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CONSTITUTIVE ANALYSIS OF ELASTIC–PLASTIC CRYSTALS AT ARBITRARY STRAIN

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Summary

A general time-independent constitutive framework is constructed for crystals capable of crystallographic shearing. No restrictions are placed on their elasticity or on the amounts of slip. In deriving properly-objective relations due account is taken of the separate motions of the material and lattice. A precise specification of the structure of the flow rule leads to conditions for the existence of plastic potentials, as well as to an exact statement of the slip criterion required for normality of the plastic strain-increment in conjugate variables. Objective hardening laws are also examined and sufficiency conditions obtained for uniqueness of the slip magnitudes.

1. Objectives

Within the usual small-strain approximation there seems to be general agreement about a constitutive description of the mechanical properties of an elastic–plastic crystal at the macroscopic level. These are that (i) distortion of the lattice is effectively elastic; (ii) the crystal deforms also by simple shears relative to specific lattice planes and directions; (iii) such 'slip systems' are active only when the corresponding shear stresses attain critical values; and (iv) each value is a functional of the entire slip-history of the crystal.

It has been customary to treat the elasticity as linear and unaffected by slip, and to regard the lattice geometry as unaltered when stating the shears. The slip-induced rotation of the lattice relative to the material has often been ignored as well when computing increments of effective stress.

We put no restrictions here on the elasticity or the amounts of slip. Our intention is to construct a comprehensive constitutive framework in which the phenomena are analysed precisely.

2. Point of Departure

As a basis suitably general for our purpose we adopt the minimal framework outlined by Hill (1972).

This allows an arbitrary choice of strain measure **e** (Hill, 1968) relative to some ground state of the crystal. A conjugate measure of stress **t** in the deformed state is defined by the requirement that $\mathbf{t}d\mathbf{e}/\rho$ shall be the work per unit mass in any differential strain, where ρ is the ground-state density. Associated with such a (**t**, **e**) pair are fourth-rank tensors of moduli and compliances, $\mathscr{L}$ and $\mathscr{M}$ say, which specify the instantaneous elastic behaviour under load.

It is supposed that crystallographic slip is the only mechanism responsible for inelastic behaviour. Then, under any incremental loading at constant temperature, we can always write

$$\mathscr{L}d\mathbf{e}-d\mathbf{t} = \sum (\boldsymbol{\lambda} d\gamma), \qquad d\mathbf{e}-\mathscr{M}d\mathbf{t} = \sum (\boldsymbol{\mu} d\gamma), \tag{2.1}$$

where

$$\left.\begin{aligned} \boldsymbol{\lambda} &= \mathscr{L}\boldsymbol{\mu} \\ \boldsymbol{\mu} &= \mathscr{M}\boldsymbol{\lambda}, \end{aligned}\right\} \tag{2.2}$$

and

with summation over the active slip systems. The $d\gamma$'s are the incremental amounts of shear, reckoned with respect to the present lattice configuration, while the $\boldsymbol{\lambda}$'s and $\boldsymbol{\mu}$'s are second-rank symmetric tensors whose precise specification is our main objective.

For the moment we simply observe that $\Sigma(\boldsymbol{\mu} d\gamma)$ is the residual increment of strain **e** after an infinitesimal loading and unloading cycle of the stress **t**, while $\Sigma(\boldsymbol{\lambda} d\gamma)$ is the residual decrement of stress **t** after a like cycle of the strain **e**. These interpretations underline the relativity of the $\boldsymbol{\lambda}$'s and $\boldsymbol{\mu}$'s to the chosen measures.

By contrast, however, it is known (HILL, 1968, 1972; and Appendix here) that the bilinear form

$$(\mathscr{L}d\mathbf{e}-d\mathbf{t})\delta\mathbf{e}/\rho, \tag{2.3}$$

where d and δ are independent differentials, is invariant under change of measure. It follows that each $\boldsymbol{\lambda}$ transforms in such a way as to preserve the Pfaffian $\boldsymbol{\lambda}\delta\mathbf{e}/\rho$ for arbitrary $\delta\mathbf{e}$; in short, each $\boldsymbol{\lambda}$ transforms like **t**. Suppose, now, that $\mathscr{L}$ and $\mathscr{M}$ have the diagonal symmetry associated with the existence of a strain-energy function in some neighbourhood of the current stress. Then (2.3) is identical with

$$(d\mathbf{e}-\mathscr{M}d\mathbf{t})\delta\mathbf{t}/\rho, \tag{2.4}$$

where $\delta\mathbf{t} = \mathscr{L}\delta\mathbf{e}$, and so each $\boldsymbol{\mu}$ transforms so as to preserve $\boldsymbol{\mu}\delta\mathbf{t}/\rho$ for arbitrary $\delta\mathbf{t}$.

Details of other consequences of changing the strain measure are recapitulated in the Appendix. Here we need only mention the transformation formulae in the case when the ground state is not varied and, further, is taken coincident with the current state. For small additional strains any measure **e** can naturally be expanded as a power series in the logarithmic measure, $\mathbf{e}_0$ say, beginning with the terms

$$\mathbf{e} = \mathbf{e}_0 + m\mathbf{e}_0 \times \mathbf{e}_0 + \ldots, \tag{2.5}$$

where the cross signifies an inner product and m is some numerical coefficient (unity for the commonly adopted Green measure). In the ground state itself we have $d\mathbf{e} = d\mathbf{e}_0$ and

$$\left.\begin{aligned} d\mathbf{t} &= d\mathbf{t}_0 - m(\boldsymbol{\sigma} \times d\mathbf{e} + d\mathbf{e} \times \boldsymbol{\sigma}), \\ d\mathbf{t}_0 &= \mathscr{D}\boldsymbol{\tau}, \end{aligned}\right\} \tag{2.6}$$

