values. In this case c_1 and c_2 should be treated as functions of γ independent of each other.

3. SHEAR-BAND ANALYSIS

Consider an infinite body undergoing an initially-homogeneous deformation and under proportional straining. The question is to determine conditions under which the governing differential equations admit non-homogeneous simple shear-type solutions, besides the fundamental, homogeneous solution (Rudnicki and Rice, 1975). To simplify the algebra, the elastic compressibility of the material is neglected. The deformation takes place in the (x_1, x_2) plane.

The Cartesian components of the homogeneous initial stress are

$$[\sigma] = \begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}, \tag{10}$$

and we assume that either $\sigma_{33} = 0$ (uniaxial initial stress) or $\sigma_{33} = \frac{1}{2}\sigma_{11}$ (plane strain). In view of (10), (2) and (3), (4) we have:

$$\dot{\sigma}'_{11} = 2G(\dot{\varepsilon}_{11} - \alpha\dot{\gamma}), \tag{11}$$

$$\dot{\sigma}'_{22} = 2G(\dot{\varepsilon}_{22} + \beta\dot{\gamma}), \tag{12}$$

$$\dot{\sigma}_{12} = 2G\dot{\varepsilon}_{12}, \tag{13}$$

$$G\alpha^{-1}\dot{\varepsilon}_{11} = (h+G)\dot{\gamma} + c_1\nabla^2\dot{\gamma} + c_2\nabla^4\dot{\gamma}, \tag{14}$$

where $h = \mathrm{d}\kappa/\mathrm{d}\gamma$ with $\alpha = \beta = \frac{1}{2}$ for the plane strain case, and $\alpha = 1/\sqrt{3}$, $\beta = 1/(2\sqrt{3})$ for the uniaxial case. The incompressibility of the material allows the introduction of a stream function ϕ such that

$$u_1 = \phi_{,2}, \quad u_2 = -\phi_{,1}, \quad (\cdot)_{,i} = \frac{\partial}{\partial x_i}(\cdot). \tag{15}$$

We insert (15) into (11)–(14) and the resulting relationship again into the equilibrium conditions $\dot{\sigma}_{ij,j} = 0$. Subsequent elimination of $\dot{p} = \frac{1}{3}\dot{\sigma}_{ii}$ gives

$$2(\alpha+\beta)\dot{\gamma}_{,12} = \nabla^4\phi, \tag{16}$$

$$\alpha^{-1}\phi_{,12} = \left(\frac{h+G}{G}\right)\dot{\gamma} + \frac{c_1}{G}\nabla^2\dot{\gamma} + \frac{c_2}{G}\nabla^4\dot{\gamma}. \tag{17}$$

We now derive the critical conditions for the existence of particular solutions of (16), (17) of the type

$$\dot{\gamma} = \dot{\gamma}_0 \exp(\mathrm{i}qy), \quad \phi = \phi_0 \exp(\mathrm{i}qy), \tag{18}$$

where:

$$q = \frac{2\pi}{\ell} \quad \text{and} \quad y = -(\sin\theta)x_1 + (\cos\theta)x_2. \tag{19}$$

This represents an inhomogeneous simple shear along the plane y = constant where θ is the angle between the normal of y = constant and the x_2 direction and ℓ is the wavelength. Upon insertion of (18) into (15), (17) we obtain the following homogeneous system of equations

$$\mathbf{A}\mathbf{x} = 0, \tag{20}$$

where

$$[\mathbf{A}] = \begin{bmatrix} (\alpha+\beta)\sin 2\theta q^2 & q^4 \\ \dfrac{h+G}{G} - \left(\dfrac{c_1}{G}q^2 - \dfrac{c_2}{G}q^4\right) & \dfrac{\alpha^{-1}}{2}\sin 2\theta q^2 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} \dot{\gamma}_0 \\ \phi_0 \end{bmatrix}. \tag{21}$$

Non-trivial solutions exist if det $\mathbf{A} = 0$ which for $q > 0$ can be written as

$$\frac{h}{G} = \frac{\alpha+\beta}{2\alpha}\sin^2 2\theta - 1 + \frac{c_1}{G}q^2 - \frac{c_2}{G}q^4. \tag{22}$$

