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ON UNIFICATION, UNIQUENESS AND NUMERICAL ANALYSIS IN PLASTICITY

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Abstract—This paper addresses various aspects of a theory of multiple-mode plastic straining which unifies constitutive equations of macroscopic solids and single crystals (for both strain-hardening and strain-softening behavior). Emphasis is given to the determination of minimal criteria for uniqueness of solution to incremental boundary value problems based upon the general theory. It is established that these criteria are sufficient to assure convergence of the finite element method in such problems.

1. OBJECTIVE AND SCOPE

It is our purpose here to interrelate (and extend) a number of scattered results from the literature of rate-independent plasticity within a unifying theory of multiple-mode plastic straining. The theory encompasses the classical, single-mode flow laws for strain-hardening solids widely adopted in applications as well as various multi-system constitutive equations useful in crystal plasticity.

The analysis in the first half of the paper (Sections 2–4) is presented for strains of arbitrary magnitude. These sections deal with identification of and alternative forms for the general constitutive theory (of essentially "non-locking" material behavior) and the subsequent relative ordering of basic constitutive inequalities. The analysis in the second half of the paper (Sections 5–7), which pertains to quasi-static boundary value problems of rate type incorporating the general theory and deals with matters of uniqueness and numerical analysis, is restricted to small strains. In these sections we establish that the criteria which assure uniqueness of solution (of the rate-type problem) also govern convergence of finite element approximations.

Throughout the paper boldface, lower case Latin letters designate vectors, boldface Greek and upper case Latin letters designate second order tensors, and upper case Latin script letters designate fourth order tensors. The only exception to this scheme is the use of $\mathbf{Z}(x, x')$ to denote a fourth order tensor influence function in Section 6.

2. IDENTIFICATION OF CONSTITUTIVE EQUATIONS

A broad range of rate-independent response in elastic-plastic solids is encompassed by the constitutive equation† (due in essence to Hill[1])

$$\overset{\circ}{\boldsymbol{\tau}} = \mathscr{L}\mathbf{D} - g^{-1}[\boldsymbol{\Lambda}\mathbf{D}]\boldsymbol{\Lambda}, \quad g > 0. \tag{2.1}$$

Here, $\overset{\circ}{\boldsymbol{\tau}}$ is the material co-rotational (Jaumann–Zaremba) derivative of Kirchhoff stress $(\rho_0/\rho)\boldsymbol{\sigma}$ (with $\boldsymbol{\sigma}$ denoting Cauchy stress); $\mathbf{D}$ is the rate of deformation (Eulerian strain rate); $\mathscr{L}$ is the positive-definite tensor of instantaneous elastic moduli, with symmetries $\mathscr{L}_{ijkl} = \mathscr{L}_{jikl} = \mathscr{L}_{klij}$; $\boldsymbol{\Lambda}$ is a symmetric, second order material tensor with units of stress; and a square bracket signifies its argument is to be replaced by zero if negative. (Both $\boldsymbol{\Lambda}$ and the modulus g may be functionals of deformation history.) In uniaxial loading the full range of response represented by (2.1) for increasing strain is indicated by the shaded region in Fig. 1, bounded by $d\tau/d\xi \to E$ as $g \to \infty$ and $d\tau/d\xi \to -\infty$ as $g \to 0$ (ξ is logarithmic strain). This range can be categorized as "non-locking" material behavior, corresponding to a unique stress increment produced by a given strain increment for all positive g (but not the converse).

Equation (2.1), which we will call the constitutive equation of *single-mode plastic straining*, includes the subclass of strain-hardening solids with a smooth yield surface. The latter are

†At a material point where additional inelastic straining is imminent.

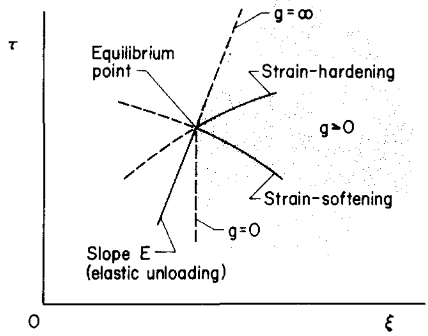

Fig. 1. The range represented by constitutive eqn (2.1) for uniaxial loading ("non-locking", rate-independent material response).

defined by[1]

$$\mathbf{D} = \mathscr{L}^{-1}\overset{\circ}{\boldsymbol{\tau}} + H^{-1}[\mathbf{M}\overset{\circ}{\boldsymbol{\tau}}]\mathbf{M}, \tag{2.2}$$

requiring

$$H = g - \mathbf{M}\mathscr{L}\mathbf{M} > 0, \tag{2.3}$$

where H is the current hardening modulus and $\mathbf{M} = \mathscr{L}^{-1}\boldsymbol{\Lambda}$. The symmetric tensor $\mathbf{M}$ delimits elastic from elastic-plastic response in stress-rate space and may be equated to the stress gradient of the yield surface $f = 0$. Thus, the plastic part of the strain rate can be expressed

$$\mathbf{D}^p = H^{-1}\left[\frac{\partial f}{\partial \boldsymbol{\tau}}\overset{\circ}{\boldsymbol{\tau}}\right]\frac{\partial f}{\partial \boldsymbol{\tau}}, \tag{2.4}$$

which at infinitesimal strain is the classical flow rule of Prager[2] and Drucker[3].