where $\boldsymbol{\sigma}$ is the current Cauchy stress, $\mathbf{t}_0$ is conjugate to $\mathbf{e}_0$, and $\mathscr{D}\boldsymbol{\tau}$ is the Jaumann differential of Kirchhoff stress (HILL, 1968). This last formula is exact, and so independent of changes in measure that affect only terms beyond the second in the series for $\mathbf{e}$. It may be re-written as

$$d\mathbf{t} = d\mathbf{t}_0 - m\mathscr{S}d\mathbf{e}, \tag{2.7}$$

where $\mathscr{S}$ is a fourth-rank symmetric tensor, which is evidently a linear function of $\boldsymbol{\sigma}$ alone. By applying (2.7) with elastic increments, in particular, we obtain the transformation rule for instantaneous moduli:

$$\mathscr{L} = \mathscr{L}_0 - m\mathscr{S}. \tag{2.8}$$

It follows that the transformation preserves symmetry of the type mentioned, when it exists. Also, for moderate values of m (of order unity in absolute magnitude), the differences in moduli are of the order of the applied stress and consequently proportionately small in metal crystals.

Lastly, by combining (2.7) and (2.8), we have

$$\mathscr{L}d\mathbf{e} - d\mathbf{t} = \mathscr{L}_0 d\mathbf{e}_0 - d\mathbf{t}_0 \tag{2.9}$$

since terms in m cancel. Thus, when the current and ground states coincide, the $\boldsymbol{\lambda}$'s are actually invariant under change of measure. This conforms with the remark after (2.3), since every $\mathbf{t} = \boldsymbol{\sigma}$ when $\mathbf{e} = \mathbf{o}$. On the other hand, the $\boldsymbol{\mu}$'s still alter, being given by $\mathscr{M}\boldsymbol{\lambda}$ where $\mathscr{M}$ is the inverse of $\mathscr{L}$ in (2.8).

3. Construction of a Flow Rule

(i) The elastoplastic behaviour of a crystal is governed by the geometry and orientation of its lattice. Since slip causes this to move *through* the material (as viewed macroscopically), we need to keep track of the separate deformations in the lattice and the material, and to distinguish stresses relative to either.

For the present we let both the strain measure and ground state be arbitrary. Then, if $d\mathbf{e}$ is a differential strain of the material and $d^*\mathbf{e}$ is the accompanying strain of the lattice,

$$d\mathbf{e} - d^*\mathbf{e} = \sum (\nu d\gamma), \tag{3.1}$$

where the α's are the associated measures of crystallographic unit shears (with respect to the *deformed* lattice).

Let $d\mathbf{t}$ and $d^*\mathbf{t}$ denote increments in $\mathbf{t}$ reckoned relative to the material and lattice respectively. We make the distinction precise a little later. However, since any relative motion of the material and lattice is caused by slip alone, it is clear in advance that

$$d\mathbf{t} - d^*\mathbf{t} = \sum (\boldsymbol{\alpha} d\gamma) \tag{3.2}$$

with certain specifiable $\boldsymbol{\alpha}$'s, depending only on lattice geometry and the current stress and strain.

The preceding equations are primarily kinematic in character. We already have a constitutive connexion between $d\mathbf{t}$ and $d\mathbf{e}$, namely (2.1) which we repeat for convenience:

$$\mathscr{L}d\mathbf{e} - d\mathbf{t} = \sum (\boldsymbol{\lambda} d\gamma). \tag{3.3}$$

It remains to state a constitutive connexion between $d^*\mathbf{t}$ and $d^*\mathbf{e}$. This is necessarily of type

$$d^*\mathbf{t} - \mathscr{L}d^*\mathbf{e} = \sum (\boldsymbol{\beta} d\gamma) \tag{3.4}$$

with the *same* modulus tensor $\mathscr{L}$, since lattice and material deform as one in the absence of slip. The $\boldsymbol{\beta}$'s represent a possible stiffening of the lattice due to microscopic phenomena associated with continued slipping. That is, an extra increment of stress, $\Sigma(\boldsymbol{\beta} d\gamma)$ relatively to the lattice, would have to be applied to maintain its deformation as it was before the $d\gamma$'s occurred.

We are now in a position to identify the $\boldsymbol{\lambda}$'s and $\boldsymbol{\mu}$'s in terms of the $\boldsymbol{v}$'s, $\boldsymbol{\alpha}$'s and $\boldsymbol{\beta}$'s, all of which may be regarded as known. Addition of (3.3) and (3.4) produces

$$\mathscr{L}(d\mathbf{e}-d^*\mathbf{e})-(d\mathbf{t}-d^*\mathbf{t}) = \sum \{(\boldsymbol{\lambda}+\boldsymbol{\beta})d\gamma\}.$$

Having regard to (3.1) and (3.2) it is apparent that we can set

$$\boldsymbol{\lambda} = (\mathscr{L}\boldsymbol{v}-\boldsymbol{\alpha})-\boldsymbol{\beta} \tag{3.5}$$

for each slip system. Further, the $\boldsymbol{v}$'s and (as we shall see) also the $\boldsymbol{\alpha}$'s do not depend on the *ratios* of the $d\gamma$'s, nor therefore in particular on how many systems are active simultaneously. Consequently neither do the $\boldsymbol{\lambda}$'s, unless it be via the $\boldsymbol{\beta}$'s.

In passing, we recall that the residual strain after an infinitesimal cycle of stress $\mathbf{t}$ is $\Sigma(\boldsymbol{\mu} d\gamma)$ where, according to (3.2) and (3.5),

$$\boldsymbol{\mu} = \boldsymbol{v}-\mathscr{M}(\boldsymbol{\alpha}+\boldsymbol{\beta}). \tag{3.6}$$

Thus, what is commonly called 'plastic' deformation is not generally the resultant $\Sigma(\boldsymbol{v} d\gamma)$ *of the slips alone.* In particular, no matter what stress measure is cycled, the residual strain-increment usually contains a dilatational component.