The critical values of (θ, q) are those making h/G a maximum [see, for example, Rudnicki and Rice (1975)]. Thus, from

$$\frac{\partial}{\partial\theta}\left(\frac{h}{G}\right)\bigg|_{\theta=\theta_{cr}} = 0$$

we find $\theta_{cr} = \pm\pi/4$, so that for $c_1 = c_2 = 0$ (or $q = 0$) we recover the results for the conventional continuum of Rudnicki and Rice (1975); namely,

$$\frac{h_{cr}}{G} = 0, \quad \text{for } \sigma_{33} = \tfrac{1}{2}\sigma_{11}, \tag{23}$$

and

$$\frac{h_{cr}}{G} = -\tfrac{1}{4}, \quad \text{for } \sigma_{33} = 0. \tag{24}$$

For $c_1 > 0$ and $c_2 = 0$, modes of type (18) exist for all $h/G \geqslant 0$ and are excluded for $h/G < 0$ if $\sigma_{33} = \frac{1}{2}\sigma_{11}$ or $h/G > -\frac{1}{4}$ if $\sigma_{33} = 0$, respectively. This case appears to be physically unrealistic. In particular, the average strain model (5) falls into this category if the Taylor expansion (7) is truncated after the second non-vanishing term. Of course, this does not exclude the existence of special cases where such a model leads to reasonable results [see, e.g. Lasry and Belytschko (1988)]. For $c_1 = -c < 0$ and $c_2 = 0$ [see Aifantis (1987)] we find

$$\frac{h_{cr}}{G} = \frac{\beta - \alpha}{2\alpha} \quad \text{and} \quad q_{cr} = 0. \tag{25}$$

i.e. the critical conditions here for shear banding are the same as for the conventional continuum with the exception that now the wavenumber at the onset of shear banding is determined, namely $q_{cr} = 0$.

If c_1, c_2 have an opposite sign, then for $c_1 < 0$ we recover (25), and for $c_1 > 0$ we arrive at the same implausible situation as for $c_2 = 0$. The latter holds also if $c_1 < 0$ and $c_2 < 0$.

An interesting case occurs if $c_1 > 0$ and $c_2 > 0$. In this case h/G has a maximum over q and from $\mathrm{d}/\mathrm{d}q(h/G) = 0$ we find

$$q_{cr} = \sqrt{\frac{c_1}{2c_2}}, \tag{26}$$

and thus

$$\frac{h_{cr}}{G} = \frac{\beta - \alpha}{2\alpha} + \frac{c_1^2}{4Gc_2}. \tag{27}$$

In particular, for the average strain model, for which c_1, c_2 are given by (9), we find $h_{cr}/G = 0$ in the plane-strain case and $h_{cr}/G = -0.833$ for axisymmetric initial stress. In the latter case of course ($h < 0$), the homogeneous ground state should be assumed in the softening regime ($h < 0$) such that h does not change sign and loss of ellipticity does not occur.

4. VARIATIONAL PRINCIPLE AND BOUNDARY CONDITIONS

In this section we supplement the proposed constitutive model by the corresponding field equations. In fact, the only remaining issue to be addressed here is the problem of the essential and natural boundary conditions for $\dot{\gamma}$. In the conventional theory of plasticity these are not required as $\dot{\gamma}$ is directly related to $\dot{\varepsilon}$ by the consistence condition. In the present model the consistency condition (3) is a fourth-order partial differential equation which according to (2)–(4) can be written as

$$\mathsf{C}[\dot{\varepsilon}] \cdot \frac{\sigma'}{2\tau} = \left(h + \mathsf{C}\left[\frac{\sigma'}{2\tau}\right] \cdot \frac{\sigma'}{2\tau}\right)\dot{\gamma} + c_1 \nabla^2 \dot{\gamma} + c_2 \nabla^4 \dot{\gamma}, \tag{28}$$

where $h = \mathrm{d}\tau/\mathrm{d}\gamma$ and c_1, c_2 are taken as constants for simplicity. For the solution of boundary value problems one has to treat a system of four simultaneous partial differential equations (instead of the three stress-equations of equilibrium of the conventional theory). Now we will deduce the non-standard boundary conditions from a variational principle. The variational principle also provides a convenient setting for the numerical solution of boundary value problems.