A theory of (rate-independent) elastic-plastic straining in multiple modes, which *appears* to have a different structure than (2.1), is defined by the equations:

$$\overset{\circ}{\boldsymbol{\tau}} = \mathscr{L}\mathbf{D} - \Sigma\gamma_k\boldsymbol{\Lambda}_k, \tag{2.5}$$

and in each critical mode (or system),

$$\left.\begin{aligned} &\boldsymbol{\Lambda}_k\mathbf{D} \le \Sigma g_{kj}\gamma_j, \qquad \gamma_k \ge 0, \\ &\gamma_k(\boldsymbol{\Lambda}_k\mathbf{D} - \Sigma g_{kj}\gamma_j) = 0. \end{aligned}\right\} \tag{2.6}$$

These equations were given independently, in somewhat different contexts, by Sewell[4] and Hill and Rice[5], with particular implications of the latter single crystal theory further investigated by Havner[6, 7]. The γ_k (which have a specific kinematic interpretation in crystals) are scalar plastic mechanism rates, and the matrix of material moduli g_{kj} is taken to be *symmetric, positive-definite.*

Equations (2.5), (2.6) include the theories of piecewise linear hardening (in stress-rate space) of Taylor[8, 9], Koiter[10], Budiansky and Wu[11], Mandel[12] and Hill[13] (also see Havner and Patel[14]). These theories are encompassed by

$$\mathbf{D} = \mathscr{L}^{-1}\overset{\circ}{\boldsymbol{\tau}} + \Sigma\gamma_k\mathbf{M}_k \tag{2.7}$$

and (in each critical system)

$$\left.\begin{aligned} &\mathbf{M}_k\overset{\circ}{\boldsymbol{\tau}} \le \Sigma h_{kj}\gamma_j, \qquad \gamma_k \ge 0, \\ &\gamma_k(\mathbf{M}_k\overset{\circ}{\boldsymbol{\tau}} - \Sigma h_{kj}\gamma_j) = 0, \end{aligned}\right\} \tag{2.8}$$

where $\mathbf{M}_k = \mathscr{L}^{-1}\boldsymbol{\Lambda}_k$ and

$$h_{kj} = g_{kj} - \mathbf{M}_k\mathscr{L}\mathbf{M}_j \tag{2.9}$$

are the effective hardening moduli (compare (2.3)).

Equations (2.5), (2.6) and (2.7), (2.8) are algebraically equivalent, with each set representing a "linear complementarity" problem. The latter equations have a unique solution for given *stress* increment, however, if and only if the matrix of hardening moduli h_{kj} is positive-definite. The former have a unique solution for given *strain* increment if only the matrix (g_{kj}) is positive-definite. Thus, (2.5), (2.6) and (2.7), (2.8) bear a similar relationship to one another as (2.1) and (2.2). Furthermore, (2.1) for single-mode plastic straining can be recognized as a *subclass* of (2.5), (2.6) for multiple modes by identifying $\gamma = g^{-1}[\boldsymbol{\Lambda}\cdot\mathbf{D}]$ as the plastic mechanism rate in the single mode. Correspondingly, *we can focus attention on* (2.5), (2.6) *with the understanding that piecewise linear hardening* (2.7), (2.8), *single-mode plastic straining* (2.1), *and the classical flow rule* (2.2) (*or* 2.4) *are included as special cases.*

3. SEWELL'S MULTIPLE-MODE SADDLE FUNCTION

An interesting (even elegant) alternate form for the general constitutive eqns (2.5)–(2.6) has been given by Sewell[15] in terms of a "saddle function" from which stress rate and plastic mechanism rates are derived. The saddle function is a potential in strain rate $\mathbf{D}$ and multiple-mode variables μ_k which are related to the γ's through

$$\boldsymbol{\Lambda}_k\mathbf{D} - \mu_k = \Sigma g_{kj}\gamma_j. \tag{3.1}$$

(Note that $\mu_k \leq 0$ from (2.6_1) and equals zero whenever $\gamma_k > 0$ from (2.6_3).) The "saddle function" is defined on the currently critical modes as

$$2W(\mathbf{D}, \mu_k) = \mathbf{D}\mathscr{L}\mathbf{D} - \Sigma\Sigma(g^{-1})_{kj}(\boldsymbol{\Lambda}_k\mathbf{D} - \mu_k)(\boldsymbol{\Lambda}_j\mathbf{D} - \mu_j). \tag{3.2}$$

It is readily established that (2.5), (2.6) are exactly equivalent to the relations (from[15])

$$\overset{\circ}{\boldsymbol{\tau}} = \frac{\partial W}{\partial \mathbf{D}}, \qquad \gamma_k = \frac{\partial W}{\partial \mu_k}, \tag{3.3}$$

$$\mu_k \leq 0, \qquad \gamma_k \geq 0, \qquad \mu_k\gamma_k = 0. \tag{3.4}$$

The saddle function for single mode plastic straining is shown in Fig. 2, which illustrates the "skewness" of the surface relative to the μ, D axes. The "solution space" is the $\overline{\mu D}$ plane, with only the indicated branches (elastic-plastic loading and elastic unloading) permitted by conditions (3.4). The curve $(\mathscr{L} - g^{-1}\Lambda^2)(D)^2$ in the plane $\mu = 0$, which appears as a solid line for $D > 0$ and a dashed line for $D < 0$, will lie below the $\overline{\mu D}$ plane for a strain-softening solid.

A more interesting and representative example is that of bi-modal plastic straining (i.e. two critical systems). The corresponding solution space is depicted in Fig. 3, where the strain-rate "axis" $\mathbf{D}$ is itself at least two dimensional.† (Obviously, we can no longer graphically represent the saddle function (3.2).) The four possible solution branches are defined as follows:

$L(+\mathbf{D}$ subspace or 'axis') – *fully active loading* $(\mu_1 = \mu_2 = 0)$;
$L_1(\mu_2 < 0$ segment of the intersection of hyperplane $\overline{\mu_2\mathbf{D}}$ with surface $\gamma_2 = 0)$ – *first system active only* $(\mu_1 = 0,\ \mu_2 < 0)$;
$L_2(\mu_1 < 0$ segment of the intersection of hyperplane $\overline{\mu_1\mathbf{D}}$ with surface $\gamma_1 = 0)$ – *second system active only* $(\mu_1 < 0,\ \mu_2 = 0)$;
E(negative segment of the intersection of surfaces $\gamma_1 = 0$, $\gamma_2 = 0$) – *elastic unloading* $(\mu_1 < 0,\ \mu_2 < 0)$.

The unloading branch E lies in the "octant" $\mathbf{D} < 0$, $\mu_1 < 0$, $\mu_2 < 0$. Lines shown on the

†It is impossible to have solutions in all four branches for positive-definite (g_{kj}) and single component (scalar) D.