(ii) We return to the specification of the $\boldsymbol{\alpha}$'s in (3.2). For this purpose it is simplest to choose the ground state coincident with the current state. Then, by applying a standard formula, the Jaumann differentials of Kirchhoff stress with respect to the material and lattice are connected by

$$\mathscr{D}\boldsymbol{\tau}-\mathscr{D}^*\boldsymbol{\tau} = \boldsymbol{\sigma}\times(d\boldsymbol{\theta}-d^*\boldsymbol{\theta})-(d\boldsymbol{\theta}-d^*\boldsymbol{\theta})\times\boldsymbol{\sigma} \tag{3.7}$$

where $d\boldsymbol{\theta}$ and $d^*\boldsymbol{\theta}$ are skew tensors that represent the incremental rotations of the material and lattice. To be exact, $d\boldsymbol{\theta}$ and $d^*\boldsymbol{\theta}$ are rotations of the respective triads of principal fibres associated with the strains $d\mathbf{e}$ and $d^*\mathbf{e}$. As remarked by TAYLOR (1938), since the relative rotation is due to crystallographic *simple* shears its components are

$$d\theta_{rs}-d^*\theta_{rs} = \tfrac{1}{2}\sum\{(m_r n_s - m_s n_r)d\gamma\}, \tag{3.8}$$

where (m_r) and (n_s) are unit vectors respectively in the slip direction and normal to the slip plane in the *deformed* lattice. Thus,

$$\mathscr{D}\boldsymbol{\tau}-\mathscr{D}^*\boldsymbol{\tau} = \sum(\boldsymbol{\alpha}_0 d\gamma), \tag{3.9}$$

where

$$(\alpha_0)_{rs} = \tfrac{1}{2}\sigma_{rp}(m_p n_s - m_s n_p)+\tfrac{1}{2}\sigma_{sp}(m_p n_r - m_r n_p).$$

Now, by analogy with (2.7),

$$d^*\mathbf{t} = d^*\mathbf{t}_0 - m\mathscr{S}d^*\mathbf{e}, \tag{3.10}$$

where $d^*\mathbf{t}_0 = \mathscr{D}^*\boldsymbol{\tau}$. Introducing (2.7), (3.9), and (3.10) into (3.2) we have finally

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}_0 - m\mathscr{S}\boldsymbol{v}, \tag{3.11}$$

where $\boldsymbol{v}$ now stands for the tensor with components

$$v_{rs} = \tfrac{1}{2}(m_r n_s + m_s n_r). \tag{3.12}$$

The operator $\mathscr{D}^*$ was introduced in the present context by HILL (1966).

Quantities unaffected by change of measure can be readily determined. From (2.8) and (3.11) one such is

$$\mathscr{L}\boldsymbol{v}-\boldsymbol{\alpha} = \mathscr{L}_0\boldsymbol{v}-\boldsymbol{\alpha}_0. \tag{3.13}$$

Remembering that $\boldsymbol{\lambda}$ is invariant, with the present choice of ground state, we see from (3.5) and (3.13) that $\boldsymbol{\beta}$ also is invariant. Or this can be recognized from (3.4) with (2.8) and (3.10). On the other hand, the difference between $\boldsymbol{\mu}$ and $\mathbf{v}$, namely $\mathscr{M}(\boldsymbol{\alpha}+\boldsymbol{\beta})$. is not invariant.

4. Normality and the Unloading Criterion

Two questions are at issue: what is the *precise* statement of the unloading criterion which leads to the normality rule in *conjugate variables* for a *finitely deformed* crystal; and to what extent can this criterion be justified on physical grounds? These questions have been posed by Hill (1972) and have been addressed by Rice (1971) for a somewhat less general crystal model than we adopt here. We shall see that the unloading criterion leading to normality reduces to that which Rice has shown to be sufficient both for a single crystal and for any composite aggregate of such crystals. However, it is here necessary to pursue the matter only for a single crystal in view of Hill's (1972) proof of the transmission of normality in conjugate variables to any such aggregate.

For normality in e-space the unloading criterion that must be taken in conjunction with (3.1) is

$$\boldsymbol{\lambda}\delta\mathbf{e} < 0 \tag{4.1}$$

for every slip system rendered potentially active by the applied stress $\boldsymbol{\sigma}$. This set of invariant inequalities delimits the local vertex of the domain in e-space attainable by elastic unloading from $\boldsymbol{\sigma}$. The $\boldsymbol{\lambda}$'s, in fact, are the outward normals to the pyramidal faces of the vertex. From (2.1) and (4.1) there follows

$$(\mathscr{L}d\mathbf{e}-d\mathbf{t})\delta\mathbf{e} = \sum (\boldsymbol{\lambda}\delta\mathbf{e}d\gamma) < 0 \tag{4.2}$$

since the $d\gamma$'s on active systems under the d-increment are positive by convention. With

$$\delta\mathbf{t} = \mathscr{L}\delta\mathbf{e},$$

where $\mathscr{L}$ is symmetric, (4.1) can be expressed as

$$\boldsymbol{\mu}\delta\mathbf{t} < 0, \tag{4.3}$$

and (4.2) re-arranged as

$$(d\mathbf{e}-\mathscr{M}d\mathbf{t})\delta\mathbf{t} < 0. \tag{4.4}$$

Thus, any plastic strain-increment has a negative scalar product with any elastic strain-increment, and so falls within another pyramid whose edges are outward normals to the faces to the yield vertex in t-space. This is a generalized version of the usual normality rule, which by (2.3) is invariant for all conjugate pairs.