We consider the generalized, incremental, total potential

$$\mathscr{F}[\dot{\mathbf{u}}, \dot{\gamma}] = \frac{1}{2}\int_B \mathsf{C}\left[\dot{\varepsilon} - \dot{\gamma}\frac{\sigma'}{2\tau}\right] \cdot \left(\dot{\varepsilon} - \dot{\gamma}\frac{\sigma'}{2\tau}\right) \mathrm{d}V + \mathsf{D}[\dot{\gamma}] - \int_{\partial_T B} \dot{\mathbf{t}} \cdot \dot{\mathbf{u}}\, \mathrm{d}A, \tag{29}$$

where

$$D[\dot{\gamma}] = \frac{1}{2}\int_B \{h\dot{\gamma}^2 - c_1(\nabla\dot{\gamma})\cdot(\nabla\dot{\gamma}) + c_2(\nabla^{(2)}\dot{\gamma})\cdot(\nabla^{(2)}\dot{\gamma})\}\, \mathrm{d}V, \tag{30}$$

and $\mathbf{t}$ are surface tractions prescribed on part $\partial_T B$ of ∂B. (Body forces have been neglected for convenience.) Next, we assume that upon equilibrium the functional $\mathscr{F}[\dot{\mathbf{u}}, \dot{\gamma}]$ subjected to the constraint $\dot{\gamma} \geqslant 0$ is stationary† with respect to arbitrary infinitesimal variations of $[\dot{\mathbf{u}}, \dot{\gamma}]$. Thus with $\delta\dot{\mathbf{u}} = 0$ on $\partial B - \partial_T B$, we have

$$\begin{aligned}\delta\mathscr{F} = 0 = &-\int_B (\nabla\dot{\sigma})\cdot\delta\dot{\mathbf{u}}\,\mathrm{d}V + \int_{\partial_T B}\{\dot{\sigma}\mathbf{n}-\mathbf{t}\}\cdot\delta\dot{\mathbf{u}}\,\mathrm{d}A \\ &-\int_B \left\{\mathbf{C}[\dot{\varepsilon}]\cdot\frac{\sigma'}{2\tau} - \left(h + \mathbf{C}\left[\frac{\sigma'}{2\tau}\right]\cdot\frac{\sigma'}{2\tau}\right)\dot{\gamma} - c_1\nabla^2\dot{\gamma} - c_2\nabla^4\dot{\gamma}\right\}\delta\dot{\gamma}\,\mathrm{d}V \\ &-\int_{\partial^P B}\{c_1\nabla\dot{\gamma} + c_2\nabla\nabla^2\dot{\gamma}\}\cdot\mathbf{n}\delta\dot{\gamma}\,\mathrm{d}A + \int_{\partial^P B}\{c_2\nabla^{(2)}\dot{\gamma}\}\mathbf{n}(\nabla\delta\dot{\gamma})\cdot\mathrm{d}A,\end{aligned} \tag{31}$$

where $\partial^P B$ designates the boundary of the plastic zone in general being made up of the elastic/plastic boundary (internal boundary) and parts of ∂B, and

$$\dot{\sigma} = \mathbf{C}\left[\dot{\varepsilon} - \dot{\gamma}\frac{\sigma'}{2\tau}\right]. \tag{32}$$

More details on the derivation of (31) are presented in the Appendix. As in the conventional theory of plasticity, the internal boundary of $\partial^P B$ is unknown *a priori*. This does not present a problem in connection with incremental finite element analyses. Also no additional difficulty is entailed with the presence of the additional non-standard boundary terms.