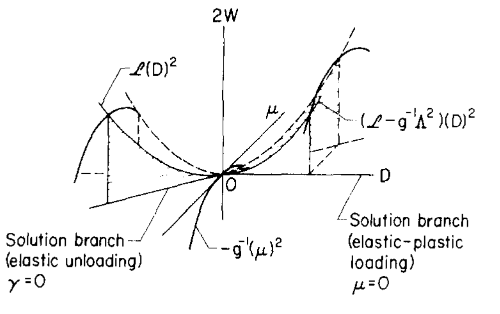

Fig. 2.

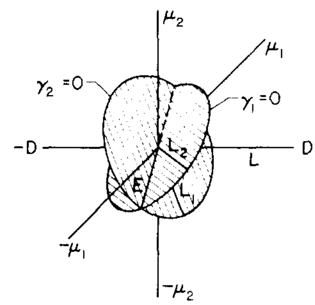

Fig. 3.

Fig. 2. Representation of Sewell's saddle function for single-mode plastic straining (shown for a strain-hardening solid).

Fig. 3. Depiction of $\boldsymbol{\mu}$, **D** solution space for bi-modal plastic straining (L, L_1, L_2, E represent the possible solution branches with two systems critical).

surface $\gamma_1 = 0$ lie in "horizontal planes" (i.e. constant μ_2), and lines shown on the surface $\gamma_2 = 0$ lie in "vertical planes" (i.e. constant μ_1).

The explicit solutions and associated inequalities (based upon $g_{11} > 0$, $g_{22} > 0$, $g = \det(g_{kj}) = g_{11}g_{22} - g_{12}g_{21} > 0$) may be summarized as:

$$L\colon \mu_1 = \mu_2 = 0,\ \gamma_1 = (g_{22}/g)\mathbf{\Lambda}_1\mathbf{D} - (g_{12}/g)\mathbf{\Lambda}_2\mathbf{D} > 0,$$
$$\gamma_2 = -(g_{21}/g)\mathbf{\Lambda}_1\mathbf{D} + (g_{11}/g)\mathbf{\Lambda}_2\mathbf{D} > 0;$$
$$L_1\colon \mu_1 = \gamma_2 = 0,\ \gamma_1 = (1/g_{11})\mathbf{\Lambda}_1\mathbf{D} > 0,$$
$$\mu_2 = -(g_{21}/g_{11})\mathbf{\Lambda}_1\mathbf{D} + \mathbf{\Lambda}_2\mathbf{D} < 0;$$
$$L_2\colon \gamma_1 = \mu_2 = 0,\ \mu_1 = \mathbf{\Lambda}_1\mathbf{D} - (g_{12}/g_{22})\mathbf{\Lambda}_2\mathbf{D} < 0,$$
$$\gamma_2 = (1/g_{22})\mathbf{\Lambda}_2\mathbf{D} > 0;$$
$$E\colon \gamma_1 = \gamma_2 = 0,\ \mu_1 = \mathbf{\Lambda}_1\mathbf{D} < 0,\ \mu_2 = \mathbf{\Lambda}_2\mathbf{D} < 0.$$

In general, the relationship between the number of possible solution branches N and the number of critical systems n is $N = (2)^n$. Thus, there are 32 solution branches associated with 5 critical systems, the latter number having significance relative to a uniqueness criterion for boundary value problems (as subsequently will be shown).

4. CONSTITUTIVE INEQUALITIES

In this section we briefly review and relate several inequalities upon which the uniqueness criteria of Section 5 depend. Let Δ signify the difference between distinct pairs of stress- and strain-rate variables satisfying the general constitutive equations (2.5), (2.6). From the linear complementarity problem represented by (2.6), we can readily establish the inequality (see Hill and Rice[5])

$$\Sigma\Delta\gamma_k\mathbf{\Lambda}_k\Delta\mathbf{D} \geq \Sigma\Sigma g_{kj}\Delta\gamma_k\Delta\gamma_j \tag{4.1}$$

which may be equivalently expressed (from (2.8))

$$\Sigma\Delta\gamma_k\mathbf{M}_k\Delta\mathring{\boldsymbol{\tau}} \geq \Sigma\Sigma h_{kj}\Delta\gamma_k\Delta\gamma_j. \tag{4.2}$$

(The latter form at *infinitesimal* strain is identical to an inequality given by Hill[13] and utilized in uniqueness and convergence arguments for numerical models by Havner[16, 17] and Havner and Patel[14].) There follows the constitutive inequality (upon substituting (2.7))

$$\Delta\mathring{\boldsymbol{\tau}}\Delta\mathbf{D} \geq \Delta\mathring{\boldsymbol{\tau}}\mathscr{L}^{-1}\Delta\mathring{\boldsymbol{\tau}} + \Sigma\Sigma h_{kj}\Delta\gamma_k\Delta\gamma_j \tag{4.3}$$

which is independent of any assumptions on the h_{kj}.

For symmetric, positive-definite g_{kj}, as assumed here, Sewell[4] has established the inequality

$$\Sigma\Sigma(g^{-1})_{kj}(\mathbf{\Lambda}_k\Delta\mathbf{D})(\mathbf{\Lambda}_j\Delta\mathbf{D}) \geq \Sigma\Delta\gamma_k\mathbf{\Lambda}_k\Delta\mathbf{D}, \tag{4.4}$$

whence, substituting (2.5),

$$\Delta\mathring{\boldsymbol{\tau}}\Delta\mathbf{D} \geq \Delta\mathbf{D}(\mathscr{L} - \Sigma\Sigma(g^{-1})_{kj}\mathbf{\Lambda}_k\otimes\mathbf{\Lambda}_j)\Delta\mathbf{D}. \tag{4.5}$$

This inequality generalizes a result of Hill[1] for single-mode plastic straining which has served as the basis for many investigations of plastic bifurcation phenomena. In turn, (4.5) has been adopted in multiple-mode plastic bifurcation analysis by Sewell[4, 18, 19].