In view of (3.5) the question then, at root, is whether

$$\mathbf{v}\delta\mathbf{t}-\boldsymbol{\alpha}\delta\mathbf{e} < \boldsymbol{\beta}\delta\mathbf{e} \tag{4.5}$$

is acceptable as the criterion of unloading. To answer this we need only consider a particular choice of ground state and measure. It is expedient to adopt logarithmic strain based on the current state, so transforming the left-hand side of (4.5) into

$$\mathbf{v}\mathscr{D}\boldsymbol{\tau}-\boldsymbol{\alpha}_0\delta\mathbf{e},$$

where

$$\mathscr{D}\boldsymbol{\tau} = \mathscr{L}_0\delta\mathbf{e}.$$

After substituting from (3.9) and (3.12) for $\boldsymbol{\alpha}_0$ and $\boldsymbol{v}$, and re-grouping terms, this becomes

$$m_r n_s(\mathscr{D}\boldsymbol{\tau}+\boldsymbol{\sigma}\times\delta\mathbf{e}-\delta\mathbf{e}\times\boldsymbol{\sigma})_{sr} = \delta\tau_m^n \quad \text{say.} \tag{4.6}$$

The expression in brackets is well known: it is the differential of one type of *mixed* components of Kirchhoff stress on a *deforming* basis embedded in the material (and in the lattice since $\delta\mathbf{e}$ is elastic). This particular convected differential is unsymmetric and (4.6) is its shear component associated with a slip system in just the way that the Schmid stress $m_r n_s \sigma_{sr}$ is. The notation $\delta\tau_m^n$ is intended as a reminder that the slip direction (regarded as a base vector) corresponds to a covariant index and the plane normal to a contravariant index. Specifically, if a_{qr} are the components of deformation gradient relative to the current state, so that an embedded unit vector m_r becomes $a_{qr}m_r$, we define

$$\tau_m^n = m_r n_s(a_{sp}^{-1}\tau_{pq}a_{qr}). \tag{4.7}$$

To verify (4.6) note that, to first order,

$$a_{rs} \approx \delta_{rs}+\delta e_{rs}+\delta\theta_{rs}, \qquad a_{rs}^{-1} \simeq \delta_{rs}-\delta e_{rs}-\delta\theta_{rs}.$$

Whence, when evaluated in the current state,

$$\delta(a_{sp}^{-1}\tau_{pq}a_{qr}) = (\delta\tau_{sr}+\sigma_{sq}\delta\theta_{qr}-\sigma_{pr}\delta\theta_{sp})+(\sigma_{sq}\delta e_{qr}-\sigma_{pr}\delta e_{sp}).$$

The first bracket on the right is $(\mathscr{D}\boldsymbol{\tau})_{sr}$, by the standard result already quoted in (3.7), while the second bracket is $(\boldsymbol{\sigma}\times\delta\mathbf{e}-\delta\mathbf{e}\times\boldsymbol{\sigma})_{sr}$ as it stands.

To summarize, the unloading criteria (4.1) or (4.3) leading to normality are equivalent to

$$\delta\tau_m^n < \boldsymbol{\beta}\delta\mathbf{e} \tag{4.8}$$

for each system, where the $\boldsymbol{\beta}$'s are such that

$$\mathscr{D}^*\boldsymbol{\tau}-\mathscr{L}_0 d^*\mathbf{e} = \sum(\boldsymbol{\beta}d\gamma) \tag{4.9}$$

after further slipping. Now any $\boldsymbol{\beta}$-effect is likely to be extremely small, it being commonly understood that the elastic response of a crystal lattice is essentially unaffected by slip. In fact, if (4.9) is re-arranged as

$$\mathscr{D}^*\boldsymbol{\tau} = \mathscr{L}_0[d^*\mathbf{e}+\sum(\mathscr{M}_0\boldsymbol{\beta}d\gamma)],$$

it is clear that each $(-\mathscr{M}_0\boldsymbol{\beta})$ can be interpreted as a ratio $d^*\mathbf{e}/d\gamma$ of additional lattice straining, per unit plastic shear, needed to maintain the same Kirchhoff stress *as referred to the lattice*. It is likely that plastic shears of order unity could be compensated in this way by small lattice stretches, perhaps typically less than a percent or so. In that event components of $\mathscr{M}_0\boldsymbol{\beta}$ would be extremely small fractions of unity. Then if (4.8) is re-written, with

$$\delta\mathbf{e} = \mathscr{M}_0\mathscr{D}\boldsymbol{\tau},$$

as

$$\delta\tau_m^n < (\mathscr{D}\boldsymbol{\tau})(\mathscr{M}_0\boldsymbol{\beta}),$$

it becomes clear that the necessary unloading criterion is virtually indistinguishable from $\delta\tau_m^n < 0$.

Certainly $\delta\tau_m^n < 0$ is a materially objective refinement of Schmid's law which, in addition, takes some account of varying lattice geometry (in contrast, for instance, to a criterion such as $\boldsymbol{v}\mathscr{D}\boldsymbol{\sigma} < 0$). But it is easy to construct equally plausible criteria which also reflect accompanying changes in geometry. For example, unloading could be characterized by a decrease in Schmid stress $\boldsymbol{v\sigma}$ when reckoned always in the deformed configuration. That is, appropriate allowance is made for changes

$$\delta m_r = (\delta_{rp} - m_r m_p) m_q (\delta e_{pq} + \delta \theta_{pq}),$$
$$\delta n_s = (\delta_{sp} - n_s n_p) n_q (\delta \theta_{pq} - \delta e_{pq})$$

in the unit vectors specifying the slip direction and slip-plane normal. With these expressions a short calculation gives

$$\delta \sigma_m^n + \sigma_{mn}(\delta e_n - \delta e_m) < 0 \qquad \text{(no summation)},$$

where δe_m and δe_n are the normal components of $\delta \mathbf{e}$ in the m and n directions. For comparison,

$$\delta \tau_m^n = \delta \sigma_m^n + \sigma_{mn} \delta e$$

where δe is the dilatational strain. In short, these and similar attempts at precise statements of the Schmid criterion differ by terms of order stress/modulus.