According to the fundamental lemma of variational calculus [e.g. Elsgolc (1961)], the first line of (31) gives the stress-equations of equilibrium and the standard boundary conditions. The second line yields the consistency condition (29) and, eventually, from the third line we can conclude the non-standard boundary conditions. This, however, is not possible directly, i.e. the desired boundary conditions cannot simply be read off from $(31)_3$. The reason for this is that $\nabla\delta\dot{\gamma}$ is not independent of $\delta\dot{\gamma}$ on $\partial^P B$ because, if $\delta\dot{\gamma}$ is known on $\partial^P B$ so is the surface gradient of $\delta\dot{\gamma}$. An analogous situation has been treated by Mindlin in his work on "second gradients of strain and surface tension in linear elasticity" (1965). In this connection it is pointed out that this dependence of the function and its surface gradient has been overlooked in recent papers dealing with gradient plasticity models.

Now, by means of the surface divergence theorem for smooth closed surfaces [the case of non-smooth surfaces is treated in the Appendix], the second term of $(31)_3$ can be written as

$$\begin{aligned}\int_{\partial^P B} c_2(\nabla^{(2)}\dot{\gamma})\nabla\dot{\gamma}\cdot\mathbf{n}\,\mathrm{d}A = &\int_{\partial^P B} c_2\{(\nabla_s\cdot\mathbf{n})(\nabla^{(2)}\dot{\gamma})\mathbf{n}\cdot\mathbf{n} - \nabla_s\cdot[(\nabla^{(2)}\dot{\gamma})\mathbf{n}]\}\delta\dot{\gamma}\,\mathrm{d}A \\ &+ \int_{\partial^P B} c_2(\nabla^{(2)}\dot{\gamma})\mathbf{n}\cdot\mathbf{n}(\nabla_n\delta\dot{\gamma})\,\mathrm{d}A,\end{aligned} \tag{33}$$

where ∇ has been resolved into a surface gradient ∇_s and a normal gradient $\mathbf{n}\nabla_n = (\mathbf{n}\otimes\mathbf{n})\nabla$, such that

† We are aware of the limitations of postulating variational principles for plasticity as this practice is related to the question of the existence of thermodynamic potentials and the associated problem of minimizing free energy functionals for the case of dissipative far from thermodynamic equilibrium processes such as the process of plastic deformation. The point of view taken here is that we do not wish to provide any specific physical meaning or interpretation to the functional $\mathscr{F}$. We simply treat it as an intermediate quantity which can motivate the extra boundary conditions and facilitate the finite element formulation of the problem.

$$\nabla_s = (1 - \mathbf{n} \otimes \mathbf{n})\nabla. \tag{34}$$

Now we combine the terms with $\delta\dot{\gamma}$ and $\nabla_n \delta\dot{\gamma}$ and thus obtain for the third line of (31)

$$\int_{\partial^P B} \Gamma_1 \delta\dot{\gamma}\, \mathrm{d}A + \int_{\partial^P B} \Gamma_2 \nabla_n \delta\dot{\gamma}\, \mathrm{d}A = 0, \tag{35}$$

where

$$\Gamma_1 = -(c_1 \nabla_n \dot{\gamma} + c_2 \nabla_n(\nabla^2 \dot{\gamma})) + c_2\{(\nabla_s \cdot \mathbf{n})[(\nabla^{(2)}\dot{\gamma})\mathbf{n}\cdot\mathbf{n}] - \nabla_s \cdot [(\nabla^{(2)}\dot{\gamma})\mathbf{n}]\}, \tag{36}$$

$$\Gamma_2 = c_2(\nabla^{(2)}\dot{\gamma})\mathbf{n}\cdot\mathbf{n}. \tag{37}$$

It follows that on complementary parts of $\partial^P B$ we have

$$\text{either } \Gamma_1 = 0 \quad \text{or} \quad \delta\dot{\gamma} = 0, \tag{38}$$

and

$$\text{either } \Gamma_2 = 0 \quad \text{or} \quad \nabla_n \delta\dot{\gamma} = 0. \tag{39}$$

Thus, the transformation (33) has led to two scalar (non-standard) boundary conditions instead of what appeared first, in $(31)_3$, to be three boundary conditions. For $c_1 = c_2 = 0$ the variational principle yields the equations of conventional plasticity. There is a formal difference to the conventional procedure in the fact that the plastic multiplier is treated here as an independent variable. For numerical applications this feature can prove to be advantageous. We will come back to this issue in the following section.