Henceforth, we will refer to (4.3) as Hill's inequality and (4.5) as Sewell's inequality. Of particular significance for uniqueness criteria is the *relative ordering* of these inequalities. This ordering can be conveniently determined utilizing the alternate form of (2.5), (2.6) in terms of the saddle function (3.2). Thus, from (3.1)–(3.3$_1$) we have the equality[15]

$$\Delta\mathring{\boldsymbol{\tau}}\Delta\mathbf{D} = \Delta\mathbf{D}(\mathscr{L} - \Sigma\Sigma(g^{-1})_{kj}\mathbf{\Lambda}_k\otimes\mathbf{\Lambda}_j)\Delta\mathbf{D} + \Sigma\Sigma(g^{-1})_{kj}\Delta\mu_k\Delta\mu_j + \Sigma\Delta\mu_k\Delta\gamma_k. \tag{4.6}$$

Sewell's inequality (4.5) obviously follows from (4.6) by dropping the last two terms, both of which are nonnegative since

$$\Delta\mu_k\Delta\gamma_k \geq 0 \tag{4.7}$$

from the linear complementarity problem (3.4) (see Sewell [15, eqn (38)]).

To establish the position of Hill's inequality (4.3) relative to (4.5) and (4.6), we first write (from (2.5))

$$\Delta\mathring{\boldsymbol{\tau}}\mathscr{L}^{-1}\Delta\mathring{\boldsymbol{\tau}} = \Delta\mathbf{D}\mathscr{L}\Delta\mathbf{D} - 2\Sigma\Delta\gamma_k\mathbf{\Lambda}_k\Delta\mathbf{D} + \Sigma\Sigma\Delta\gamma_k\mathbf{M}_k\mathscr{L}\mathbf{M}_j\Delta\gamma_j \tag{4.8}$$

and thence obtain (from (2.9) and (3.1))

$$\Delta\mathring{\boldsymbol{\tau}}\mathscr{L}^{-1}\Delta\mathring{\boldsymbol{\tau}} + \Sigma\Sigma h_{kj}\Delta\gamma_k\Delta\gamma_j = \Delta\mathbf{D}(\mathscr{L} - \Sigma\Sigma(g^{-1})_{kj}\mathbf{\Lambda}_k\otimes\mathbf{\Lambda}_j)\Delta\mathbf{D} + \Sigma\Sigma(g^{-1})_{kj}\Delta\mu_k\Delta\mu_j. \tag{4.9}$$

Upon comparing (4.9) with (4.3) and (4.6), we see that Hill's inequality follows by deleting only the last term in (4.6). Thus, we have the *ordered* relation

$$\begin{aligned}\Delta\mathring{\boldsymbol{\tau}}\Delta\mathbf{D} &= \Delta\mathbf{D}(\mathscr{L} - \Sigma\Sigma(g^{-1})_{kj}\mathbf{\Lambda}_k\otimes\mathbf{\Lambda}_j)\Delta\mathbf{D} + \Sigma\Sigma(g^{-1})_{kj}\Delta\mu_k\Delta\mu_j + \Sigma\Delta\mu_k\Delta\gamma_k \\ &\geq \text{R.H.S. } (4.3) \geq \text{R.H.S. } (4.5)\end{aligned} \tag{4.10}$$

(where R.H.S. denotes right-hand side).

Lastly, we identify the counterpart of (4.10) for single-mode plastic straining:

$$\begin{aligned}\Delta\mathring{\boldsymbol{\tau}}\Delta\mathbf{D} &= \Delta\mathbf{D}(\mathscr{L} - g^{-1}\mathbf{\Lambda}\otimes\mathbf{\Lambda})\Delta\mathbf{D} + g^{-1}(\Delta\mu)^2 + \Delta\mu\Delta\gamma \\ &\geq \Delta\mathring{\boldsymbol{\tau}}\mathscr{L}^{-1}\Delta\mathring{\boldsymbol{\tau}} + H(\Delta\gamma)^2 \geq \Delta\mathbf{D}(\mathscr{L} - g^{-1}\mathbf{\Lambda}\otimes\mathbf{\Lambda})\Delta\mathbf{D}.\end{aligned} \tag{4.11}$$

Clearly, the presumption of *strain-hardening* ($H > 0$) is sufficient to guarantee the inequality $\Delta\mathring{\boldsymbol{\tau}}\Delta\mathbf{D} > 0$ and is less strict than would be the requirement of positive-definite $\mathscr{L} - g^{-1}\mathbf{\Lambda}\otimes\mathbf{\Lambda}$. This point (and its generalization in (4.10)) is significant to uniqueness criteria, as shown in the following section.

5. UNIQUENESS CRITERIA AT SMALL STRAIN

Henceforth we restrict consideration to small strain to obtain definitive results and enable a precise connection with the analysis of Havner and Patel[14]. (Uniqueness theorems and minimum principles at finite strain are presented in Havner[20].) Accordingly, $\mathring{\boldsymbol{\tau}}$ and $\mathbf{D}$ may be replaced by ordinary Cauchy stress rate (or increment) $\dot{\boldsymbol{\sigma}}$ and small strain rate (or increment) $\dot{\boldsymbol{\epsilon}}$

with respect to an appropriate reference frame. In addition, we assume the symmetric tensors $\mathbf{M}_k$ to be deviatoric (i.e. tr $\mathbf{M}_k = 0$), corresponding to zero volumetric plastic strain rate, and adopt the symbol $\mathbf{N}_k$ (as in [14, 16, 17] for this class).

In a quasi-static boundary value problem of rate type in an elastic-plastic solid, body force rates $\dot{\mathbf{f}}$ are prescribed throughout the volume V, traction rates $\dot{\mathbf{t}}$ are prescribed on a portion of the surface S_F, and displacement rates $\mathbf{v}$ are prescribed on the remainder S_D.† We suppose the current values of $\mathscr{L}$, g_{kj} (or h_{kj}), and the equilibrium stress field $\boldsymbol{\sigma}(x)$ are known throughout V and that the critical modes or systems (if any) at each material point are identified. (A currently critical system may be formally defined by the requirement

$$\int \mathbf{N}_k \dot{\boldsymbol{\sigma}}\, \mathrm{d}\theta = \Sigma \int h_{kj}\gamma_j\, \mathrm{d}\theta + \tau_k{}^0, \tag{5.1}$$

where θ is a time-like variable, the integration is taken over the history of the deformation, and $\tau_k{}^0$ is a material strength parameter which defines the critical system in the plastically unstrained state.)