In typical cases the stresses are small fractions of some representative modulus and the $\boldsymbol{\beta}$-effect is presumably small as here estimated. Hence, to the extent that a Schmid-like criterion is appropriate, any deviations from the normality rule will remain barely observable at finite strain (provided, of course, that the rule is expressed in *conjugate variables*).

However, the normality rule will apply *precisely* only if (4.8) *as it stands* is the unloading criterion. Although the variables entering have an interesting interpretation as energetic 'forces' conjugate to the amounts of slip (RICE, 1971; and Section 5), we can suggest no argument why this criterion should apply exactly, especially when large lattice strains are considered. For example, to the extent that a $\boldsymbol{\beta}$-effect exists, it is not clear that such lattice stiffening with continuing slip should enter an unloading criterion. Nor is there reason to single out τ_m^n over other candidates for the shear stress measure. And, perhaps most important, it is unlikely that any choice of a *shear stress* measure could adequately reflect the influence of very large pressures on the slip criterion. Hence *strict* normality of the kind described does not seem plausible.

5. An Equivalent Formulation

The flow rule for a crystal can also be approached by a different route. The change in formal analysis is slight, but the shift in viewpoint is substantial. Our aim here is to make contact with the framework of RICE (1971).

We begin with Hill's bilinear form and re-arrange it so as to make explicit its connexion with work differentials:

$$\delta \mathbf{t} d\mathbf{e} - d\mathbf{t} \delta \mathbf{e} = \delta(\mathbf{t} d\mathbf{e}) - d(\mathbf{t} \delta \mathbf{e}) = d(\mathbf{e} \delta \mathbf{t}) - \delta(\mathbf{e} d\mathbf{t}) \tag{5.1}$$

since $\delta(d\mathbf{e}) = d(\delta \mathbf{e})$ and $\delta(d\mathbf{t}) = d(\delta \mathbf{t})$. We now identify d with any increment involving slips, typically $d\gamma$, and δ with any purely elastic increment. At constant temperature we assume that, within an elastic domain,

$$\mathbf{t} \delta \mathbf{e} = \delta \phi(\mathbf{e}), \qquad \mathbf{e} \delta \mathbf{t} = \delta \psi(\mathbf{t}), \qquad \phi + \psi = \mathbf{t}\mathbf{e}, \tag{5.2}$$

where the strain–energy density ϕ and complementary-energy density ψ (per unit ground-state volume) are of course functionals also of the slip history. Then dual variants of (5.1) are

$$\left.\begin{aligned} (\mathscr{L} d\mathbf{e} - d\mathbf{t}) \delta \mathbf{e} &= \delta(\mathbf{t} d\mathbf{e} - d\phi), \qquad & \mathscr{L} &= \partial^2 \phi / \partial \mathbf{e}^2, \\ (d\mathbf{e} - \mathscr{M} d\mathbf{t}) \delta \mathbf{t} &= \delta(d\psi - \mathbf{e} d\mathbf{t}), \qquad & \mathscr{M} &= \partial^2 \psi / \partial \mathbf{t}^2, \end{aligned}\right\} \tag{5.3}$$

where it is to be understood that $d\phi$ and $d\psi$ are increments on a path from a state $(\mathbf{t}, \mathbf{e})$ inside one elastic domain to a state $(\mathbf{t}+d\mathbf{t}, \mathbf{e}+d\mathbf{e})$ inside another. Equivalently

$$\mathscr{L}d\mathbf{e}-d\mathbf{t} = \frac{\delta}{\delta \mathbf{e}}(\mathbf{t}d\mathbf{e}-d\phi), \qquad d\mathbf{e}-\mathscr{M}d\mathbf{t} = \frac{\delta}{\delta \mathbf{t}}(d\psi-\mathbf{e}d\mathbf{t}), \tag{5.4}$$

where the notation emphasizes that the partial derivatives are generated via the limiting difference of a pair of such paths. These start from neighbouring states $(\mathbf{t}, \mathbf{e})$ and $(\mathbf{t}+\delta\mathbf{t}, \mathbf{e}+\delta\mathbf{e})$ in the same elastic domain and need coincide only along their plastic portions.

To establish the contact it is convenient to adopt a measure of slip increments that is the same for any given structural re-arrangement of the crystal, regardless of the lattice strain prevailing when the slips occurred. We recall that each $d\gamma$ is an increment of m-directed displacement (relative to the lattice) per unit distance in the n-direction; this does not have the desired invariance to lattice strain. A measure $d\tilde{\gamma}$ that does may be defined in a similar way, however, except that the m-directed 'displacement' and the n-directed 'distance' are measured in *units of lattice spacing*. These are defined by the current separations between lattice points which were some unit standard length apart in the geometry of the adopted ground-state. Let $\tilde{m}_r$ and $\tilde{n}_s$ be the unit direction and normal of a typical slip system in the ground-state lattice, and let a_{qr} be the lattice deformation gradient in some other state. Then $a_{qr}\tilde{m}_r$ is equal to the unit slip-direction vector in that state multiplied by the lattice stretch ratio for the slip direction, and $\tilde{n}_s a_{sp}^{-1}$ is equal to the unit slip-plane normal divided by the lattice stretch ratio for the distance between parallel slip planes. In particular, if a_{qr} is the lattice deformation gradient when slip takes place, it follows that

$$(a_{qr}\tilde{m}_r)(\tilde{n}_s a_{sp}^{-1})d\tilde{\gamma} = m_q n_p d\gamma.$$