As has already been mentioned in Section 2, for $c_2 = 0$ our models yields the elasto-plastic generalization of the rigid models of Aifantis (1987) and Coleman and Hodgdon (1985). Now we have completed this theory by equipping it on the basis of the variational principle with boundary conditions for $\dot{\gamma}$. For $c_2 = 0$ these assume the relatively simple form

$$\Gamma_1 = -c_1 \nabla_n \dot{\gamma} = 0 \quad \text{or} \quad \delta\dot{\gamma} = 0, \quad \text{on} \quad \partial^P B. \tag{40}$$

In the formulation of (33) we have assumed that $\partial^P B$ is a smooth closed surface. If $\partial^P B$ has edges, additional terms have to be included in (33). We deal with this problem in the Appendix. [Note that this concerns the case $c_2 \neq 0$ only.]

In concluding this section, we address briefly the question of ellipticity of the governing differential equations and the uniqueness of the solution. The governing differential equations are strongly elliptic if the characteristic form of their principal part, i.e. the term with the highest-order derivative, is positive definite [e.g. Aubin (1972)]. According to (29) and (30) this is the case if $c_2 > 0$, or for the special case $c_2 \equiv 0$ if $-c_1 > 0$ (positive definiteness of $\mathbf{C}[\cdot]$ is assumed). Note that for c_1 and/or $c_2 \neq 0$ it was only within the ellipticity regime that the shear band analyses in Section 3 have yielded physically plausible results. The solution of the variational principle is unique if the second variation of the functional of the so-called linear comparison solid [which is obtained by dropping the constraint $\dot{\gamma} \geqslant 0$ in the evaluation of (31)] is positive definite. The proof for this is straightforward and follows along the lines of Hill's (1958) proof for the conventional continuum. The first term on the right-hand side of (29) is obviously positive semi-definite if $\mathbf{C}[\cdot]$ is positive definite and in particular positive if $\delta\dot{\gamma} = 0$. Sufficient conditions for the positive definiteness of $\mathbf{D}[\delta\dot{\gamma}]$ are

$$h > 0, \quad c_1 \leqslant 0, \quad c_2 \geqslant 0. \tag{41}$$

Thus, if the above conditions are satisfied and the boundary value problem at hand is solvable, then there exists only one solution. It should be noted that (41) ensures a specific property of the governing differential equation and by no means is assigned a particular physical interpretation or represents a physical requirement.

5. FINITE ELEMENT SOLUTION OF THE VARIATIONAL EQUATIONS

In this section the governing equations are derived for a formal direct solution of the variational principle (29ff) by the finite element method (Zienkiewicz, 1977; Bathe, 1984). Applications of the theory with respect to strain localization will be presented in a forthcoming paper by de Borst and Mühlhaus (1991). We restrict ourselves to the case where κ in (4) depends on $\nabla^2\dot{\gamma}$ only. This case can be implemented rather easily in existing finite element codes; $\dot{u}$ and $\dot{\gamma}$ have to satisfy the same smoothness requirements (C^0 continuity) so that also the same shape functions can be used for the interpolation. For the global structure of the code this means that we now have only one additional degree of freedom per nodal point besides the nodal-point displacements. In many codes (e.g. for coupled thermal or coupled fluid-flow analyses) four degrees of freedom (or three in plane strain) per node are already provided so that the global program structure can be left unaltered and only the element routines have to be modified.