As is well known, a sufficient condition for uniqueness of solution to the considered boundary value problem is that

$$\int \Delta\dot{\boldsymbol{\sigma}} \Delta\dot{\boldsymbol{\epsilon}}\, \mathrm{d}V > 0 \tag{5.2}$$

for every pair of continuous, piecewise differentiable displacement-rate fields whose difference $\Delta\mathbf{v}$ vanishes on S_D, with each $\dot{\boldsymbol{\sigma}}$ related to the corresponding $\dot{\boldsymbol{\epsilon}}$ through the constitutive equations (2.5), (2.6) or (2.7), (2.8). (Refer to Hill [1] for the original statement of uniqueness at finite strain in terms of $\mathring{\boldsymbol{\tau}}$ and $\mathbf{D}$.) Thus, from (4.10), uniqueness of solution follows if (see Hill [13] or Havner and Patel [14])

$$\int (\Delta\dot{\boldsymbol{\sigma}} \mathscr{L}^{-1} \Delta\dot{\boldsymbol{\sigma}} + \Sigma\Sigma h_{kj} \Delta\gamma_k \Delta\gamma_j)\, \mathrm{d}V > 0, \tag{5.3}$$

where each $\dot{\boldsymbol{\sigma}}$, $\boldsymbol{\gamma}$ pair is determined from the associated $\dot{\boldsymbol{\epsilon}} = \partial\mathbf{v}$ (the symmetric gradient) via (2.5), (2.6) (requiring positive-definite g_{kj}). An *over*sufficient condition is (also from (4.10))

$$\int \Delta\dot{\boldsymbol{\epsilon}} (\mathscr{L} - \Sigma\Sigma (g^{-1})_{kj} \boldsymbol{\Lambda}_k \otimes \boldsymbol{\Lambda}_j) \Delta\dot{\boldsymbol{\epsilon}}\, \mathrm{d}V > 0, \tag{5.4}$$

the latter being a small strain specialization of the uniqueness criterion in Sewell [4]. Since L.H.S. (5.3) $\geq$ L.H.S. (5.4) from (4.10), *we focus attention on the less strict criterion* (5.3) and its single-mode counterpart

$$\int (\Delta\dot{\boldsymbol{\sigma}} \mathscr{L}^{-1} \Delta\dot{\boldsymbol{\sigma}} + H(\Delta\gamma)^2)\, \mathrm{d}V > 0. \tag{5.5}$$

This last obviously is satisfied for $H > 0$, corresponding to the classical flow rule (2.4) (see Drucker [21]). More generally, positive-definite moduli h_{kj} assure (5.3) and nonnegative-definite moduli at least assure uniqueness of stress rate $\dot{\boldsymbol{\sigma}}$. We further investigate the latter case in Section 6.

Within the context of crystalline slip models at small strain, the h_{kj} are hardening moduli in the crystallographic slip systems. These moduli connect increments in critical shear strengths in both active and latent systems to the incremental plastic slips. (The γ_k here are slip rates.) The most widely applied crystal hardening rule was first proposed by G. I. Taylor [8]: $h_{kj} = H$ for all k, j ($H > 0$ denoting the single slip modulus). The matrix of moduli h_{kj} in this case is positive-*semi*definite if two or more systems are critical. Budiansky and Wu [11] adopted the rule $h_{kj} = 2H\mathbf{N}_k \cdot \mathbf{N}_j$, which includes a simple Bauschinger effect and is positive-definite if the $\mathbf{N}_k$ are linearly independent. Koiter [10] suggested the uncoupled hardening rule $h_{kj} = H\delta_{kj}$, but not in the context of single crystal models. Taking into account what is known about active vs. latent hardening from experimental test (see Kocks [22]), Taylor's rule remains the best *simple*

†Mixed boundary conditions are of course accommodated by assigning individual component pairs of force and displacement (at a boundary point) to S_F and S_D as appropriate.

approximation to the complexities of crystalline slip at small deformations. (For macroscopic materials, multiple-mode hardening rules of the above forms have been employed with a piecewise-linear yield surface which approximates the von Mises criterion[23]. One then obtains piecewise-linear approximations to isotropic hardening and Reuss-Prager "kinematic" hardening, for example.)

6. PROBLEM PARTITIONING AND A GREEN'S FUNCTION APPROACH

Some further insight into the question of uniqueness of solution for positive-*semi*definite moduli h_{kj} may be gained through a partitioning of the rate-type boundary value problem into two parts: a (pseudo-) elastic problem and a self-straining problem whose solution depends upon the elastic solution.

In the elastic problem the unique solution $\mathbf{u}_e(x)$, which equilibrates $\dot{\mathbf{f}}$ in V and $\dot{\mathbf{t}}$ on S_F, minimizes the "potential energy" functional

$$2I_1(\mathbf{v}) = \int \dot{\boldsymbol{\epsilon}}(\mathbf{v})\mathscr{L}\dot{\boldsymbol{\epsilon}}(\mathbf{v})\,\mathrm{d}V - 2\{\int \mathbf{v}\dot{\mathbf{f}}\,\mathrm{d}V + \int \mathbf{v}\dot{\mathbf{t}}\,\mathrm{d}S_F\} \tag{6.1}$$

on the class of continuous displacement-rate fields $\mathbf{v}(x)$ taking the prescribed values on S_D. For the self-straining problem, in which the body is fully constrained on S_D, with zero body-force rate in V and zero traction rate on S_F, we adopt a "Green's function approach" to investigate uniqueness, as follows.