Of course $d\gamma = d\tilde{\gamma}$ when the current state is adopted as ground state. More generally, consider any two neighbouring strains $\mathbf{e}$ and $\mathbf{e}+d\mathbf{e}$ (not necessarily at yield) that are associated with lattice deformation gradients a_{qr} and $a_{qr}+da_{qr}$ as well as intervening shear increments $d\tilde{\gamma}$. The *spatial* gradient of the resultant displacement increment is the direct sum of the spatial gradients in the lattice deformation da_{qr} and in the shears $d\tilde{\gamma}$:

$$da_{qr}a_{rp}^{-1} + a_{qr}\sum(\tilde{m}_r\tilde{n}_s d\tilde{\gamma})a_{sp}^{-1}. \tag{5.5}$$

Here we can regard $a_{qr}\tilde{m}_r$ as a convected base-vector in the slip direction and $\tilde{n}_s a_{sp}^{-1}$ as a corresponding reciprocal base-vector along the slip-plane normal.

With these invariant slip measures we may write

$$\mathbf{t}d\mathbf{e}-d\phi = d\psi-\mathbf{e}d\mathbf{t} = \sum(\chi d\tilde{\gamma}), \tag{5.6}$$

where the χ's are functions of stress or strain within the elastic domain, and must generally be assumed to depend also on the yield point at which the $d\tilde{\gamma}$'s occurred. Each χ is defined to within an additive constant, and in terms of them (5.4) becomes

$$\mathscr{L}d\mathbf{e}-d\mathbf{t} = \sum\left(\frac{\delta\chi}{\delta\mathbf{e}}d\tilde{\gamma}\right), \qquad d\mathbf{e}-\mathscr{M}d\mathbf{t} = \sum\left(\frac{\delta\chi}{\delta\mathbf{t}}d\tilde{\gamma}\right). \tag{5.7}$$

Notwithstanding the gradient structure of this flow rule, an interpretation of the χ's as plastic potentials in the conventionally understood sense is not justified at this stage, in view of the meaning given to the δ-derivatives.

The χ's correspond to energetic 'forces' conjugate to the amount of slip (or to any other suitable set of anholonomic 'internal variables') in RICE's (1971) framework. Indeed, (5.7) was derived there as a set of generalized reciprocal relations for the semi-perfect differential forms $d\phi$ and $d\psi$ in (5.6). It is characteristic of this approach that inelastic strains are not treated directly but enter instead via the history dependence of the elastic energy potential.

To identify the χ's note that a general strain increment from a point in one elastic domain to a point in another corresponds to the spatial gradient of displacement increment given by (5.5). Its scalar product with Kirchhoff stress is the increment of work per unit ground-state volume, so that

$$\mathbf{t}d\mathbf{e} = a_{rp}^{-1}\tau_{pq}da_{qr} + \sum (\tau_m^n d\tilde{\gamma}), \tag{5.8}$$

where τ_m^n is the mixed shear stress defined analogously to that of (4.7), but now referred to the lattice geometry of the *ground* state. The leading term is clearly the change in strain energy density when no slip occurs. In general, therefore,

$$d\phi = a_{rp}^{-1}\tau_{pq}da_{qr} + \sum (bd\tilde{\gamma}), \tag{5.9}$$

where, since da_{qr} denotes the change in lattice deformation, the b's account for the $\boldsymbol{\beta}$-effect (each being determined, like its associated χ, to within an additive constant in an elastic domain). From (5.6) it is evident that we can make the identification

$$\chi = \tau_m^n - b, \tag{5.10}$$

so that

$$\boldsymbol{\lambda}d\gamma = \frac{\delta}{\delta\mathbf{e}}(\tau_m^n - b)d\tilde{\gamma}, \qquad \boldsymbol{\mu}d\gamma = \frac{\delta}{\delta\mathbf{t}}(\tau_m^n - b)d\tilde{\gamma}. \tag{5.11}$$

On adopting the current state as ground state we recover the previous expression for the invariant $\boldsymbol{\lambda}\delta\mathbf{e}$ embodied in (4.8), when $\boldsymbol{\beta}$ is written for $\delta b/\delta\mathbf{e}$.

This interpretation of the χ's is the same as that established by RICE (1971) in the restricted case when they are assumed to have no explicit dependence on the point of departure from an elastic domain. Indeed, we see that the τ_m^n part of χ has no such dependence, so that the δ-derivatives of it in (5.11) are the same as conventional derivatives. The question is open as to whether the b part contains such a dependence. If it does not, then (5.7) implies the existence of plastic potentials $\chi \equiv \tau_m^n - b = \text{const.}$ in the conventionally understood sense. If it does, plastic potentials may yet be defined but only when the stress state at yield is specified. In any event it is only the b part which causes difficulty and, as regards its stress dependence, we have estimated that it will generally be negligible in comparison to τ_m^n.

6. STRAIN HARDENING

We discuss briefly how the framework (2.1) with (3.5) and (3.6), or its equivalent (5.7) with (5.10), might be completed by adjoining an appropriate hardening rule. This must be properly objective and permit the crystal slips to be computed unambiguously in terms of prescribed increments of stress or strain. It must naturally also be consistent with the criterion of unloading. For this we choose, by way of illustration and with the reservations already noted, (4.1) and (4.3). We then have a normality structure which allows some definite statements in regard to uniqueness.