We assume

$$\dot{u}_i = \phi^M \dot{u}_i^M, \quad \dot{\gamma} = \phi^M \dot{\gamma}^M \quad \text{and}$$
$$\delta\dot{u}_i = \phi^M \delta\dot{u}_i^M, \quad \delta\dot{\gamma} = \phi^M \delta\dot{\gamma}^M, \quad M = 1, 2, \ldots, M^e \tag{42}$$

where summation over M is assumed, M^e is the number of nodal points of each element and ϕ^M are the corresponding shape functions. In view of (42), $\delta\mathcal{F}$ [see (29)] becomes

$$\sum_{e\in B}\left\{\left[\int_{B^e} c_{ijkl}\phi_{,j}^M\phi_{,l}^N \,\mathrm{d}V\right]\dot{u}_k^N\delta\dot{u}_i^M - \left[\int_{B^e} c_{ijkl}\frac{\sigma'_{kl}}{2\tau}\phi_{,j}^M\phi^N\,\mathrm{d}V\right]\delta\dot{u}_i^M\dot{\gamma}^N\right.$$
$$\left. - \left[\int_{B^e} c_{ijkl}\frac{\sigma'_{ij}}{2\tau}\phi_{,l}^N\phi^M\,\mathrm{d}V\right]\delta\dot{u}_k^N\delta\dot{\gamma}^M + \left[\int_{B^e}\{h\phi^M\phi^N - c_1\phi_{,i}^M\phi_{,i}^N\}\,\mathrm{d}V\right]\delta\dot{\gamma}^M\dot{\gamma}^N\right\}$$
$$= \sum_{e\in\partial_1 B}\left\{\left[\int_{\partial_1 B^e} t_i\phi^M\,\mathrm{d}A\right]\delta\dot{u}_i^M\right\}, \tag{43}$$

where B^e is the volume of each element and ∂B^e is the boundary of it. For applications it is more convenient to write (43) in matrix notation. For this we first introduce the vector of the generalized nodal degrees of freedom

$$(\mathbf{q}^M) = (\dot{u}_1^M, \dot{u}_2^M, \dot{u}_3^M, \dot{\gamma}^M), \tag{44}$$

and thus (43) can be written as

$$\sum_{e\in B}\delta\mathbf{q}_i^M(\mathbf{K}^{MN}\mathbf{q}^N) = \sum_{e\in\partial_1 B}\delta\mathbf{q}_i^M\mathbf{f}^M, \tag{45}$$

where

$$[\mathbf{K}^{MN}] = \left[\begin{array}{c|c} \mathbf{K}_{uu}^{MN} & \mathbf{K}_{u\dot\gamma}^{MN} \\ \hline \text{symm.} & \mathbf{K}_{\dot\gamma\dot\gamma} \end{array}\right]. \tag{46}$$

$$\sum_{e \in \partial_T B} [\mathbf{f}^M] = \left[\begin{array}{c} \sum_{e \in \partial_T B} \int_{\partial_T B^e} \mathbf{t}\phi^M \, \mathrm{d}A \\ \hline 0 \end{array}\right]. \tag{47}$$

$$[\mathbf{K}_{uu}^{MN}]_{ij} = \int_{B^e} C_{ikjl} \phi_{,k}^M \phi_{,l}^N \, \mathrm{d}V, \tag{48}$$

is the standard, linear elastic element stiffness matrix of the conventional continuum. The coupling matrix $\mathbf{K}_{u\dot\gamma}$ is given by

$$[\mathbf{K}_{u\dot\gamma}^{MN}]_k = -\int_{B^e} C_{ijkl} \frac{\sigma'_{ij}}{2\tau} \phi_{,l}^N \phi^M \, \mathrm{d}V, \tag{49}$$

and

$$\mathbf{K}_{\dot\gamma\dot\gamma}^{MN} = \int_{B^e} \left\{ \left(h + \mathbf{C}\left[\frac{\boldsymbol{\sigma}'}{2\tau}\right] \cdot \frac{\boldsymbol{\sigma}'}{2\tau} \right) \phi^M \phi^N - c_1 (\nabla\phi^M) \cdot (\nabla\phi^N) \right\} \mathrm{d}V. \tag{50}$$

For the assembly of the global stiffness matrix and the global nodal force vector one proceeds as in the conventional continuum; thus further explanation is not necessary here. One has to note, however, that the $\dot\gamma$ degrees of freedom have to be constrained at nodal points within an elastic zone. The explicit implementation of such a constraint may be inconvenient because one has then to modify the global code structure. Alternatively, one might proceed quite pragmatically in the sense of a penalty method by "penalizing" $\dot\gamma$ at integration points where $F < 0$ and/or $\dot\gamma < 0$ with an artificial hardening modulus $h = h^* \gg E$, where E is the Young's modulus. At the same time one sets the contributions of this integration point to the components of the coupling matrix (49) equal to zero.