Let $\dot{\mathbf{f}}^*(x)$ denote an arbitrary body force rate which is separate from and unrelated to the body force rate $\dot{\mathbf{f}}(x)$ in the elastic part of the boundary value problem. Imagine a *second* elastic-problem corresponding to the body force rate $\dot{\mathbf{f}}^*(x)$ but with the boundary conditions of the self-straining problem. The solution $\mathbf{u}^*(x)$ to this second elastic problem is unique and is characterized by the minimization of

$$2I_1(\mathbf{w}) = \int \dot{\boldsymbol{\epsilon}}(\mathbf{w})\mathscr{L}\dot{\boldsymbol{\epsilon}}(\mathbf{w})\,\mathrm{d}V - 2\int \mathbf{w}\dot{\mathbf{f}}^*\,\mathrm{d}V \tag{6.2}$$

over the vector space of continuous velocity fields $\mathbf{w}(x)$ identically zero on S_D. The associated stress rate $\dot{\boldsymbol{\sigma}}^* = \mathscr{L}\dot{\boldsymbol{\epsilon}}(\mathbf{u}^*)$ equilibrates $\dot{\mathbf{f}}^*(x)$ in V and zero traction rates on S_F.

Consider a generalization of the self-straining problem to one caused by *any* imposed, inelastic strain-rate distribution $\dot{\boldsymbol{\epsilon}}_I(x)$. The stress-rate corresponding to the self-straining velocity field $\mathbf{u}_s(x)$ is

$$\dot{\boldsymbol{\sigma}}_s = \mathscr{L}(\partial\mathbf{u}_s - \dot{\boldsymbol{\epsilon}}_I), \qquad \mathbf{u}_s = \mathbf{u}_s(\dot{\boldsymbol{\epsilon}}_I). \tag{6.3}$$

The "second elastic" and self-straining problems are connected by

$$\int \mathbf{u}_s(\dot{\boldsymbol{\epsilon}}_I)\dot{\mathbf{f}}^*\,\mathrm{d}V = \int \dot{\boldsymbol{\epsilon}}(\mathbf{u}^*)\mathscr{L}\dot{\boldsymbol{\epsilon}}_I\,\mathrm{d}V, \tag{6.4}$$

which is equivalent to a result in Maier[24], derived therein from the Maxwell-Betti reciprocal theorem and the Gauss-Green transformation. Alternatively, (6.4) can be proved using the principle of virtual work as applied to any kinematically admissible $\mathbf{w}(x)$. Thus, in the second elastic problem

$$\int \dot{\boldsymbol{\sigma}}^*\dot{\boldsymbol{\epsilon}}(\mathbf{w})\,\mathrm{d}V \equiv \int \partial\mathbf{u}^*\mathscr{L}\partial\mathbf{w}\,\mathrm{d}V = \int \mathbf{w}\dot{\mathbf{f}}^*\,\mathrm{d}V, \tag{6.5}$$

and in the self-straining problem $\int \dot{\boldsymbol{\sigma}}_s\dot{\boldsymbol{\epsilon}}(\mathbf{w})\,\mathrm{d}V = 0$, whence (from (6.3))

$$\int \partial\mathbf{u}_s\mathscr{L}\partial\mathbf{w}\,\mathrm{d}V = \int \partial\mathbf{w}\mathscr{L}\dot{\boldsymbol{\epsilon}}_I\,\mathrm{d}V. \tag{6.6}$$

Both $\mathbf{u}_s(x)$ and $\mathbf{u}^*(x)$ belong to the class of kinematically admissible $\mathbf{w}(x)$. Upon substituting $\mathbf{u}_s$ for $\mathbf{w}$ in (6.5) and $\mathbf{u}^*$ for $\mathbf{w}$ in (6.6), the equality (6.4) immediately follows.

Equation (6.4) is the key relationship in the Green's function approach to the self-straining problem. Let $G_{pm}(x', x)$ denote the displacement rate u_p^* at x' in the second elastic problem due to a unit force rate $\dot{F}_m^*$ at x (i.e. $\lim_{\Delta V\to 0} \int_{\Delta V} \dot{f}_m^*\,\mathrm{d}V = 1$, x in ΔV, with $\dot{f}_m^* \equiv 0$ outside ΔV and the other components of $\dot{\mathbf{f}}^*$ everywhere zero). Then, the formal solution to the self-straining problem for arbitrary $\dot{\boldsymbol{\epsilon}}_I$ is, from (6.4),

$$\mathbf{u}_s(x) = \int \nabla' \mathbf{G}(x', x) \mathscr{L}(x') \dot{\boldsymbol{\epsilon}}_I(x') \, \mathrm{d}V'. \tag{6.7}$$

($\nabla' \mathbf{G}(x', x)$ has components $\partial G_{pm}(x', x)/\partial x'_q$.) Substituting (6.7) into eqn (6.3) for the stress rate,

$$\dot{\sigma}^s_{ij}(x) = -\int Z_{ijkl}(x, x') \dot{\epsilon}^I_{kl}(x') \, \mathrm{d}V' \tag{6.8}$$

in which the kernel influence function $\mathbf{Z}(x, x')$ is given by

$$Z_{ijkl}(x, x') = \mathscr{L}_{ijkl}(x)\delta(x, x') - \mathscr{L}_{ijmn}(x) \frac{\partial}{\partial x_n} \frac{\partial}{\partial x'_q} G_{mp}(x, x') \mathscr{L}_{pqkl}(x'). \tag{6.9}$$