Remembering that $\lambda d\mathbf{e}/\rho$ is invariant under change of measure and ground state, we suppose that

$$\left.\begin{aligned}\boldsymbol{\lambda}_i d\mathbf{e} &= g_{ij}d\gamma_j \text{ when the } i\text{th system is active,}\\ \boldsymbol{\lambda}_i d\mathbf{e} &\leqslant g_{ij}d\gamma_j \text{ when the } i\text{th system is inactive,}\end{aligned}\right\} \tag{6.1}$$

where j is summed and i, j may take values $1, \ldots, n$, n being the number of systems made critical (or potentially active) in a considered state by given loads. The moduli g_{ij} are presumed not to depend on how many systems are activated, but can take account of any linear coupling. When the applied $d\mathbf{e}$ does not cause slip, (6.1) reduces to (4.1) as required.

To transform these relations into a hardening rule more familiar in appearance, we introduce new moduli

$$h_{ij} = g_{ij} - \boldsymbol{\lambda}_i \boldsymbol{\mu}_j. \tag{6.2}$$

Then, by resolving the first of (2.1) on the direction $\boldsymbol{\mu}_i$,

$$\boldsymbol{\mu}_i d\mathbf{t} - h_{ij}d\gamma_j = \boldsymbol{\lambda}_i d\mathbf{e} - g_{ij}d\gamma_j,$$

provided that $\mathscr{L}$ is symmetric. Thus, by (6.1),

$$\left.\begin{aligned}\boldsymbol{\mu}_i d\mathbf{t} &= h_{ij}d\gamma_j \text{ when the } i\text{th system is active,}\\ \boldsymbol{\mu}_i d\mathbf{t} &\leqslant h_{ij}d\gamma_j \text{ when the } i\text{th system is inactive,}\end{aligned}\right\} \tag{6.3}$$

consistent with the no-slip criterion (4.3). The coefficients h_{ij} are seen to have the character of rates of slip-hardening, but are not measure-invariant like the g_{ij}'s. Indeed, $\boldsymbol{\mu}_i \boldsymbol{\lambda}_j = \boldsymbol{\lambda}_i \mathscr{M} \boldsymbol{\lambda}_j$ changes with measure even when the current state is used for reference, since the elastic moduli and compliances still change in accordance with (2.8).

Suppose, now, that the strain measure $d\mathbf{e}$ is assigned. Following the method of HILL (1966) we show that the $d\gamma$'s are unique, and hence also the motion of the lattice relative to the material, when

$$\text{matrix } (g_{ij}) \text{ is positive-definite.} \tag{6.4}$$

This sufficiency condition is invariant, by what has been said. Let the prefix Δ denote the difference of pairs of corresponding quantities in two presumed distinct modes of slip. By (2.1) we have

$$\Delta(d\mathbf{e})\Delta(\mathscr{L}d\mathbf{e} - d\mathbf{t}) = \Delta(\boldsymbol{\lambda}_i d\mathbf{e})\Delta(d\gamma_i)$$

with summation over the critical systems. Now, by (6.1),

$$\Delta(\boldsymbol{\lambda}_i d\mathbf{e})\Delta(d\gamma_i) = g_{ij}\Delta(d\gamma_i)\Delta(d\gamma_j) \qquad \text{(no sum over } i)$$

when the ith system is active in both modes or in neither, while

$$\Delta(\boldsymbol{\lambda}_i d\mathbf{e})\Delta(d\gamma_i) \geqslant g_{ij}\Delta(d\gamma_i)\Delta(d\gamma_j) \qquad \text{(no sum over } i)$$

when the ith system is active in only one mode (with equality only when the system stays critical in the other). Consequently, taking account of all systems,

$$\Delta(d\mathbf{e})\Delta(\mathscr{L}d\mathbf{e} - d\mathbf{t}) \geqslant g_{ij}\Delta(d\gamma_i)\Delta(d\gamma_j) \tag{6.5}$$

with summation over both i and j. The inequality is strict when and only when some system is active in one mode but becomes non-critical in the other. In any event (6.4) ensures that the left-hand side of (6.5) would be positive if any $\Delta(d\gamma)$ could be non-zero. But prescription of $d\mathbf{e}$ makes the left-hand side vanish, and consequently every

$d\gamma$ must be the same in both modes. This establishes uniqueness of the slips and hence that of $d\mathbf{t}$ calculated from (2.1).

An analogous argument applied with prescribed $d\mathbf{t}$, instead of $d\mathbf{e}$, succeeds only if matrix (h_{ij}) is positive-definitie. Since this is a non-invariant condition, uniqueness of the $d\gamma$'s and $d\mathbf{e}$ is not provable by this method for arbitrary stress-measures. Indeed, unqualified uniqueness is not to be expected on general grounds. We can note, however, that for any measure such that (h_{ij}) *is* positive-definite (6.4) can be ensured by requiring that the associated tensor of elastic moduli is also positive-definite (likewise a non-invariant condition).

There remains the question whether a rule of type (6.3) could hold in principle, irrespective of how the lattice moves in the material. To answer this we note that

$$h_{ij} - h_{ij}^* = \boldsymbol{\lambda}_i(\mathbf{v}_j - \boldsymbol{\mu}_j) = \boldsymbol{\mu}_i(\boldsymbol{\alpha}_j + \boldsymbol{\beta}_j)$$

where the new moduli

$$h_{ij}^* = g_{ij} - \boldsymbol{\lambda}_i \mathbf{v}_j \tag{6.6}$$

are measure-invariant. Then (6.1) becomes

$$\left.\begin{aligned} \boldsymbol{\lambda}_i d^*\mathbf{e} &= h_{ij}^* d\gamma_j \text{ when the } i\text{th system is active,} \\ \boldsymbol{\lambda}_i d^*\mathbf{e} &\leqslant h_{ij}^* d\gamma_j \text{ when the } i\text{th system is inactive,} \end{aligned}\right\} \tag{6.7}$$

by virtue of (3.1). This rule is plainly objective for the lattice, and it follows that the h_{ij}'s in (6.3) are well defined. We see also that the moduli h_{ij}^* represent slip hardening over and above the lattice stiffening described after (3.4). Indeed by means of the latter we can transform (6.7) to

$$\left.\begin{aligned} \boldsymbol{\mu}_i(d^*\mathbf{t} - \boldsymbol{\beta}_j d\gamma_j) &= h_{ij}^* d\gamma_j \text{ when the } i\text{th system is active,} \\ \boldsymbol{\mu}_i(d^*\mathbf{t} - \boldsymbol{\beta}_j d\gamma_j) &\leqslant h_{ij}^* d\gamma_j \text{ when the } i\text{th system is inactive.} \end{aligned}\right\} \tag{6.8}$$