Eventually it should be noted that the present approach is applicable for the conventional continuum as well. In this case we simply let $c_1 \to 0$ in (50). It is conjectured that even in this degenerate case the present approach has certain advantages over the conventional procedure where $\dot\gamma$ does not appear as an independent variable. We expect that these advantages are particularly significant in connection with low order interpolation functions.

6. CONCLUSIONS

(1) We have provided a modification to the classical rate-independent theory of plasticity by incorporating higher-order gradients of the equivalent plastic strain into the yield condition. The flow rule and the elasticity law were left unaltered.

(2) Implications of the gradient terms were studied in connection with a shear-band analysis for an infinite medium under uniaxial and plane-strain initial stress. It has been shown that for certain ratios of the non-standard material parameters a wave number selection is possible leading to estimates for the width and/or spacing of shear bands.

(3) Due to the presence of strain gradients in the constitutive relations, additional (non-standard) boundary conditions are required for the solution of equilibrium states. Such boundary conditions are deduced here from the assumption that the equilibrium conditions and the consistency conditions are the Euler–Lagrange equations of an appropriate functional. Sufficient conditions for the ellipticity of the governing equations and the uniqueness of the solution are given. The variational principle can be used as a starting point for the construction of approximate solutions of equilibrium states by the finite

element method. In this respect, we have derived the salient expressions for the application of the finite element method in connection with the present gradient plasticity model. Finally, an Appendix is given where details of various calculations are included.

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APPENDIX: MORE DETAILS ON THE DERIVATION OF THE EULER-LAGRANGE EQUATIONS AND BOUNDARY CONDITIONS AT EDGES

In Section 4 the derivation of the non-standard boundary conditions was based on the assumption that upon equilibrium states the first variation of the function $\mathscr{F}[\dot{\mathbf{u}}, \dot{\gamma}]$ (29) vanishes; thus

$$\delta F = \int_B \mathbf{c}\left[\dot{\boldsymbol{\varepsilon}} - \dot{\gamma}\frac{\boldsymbol{\sigma}'}{2\tau}\right]\cdot\delta\dot{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \int_{\partial_T B} \mathbf{t}\cdot\delta\dot{\mathbf{u}}\,\delta A - \int_B \left\{\mathbf{c}\left[\dot{\boldsymbol{\varepsilon}} - \dot{\gamma}\frac{\boldsymbol{\sigma}'}{2\tau}\right]\cdot\frac{\boldsymbol{\sigma}'}{2\tau} - h\dot{\gamma}\right\}\delta\dot{\gamma}\,\mathrm{d}V$$
$$- \int_B c_1(\nabla\dot{\gamma})\cdot(\nabla\delta\dot{\gamma})\,\mathrm{d}V + \int_B c_2(\nabla^{(2)}\dot{\gamma})\cdot(\nabla^{(2)}\delta\dot{\gamma})\,\mathrm{d}V = 0. \quad \text{(A1)}$$

By applying Gauss' theorem to the first two terms of (A1) we obtain the first line of (31). Now we consider the second line of (A1): we imagine the plastified part of $B(=B^{\mathrm{p}})$ to be cut out. The boundary of B^{p} is designated as $\partial^{\mathrm{p}}B$. It should be noted that for the volume integrals a formal distinction between B and B^{p} is not necessary because $\dot{\gamma} \equiv 0$ in $B^{\mathrm{e}} = B - B^{\mathrm{p}}$. Application of Gauss' theorem on the first term of the second line of (A1) gives the identity:

$$\int_B c_1(\nabla\dot{\gamma})\cdot(\nabla\delta\dot{\gamma})\,\mathrm{d}V = \int_{\partial^{\mathrm{p}}B} (c_1\nabla\dot{\gamma}\cdot\mathbf{n})\delta\dot{\gamma}\,\mathrm{d}A - \int_B (c_1\nabla^2\gamma)\delta\dot{\gamma}\,\mathrm{d}V. \quad \text{(A2)}$$