Here we have utilized the symmetries of the elastic moduli and the basic reciprocity relations of the Green's function (viz. $G_{mp}(x', x) = G_{mp}(x, x')$) and have introduced the Dirac-delta function $\delta(x, x')$, scaled such that $\int \delta(x, x') f(x') \, \mathrm{d}V' = f(x)$. Note that $\mathbf{Z}(x, x')$ also has the reciprocal property

$$Z_{ijkl}(x, x') = Z_{klij}(x', x). \tag{6.10}$$

From virtual work,

$$\int \dot{\boldsymbol{\sigma}}_s \partial \mathbf{u}_s \, \mathrm{d}V = 0 = \int \dot{\boldsymbol{\sigma}}_s \mathscr{L}^{-1} \dot{\boldsymbol{\sigma}}_s \, \mathrm{d}V + \int \dot{\boldsymbol{\sigma}}_s \dot{\boldsymbol{\epsilon}}_I \, \mathrm{d}V, \tag{6.11}$$

whence, substituting (6.8) for $\dot{\boldsymbol{\sigma}}_s$ in the last term,

$$\iint \dot{\boldsymbol{\epsilon}}_I(x) \mathbf{Z}(x, x') \dot{\boldsymbol{\epsilon}}_I(x') \, \mathrm{d}V' \, \mathrm{d}V = \int \dot{\boldsymbol{\sigma}}_s \mathscr{L}^{-1} \dot{\boldsymbol{\sigma}}_s \, \mathrm{d}V. \tag{6.12}$$

Obviously, the kernel $\mathbf{Z}(x, x')$ is at least positive-semidefinite for arbitrary $\dot{\boldsymbol{\epsilon}}_I(x)$.

Consider now the specific inelastic strain-rate distribution

$$\dot{\boldsymbol{\epsilon}}_I(x) = \Sigma \lambda_k \mathbf{N}_k(x) \tag{6.13}$$

in critical systems, where the λ's are arbitrary scalar rates which may be negative.† From (6.12),

$$\iint \Sigma\Sigma \lambda_k(x) p_{kj}(x, x') \lambda_j(x') \, \mathrm{d}V' \, \mathrm{d}V = \int \dot{\boldsymbol{\sigma}}_s(\lambda) \mathscr{L}^{-1} \dot{\boldsymbol{\sigma}}_s(\lambda) \, \mathrm{d}V \geq 0 \tag{6.14}$$

in which

$$p_{kj}(x, x') = \mathbf{N}_k(x) \mathbf{Z}(x, x') \mathbf{N}_j(x') \tag{6.15}$$

(with $p_{kj}(x, x') = p_{jk}(x', x)$ from (6.10)). For linearly independent $\mathbf{N}_k(x)$ (i.e. no more than five critical modes at any material point), the matrix of influence functions $p_{kj}(x, x')$ is positive-definite unless there is a critical-systems distribution $\boldsymbol{\lambda}(x)$ which produces identically zero $\dot{\boldsymbol{\sigma}}_s(x)$ from (6.8).

Upon substituting (6.14) into (5.3), the implications for uniqueness are immediate. For positive-*semi*definite h_{kj}, the solution to the rate-type boundary value problem is unique in plastic strain rate *unless two distributions* $\gamma(x)$ *can be found which satisfy the constitutive equations and differ by a purely kinematical "mechanism."* The final uniqueness criterion is

$$\iint \Sigma\Sigma \Delta\gamma_k(x) \{h_{kj}(x)\delta(x, x') + p_{kj}(x, x')\} \Delta\gamma_j(x') \, \mathrm{d}V' \, \mathrm{d}V > 0, \tag{6.16}$$

generalizing similar criteria in Maier[24] and Havner and Singh[25].

†$\lambda_k(x)$ is identically zero at all points x where the kth system is not critical.

As with (5.3), a general conclusion about absolute uniqueness of solution can be made only in the case of positive-definite h_{kj}. In the experience of computations with the positive-*semi*definite Taylor hardening rule, however, ***a mechanism state apparently has not been reached within the small strain approximation.*** The matrices of influence functions $p_{kj}(x, x')$ were found to be ***positive-definite*** (thereby assuring uniqueness) in calculations by Havner *et al.* [25–27] incorporating up to five active modes at material points. For the same hardening rule, all incremental solutions (apparently) were found unique in calculations by Lin *et al.* [28, 29] and DeDonato and Franchi[23]. (Even for an elastic-perfectly plastic solid, the limit load and associated mechanism state are usually only approached asymptotically in tracing a deformation history. Exceptions are those simple cases where additional kinematic and stress approximations are made, as in frame analysis.)

7. CONVERGENCE OF FINITE ELEMENT APPROXIMATIONS

In this final section we show the connection between uniqueness of solution and convergence of the finite element method in quasi-static boundary value problems of rate type. To this end we introduce a minimum principle established in Havner and Patel[14] which permits the *independent* variation of displacement rate and plastic mechanism rates in the self-straining problem.†

Consider the functional

$$2I_2(\mathbf{w},\boldsymbol{\lambda}) = \int\{\dot{\boldsymbol{\sigma}}_s(\mathbf{w}, \boldsymbol{\lambda})\mathscr{L}^{-1}\dot{\boldsymbol{\sigma}}_s(\mathbf{w}, \boldsymbol{\lambda}) + \Sigma\Sigma h_{kj}\lambda_k\lambda_j\}\,\mathrm{d}V - 2\int\Sigma\lambda_k\boldsymbol{\Lambda}_k\partial\mathbf{u}_e\,\mathrm{d}V \tag{7.1}$$

on the space of continuous (vector) functions $\mathbf{w}(x)$, indentically zero on S_D, and the field of nonnegative scalar rates $\lambda_k(x)$ in critical systems, with

$$\dot{\boldsymbol{\sigma}}_s(\mathbf{w}, \boldsymbol{\lambda}) = \mathscr{L}(\partial\mathbf{w} - \Sigma\lambda_k\mathbf{N}_k). \tag{7.2}$$

For *nonnegative-definite* h_{kj}, the true self-straining solution $\mathbf{u}_s(x)$, $\boldsymbol{\lambda}(x)$, statically admissible (through $\dot{\boldsymbol{\sigma}}_s$) and satisfying the constitutive equations (2.5), (2.6), minimizes I_2 on the admissible class $\mathbf{w}(x)$, $\boldsymbol{\lambda}(x)$. (Refer to [14] for a formal proof.) The counterpart of this principle for single-mode plastic straining is obvious. The true solution $\mathbf{u}_s(x)$, $\gamma(x)$ to the self-straining problem minimizes the functional

$$2I_2(\mathbf{w}, \lambda) = \int\{\dot{\boldsymbol{\sigma}}_s\mathscr{L}^{-1}\dot{\boldsymbol{\sigma}}_s + H(\lambda)^2\}\,\mathrm{d}V - 2\int\lambda\boldsymbol{\Lambda}\partial\mathbf{u}_e\,\mathrm{d}V, \tag{7.3}$$

with $\dot{\boldsymbol{\sigma}}_s(\mathbf{w}, \lambda) = \mathscr{L}(\partial\mathbf{w} - \lambda\boldsymbol{\Lambda})$.