Further, when the $\boldsymbol{\beta}$'s vanish, $\boldsymbol{\mu} d^*\mathbf{t} = d\tau_m^n$ according to (5.11), the mixed components being based on the current state. In that event (6.8) can be interpreted as an objective hardening rule for the critical lattice shear strengths.

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APPENDIX

Effects of changing stress and strain measures

We record here some effects of changing from one conjugate pair of stress and strain measures to another, say from (**t**, **e**) to (**t**′, **e**′) where

$$\mathbf{t}d\mathbf{e}/\rho \equiv \mathbf{t}'d\mathbf{e}'/\rho' \tag{A.1}$$

and ρ, ρ' are the densities in the respective ground states. To simplify the analysis we treat second-rank tensors as 9×1 vectors, and fourth-rank tensors as 9×9 matrices, in the customary manner. Then (A.1) leads successively to

$$\frac{\rho}{\rho'}\, t_i' = \frac{\partial e_k}{\partial e_i'}\, t_k \; (i,k = 1, \ldots, 9;\ \text{summation convention}), \tag{A.2}$$

$$\frac{\rho}{\rho'}\, dt_i' = \frac{\partial e_k}{\partial e_i'}\, dt_k + \frac{\partial^2 e_k}{\partial e_i' \partial e_l'}\, t_k\, de_l'. \tag{A.3}$$

Suppose that incremental elastic relations $\delta t_k = \mathscr{L}_{kl}\delta e_l$ transform to $\delta t_i' = \mathscr{L}'_{ij}\delta e_j'$. The δ-differentials satisfy equations similar to (A.3), from which we obtain

$$\frac{\rho}{\rho'}\, \mathscr{L}'_{ij} = \frac{\partial e_k}{\partial e_i'}\frac{\partial e_l}{\partial e_j'}\, \mathscr{L}_{kl} + \frac{\partial^2 e_k}{\partial e_i' \partial e_j'}\, t_k, \tag{A.4}$$

connecting the new and old moduli. Their skew parts are thus related by

$$\frac{\rho}{\rho'}\, (\mathscr{L}'_{ij} - \mathscr{L}'_{ji}) = \frac{\partial e_k}{\partial e_i'}\frac{\partial e_l}{\partial e_j'}\, (\mathscr{L}_{kl} - \mathscr{L}_{lk}), \tag{A.5}$$

from which it follows that diagonal symmetry of moduli is preserved under change of measure.

By combining (A.3) and (A.4) we can generate

$$\frac{\rho}{\rho'}\, (dt_i' - \mathscr{L}'_{ij}de_j') = (dt_k - \mathscr{L}_{kl}de_l)\, \frac{\partial e_k}{\partial e_i'}.$$

Equivalent to these component equations is the single scalar identity

$$(dt_i' - \mathscr{L}'_{ij}de_j')\delta e_i'/\rho' = (dt_k - \mathscr{L}_{kl}de_l)\delta e_k/\rho \tag{A.6}$$

in the independent differentials d and δ. This corresponds to (2.3) in the text of this paper.

Similarly,

$$\frac{\rho}{\rho'}\, (dt_i' - \mathscr{L}'_{ji}de_j') = (dt_k - \mathscr{L}_{lk}de_l)\, \frac{\partial e_k}{\partial e_i'},$$

which is equivalent to

$$(dt_i' - \mathscr{L}'_{ji}de_j')\delta e_i'/\rho' = (dt_k - \mathscr{L}_{lk}de_l)\delta e_k/\rho. \tag{A.7}$$

This invariant can be re-written as

$$(d\mathbf{t} - \mathscr{L}^T d\mathbf{e})\delta\mathbf{e}/\rho,$$

where $\mathscr{L}^T$ is the transpose of $\mathscr{L}$, or as

$$(d\mathbf{t}\delta\mathbf{e} - \delta\mathbf{t}d\mathbf{e})/\rho, \tag{A.8}$$

where $\delta\mathbf{t} = \mathscr{L}\delta\mathbf{e}$. This is the bilinear form studied by HILL (1972) in connexion with the work in a certain *virtual* cycle of both stress and strain.

By contrast, the work (per unit mass) in an *actual* cycle of strain alone, namely $\mathbf{e}+\delta\mathbf{e} \to \mathbf{e} \to \mathbf{e}+d\mathbf{e} \to \mathbf{e}+\delta\mathbf{e}$ where the intermediate arc is plastic and the others elastic, is

$$\oint \mathbf{t}d\mathbf{e}/\rho = (d\mathbf{t}-\mathscr{L}d\mathbf{e})\delta\mathbf{e}/\rho+\tfrac{1}{2}d\mathbf{e}(\mathscr{L}^T-\mathscr{L})\delta\mathbf{e}/\rho \tag{A.9}$$

by the trapezoidal rule, correct to first order in each differential. Not only is the expression as a whole therefore invariant, but also its separate parts by virtue of (A.4) and (A.5).