Accordingly, we find for the second term the representation

$$\int_B c_2(\nabla^{(2)}\dot{\gamma})\cdot(\nabla^{(2)}\delta\dot{\gamma})\,\mathrm{d}V = \int_{\partial^{\mathrm{p}}B} ([c_2\nabla^{(2)}\dot{\gamma}]\mathbf{n})\cdot\nabla\delta\gamma\,\mathrm{d}A - \int_B [c_2\nabla(\nabla^2\dot{\gamma})]\cdot\nabla\delta\gamma\,\mathrm{d}V$$
$$= \int_{\partial^{\mathrm{p}}B} ([c_2\nabla^{(2)}\dot{\gamma}]\mathbf{n})\cdot\nabla\delta\gamma\,\mathrm{d}A - \int_{\partial^{\mathrm{p}}B} [c_2\nabla(\nabla^2\dot{\gamma})]\cdot\mathbf{n}\delta\gamma\,\mathrm{d}A + \int_B (c_2\nabla^4\gamma)\delta\dot{\gamma}\,\mathrm{d}V. \quad \text{(A3)}$$

Inserting (A2) and (A3) into (A1) gives the second and third line of (31).

Also in Section 4 it was assumed that the elastic/plastic boundary surface $\partial^{\mathrm{p}}B$ is smooth. Additional boundary conditions are required if $\partial^{\mathrm{p}}B$ has edges (Mindlin, 1965). Note that this affects only cases where the term $c_2\nabla^4\gamma$ is included in the hardening/softening rule.

Suppose $\partial^{\mathrm{p}}B$ has an edge c, formed by the intersection of two segments ∂^{p}_1B and ∂^{p}_2B of $\partial^{\mathrm{p}}B$. Then for each segment we have

$$c_2\int_{\partial^{\mathrm{p}}_{\alpha}B} \nabla_s\cdot[(\nabla^{(2)}\dot{\gamma})\mathbf{n}\delta\dot{\gamma}]\,\mathrm{d}A = c_2\left\{\int_{\partial^{\mathrm{p}}_{\alpha}B} (\nabla_s\cdot\mathbf{n})(\nabla^{(2)}\dot{\gamma})\mathbf{n}\cdot\mathbf{n}\,\delta\dot{\gamma}\,\mathrm{d}A + \int_c (\nabla^{(2)}\dot{\gamma})\mathbf{n}_{(\alpha)}\cdot\mathbf{m}_{(\alpha)}\delta\dot{\gamma}\,\mathrm{d}s\right\}, \quad \text{(A4)}$$

where $\alpha = 1, 2$ and s is measured along c in the direction of its unit tangent s_{α}; $\mathbf{m}_{(\alpha)} = \mathbf{s}_{(\alpha)} \times \mathbf{n}_{(\alpha)}$ is the unit outward normal to c tangent to $\mathbf{s}_{(\alpha)}$ and we also have $\mathbf{s}_1 = -\mathbf{s}_2$. Thus to the right-hand side of (33) we have to add the term

$$\int_c [(\nabla^{(2)}\dot{\gamma})\mathbf{n}\cdot\mathbf{m}]\delta\dot{\gamma}\,\mathrm{d}s, \quad \text{(A5)}$$

where $[(\cdot)]$ denotes the jump of $(\cdot)$ when c is approached from ∂^{p}_1B minus its value when it is approached from ∂^{p}_2B; and $\mathrm{d}s$ is positive in the direction $\mathbf{s}_1$. Thus, in addition to (38), (39) along c, we also have to satisfy the condition

$$\Gamma_c = c_2[(\mathbf{m}\otimes\mathbf{m})\cdot\nabla^{(2)}\dot{\gamma}] = 0 \quad \text{or} \quad \delta\dot{\gamma} = 0. \quad \text{(A6)}$$