The usefulness of this principle, in either its multiple- or single-mode form, as compared with other minimum principles for elastic-plastic solids at small strain (viz. Drucker[21], Hill[13] and Havner[17]) lies in the *independence* of $\mathbf{w}(x)$ and $\boldsymbol{\lambda}(x)$. Combining this principle with the elastic minimum principle (6.1) leads to a pair of inequalities on the discretization errors in a finite element approximation, as follows.

Let the body be subdivided into a large number of tetrahedral subregions q, the *finite elements* (making certain that no element cuts across a material interface). Assume all elements to be of equal order of magnitude in size and let h denote a representative element dimension. Further, suppose the current distribution of stress and constitutive properties is known throughout the body. Introducing *piecewise-linear* interpolating polynomials with a local basis and distinguishing the finite element solution from the exact solution by a superscript h, it may be proved (utilizing (6.1) and (7.1)) that [14]

$$\int\partial(\mathbf{u}_e - \mathbf{u}_e^h)\mathscr{L}\partial(\mathbf{u}_e - \mathbf{u}_e^h)\,\mathrm{d}V \le 0(h^2), \tag{7.4}$$

$$\begin{aligned}\int(\dot{\boldsymbol{\sigma}}_s - \dot{\boldsymbol{\sigma}}_s^h)\mathscr{L}^{-1}(\dot{\boldsymbol{\sigma}}_s - \dot{\boldsymbol{\sigma}}_s^h)\,\mathrm{d}V + \int\Sigma\Sigma h_{kj}(\gamma_k - \gamma_k^h)(\gamma_j - \gamma_j^h)\,\mathrm{d}V + 2\int\Sigma\gamma_k^h(\Sigma h_{kj}\gamma_j \\ - \mathbf{N}_k\dot{\boldsymbol{\sigma}})\,\mathrm{d}V \le \int\partial(\mathbf{u}_e - \mathbf{u}_e^h)\mathscr{L}\partial(\mathbf{u}_e - \mathbf{u}_e^h)\,\mathrm{d}V + 2\int\Sigma(\gamma_k - \gamma_k^h)\boldsymbol{\Lambda}_k\partial(\mathbf{u}_e - \mathbf{u}_e^h)\,\mathrm{d}V.\end{aligned} \tag{7.5}$$

†The implied restriction of this principle to piecewise-linear yield surfaces in [14] is unnecessary, and the principle and proof therein are directly applicable to the constitutive theory of (2.5), (2.6).

The inequality (7.4) can be considered a special case of the "fundamental Theorem 1.1" in Strang and Fix [30, pp. 39–40 and 106]. The proof of (7.5), which is moderately long, is given in full in Havner and Patel[14].

The convergence of the (incremental) elastic solution from (7.4) (i.e. $\mathbf{u}_e^h \to \mathbf{u}_e$ as $h \to 0$) ensures that the right-hand side of (7.5) converges to zero. Thus, the nonnegative integrals on the left-hand side must *individually* converge to zero, whence $\dot{\boldsymbol{\sigma}}_s^h \to \dot{\boldsymbol{\sigma}}_s$ and $\dot{\boldsymbol{\sigma}}^h \to \dot{\boldsymbol{\sigma}}$, *the unique stress rate assured by the uniqueness criterion* (5.3) ($\dot{\boldsymbol{\sigma}}_e^h \to \dot{\boldsymbol{\sigma}}_e$ from (7.4)). Moreover, for *positive-definite* h_{kj}, $\gamma_k^h \to \gamma_k$, *the unique plastic mechanism rates from* (5.3). Inequality (7.5) was established by Havner and Patel[14] for piecewise-linear yield surfaces. Here we recognize for the first time its direct applicability to the general constitutive theory (2.5), (2.6) (or (3.3), (3.4)).

Lastly, we write the convergence inequality for the case of single-mode plastic straining:

$$\int(\dot{\boldsymbol{\sigma}}_s - \dot{\boldsymbol{\sigma}}_s^h)\mathscr{L}^{-1}(\dot{\boldsymbol{\sigma}}_s - \dot{\boldsymbol{\sigma}}_s^h)\,\mathrm{d}V + \int H(\gamma - \gamma^h)^2\,\mathrm{d}V + 2\int \gamma^h(H\gamma - \mathbf{N}\dot{\boldsymbol{\sigma}})\,\mathrm{d}V$$
$$\leq 2\int(\gamma - \gamma^h)\Lambda\partial(\mathbf{u}_e - \mathbf{u}_e^h)\,\mathrm{d}V + 0(h^2), \tag{7.6}$$

with $\mathbf{u}_e^h \to \mathbf{u}_e$ from (7.4). For $H > 0$, *this is a proof of convergence in the incremental problem for the classical flow rule of Prager*[2] *and Drucker*[3] (i.e. (2.2) or (2.4)). For the elastic-perfectly plastic solid with a smooth yield surface, $H = 0$, (7.6) assures convergence of stress rate in the incremental problem and further assures that γ^h converges to a nonzero value only where $\mathbf{N} \cdot \dot{\boldsymbol{\sigma}} = 0$.

As remarked in Havner and Patel[14], the real issue in actual calculations is the absolute convergence of the finite element method for a *sequence of incremental solutions*. Convergence of the rate-type problem as proved in[14] and interpreted more broadly here is a *necessary* test for the finite element method but is not sufficient (of itself) to establish sequential convergence. The latter proof remains a significant open problem in numerical analysis and theoretical plasticity.

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