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A DISCRETE MODEL FOR THE PREDICTION OF SUBSEQUENT YIELD SURFACES IN POLYCRYSTALLINE PLASTICITY

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Abstract—A discrete model suitable for the analysis of polycrystalline aggregate response under macroscopically uniform, quasi-static loading is developed, with particular emphasis on the characteristics of subsequent yield surfaces in stress or strain space. Internal stress and deformation states are determined from approximating, piecewise linear infinitesimal displacement fields within crystal grains, based upon broadly defined constitutive behavior which permits inclusion of cubic or hexagonal crystal anisotropy and relatively general hardening laws over crystallographic slip systems. Appropriate aggregate matrices are established as symmetric, positive-definite, and internal fields corresponding to the solution of the discrete model are proved to be unique. It is further shown that the final calculation of incremental crystal shears can be posed as a quadratic programming problem.

1. INTRODUCTION

THE first satisfactory theory for predicting the plastic deformation of polycrystalline aggregates from phenomenological laws of single crystal behavior was advanced by Taylor [1, 2]. In Taylor's now classic work, the simplest possible kinematic model was adopted consistent with the concept of a deformed continuum–uniform strain throughout the crystal grains. This theory was generalized by Bishop and Hill [3–5] to enable the approximate calculation of macroscopic yield surfaces of pronounced yielding (neglecting elastic behavior) and modified by Lin [6] to incorporate elastic strains. Subsequent studies were made by Payne *et al.* [7, 8]. Other theories and models of interacting crystals, all utilizing isotropic elastic field solutions in one form or another, have been proposed and/or investigated by Kröner [9], Budiansky and Wu [10], Hutchinson [11, 12], Hill [13], and Lin *et al.* [14–23], with the models of Lin *et al.*, most nearly satisfying all equilibrium and kinematic conditions in numerical evaluations.

In the present paper, a new discrete aggregate model suitable for predicting macroscopic stress–strain relations and aggregate yield surfaces is presented which incorporates certain features of previous models but is more general in several important respects. Moreover, the model is closely related to theoretical characteristics of anisotropic crystal and aggregate behavior established by Hill [24, 25].

2. RELATIONS BETWEEN MICRO- AND MACRO-FIELDS

Before proceeding to a general presentation and analysis of the discrete model, we first derive some general relationships involving volume averages of aggregate continuum micro-fields. Consider an arbitrary volume V of surface S within a polycrystalline metal

specimen. We denote any statically admissible stress field in V, corresponding to a system of self-equilibrating tractions $\mathbf{T}^*$ on S, by $\boldsymbol{\zeta}^*$ (with tensor components ζ_{ij}^*) and any continuous, piecewise differentiable infinitesimal displacement field by $\delta\mathbf{u}^0$. A straightforward application of Gauss' theorem then yields

$$\int_V (\boldsymbol{\zeta}^* \,.\, \delta\boldsymbol{\xi}^0)\, \mathrm{d}V = \int_S (\mathbf{T}^* \,.\, \delta\mathbf{u}^0)\, \mathrm{d}S \tag{2.1}$$

wherein

$$\delta\boldsymbol{\xi}^0 = \boldsymbol{D}^T \delta\mathbf{u}^0 \tag{2.2}$$

locally within each crystal grain V_M of V. (See the Appendix for definitions.) To obtain an equivalent expression for the right-hand side of (2.1) in terms of macroscopic stress and strain over the smallest possible volume sample, we introduce the mathematical model of an aggregate of identical "unit cubes" and define macroscopically uniform fields

$$\delta\mathbf{u}^0(A_i^+) = \delta\mathbf{u}^0(A_i^-) + \overset{i}{\mathbf{c}}{}^0 \tag{2.3}$$

$$\overset{i}{\mathbf{T}}{}^*(A_i^+) = -\overset{i}{\mathbf{T}}{}^*(A_i^-) \tag{2.4}$$

(respectively kinematically and statically admissible). A_i^+ denotes the unit cube face corresponding to the positive coordinate axis x_i and $\overset{i}{\mathbf{c}}{}^0$ is a constant vector independent of position over A_i^+ (unless the aggregate extends in only two directions and A_i^+ is a free face). Macroscopic stress and incremental strain are evaluated in a natural way as

$$\sigma_{ij}^* = \int \overset{i}{T}{}_j^* \, \mathrm{d}A_i^+ \tag{2.5}$$

$$\delta\varepsilon_{ij}^0 = \tfrac{1}{2}\left(\int \overset{i}{c}{}_j^0 \, \mathrm{d}A_i^+ + \int \overset{j}{c}{}_i^0 \, \mathrm{d}A_j^+ \right). \tag{2.6}$$

Upon substitution of (2.3)–(2.5) into (2.1), we find

$$\int \mathbf{T}^* \,.\, \delta\mathbf{u}^0 \, \mathrm{d}S = \int \sigma_{ij}^* \overset{i}{c}{}_j^0 \, \mathrm{d}A_i^+ . \tag{2.7}$$

From considerations of moment equilibrium

$$\int \overset{i}{T}{}_j^* \, \mathrm{d}A_i^+ = \int \overset{j}{T}{}_i^* \, \mathrm{d}A_j^+ . \tag{2.8}$$

Hence, the macroscopic stress tensor is symmetric and, from (2.6) and (2.7), (2.1) can be written

$$\int (\boldsymbol{\zeta}^* \,.\, \delta\boldsymbol{\xi}^0)\, \mathrm{d}V = \boldsymbol{\sigma}^* \,.\, \delta\boldsymbol{\varepsilon}^0 \tag{2.9}$$

with V now representing the unit volume of the polycrystalline cube. Furthermore, from (2.2), (2.3) and (2.6),

$$\delta\boldsymbol{\varepsilon}^0 = \int (\delta\boldsymbol{\xi}^0)\, \mathrm{d}V \tag{2.10}$$

and, from (2.4) and (2.5) and force equilibrium over any interior plane area normal to a coordinate axis,

$$\boldsymbol{\sigma}^* = \int \boldsymbol{\zeta}^* \, \mathrm{d}V. \tag{2.11}$$

Equations (2.10) and (2.11) are of course equivalent to (2.6) and (2.5), and equation (2.9) (together with these definitions) is the well known virtual work equation for the polycrystalline aggregate. We merely remark here that by mathematically defining states of homogeneous macrostrain and macrostress (2.3), (2.4) the relationship (2.9) follows immediately and the various additional arguments of Bishop and Hill [3], Kocks [26] and Hill [25] are unnecessary. Bishop and Hill's criterion, which can be written

$$\int (\overset{i}{T}{}_j^* \delta u_k^0) \, \mathrm{d}A_i = \left(\int \overset{i}{T}{}_j^* \, \mathrm{d}A_i \right) \int (\delta u_k^0) \, \mathrm{d}A_i \tag{2.12}$$

for arbitrary i, j, k, is in fact distinctly different from (2.3), (2.4), and neither condition implies the other. In addition, although the macroscopic stress tensor is symmetric, equations (2.3) and (2.4) do not preclude the existence of small macroscopic couple stresses (depending upon the distribution of crystal orientations within the cube). These are determined as

$$\overset{i}{\mathbf{m}}{}^* = \int (\mathbf{r} \times \overset{i}{\mathbf{T}}{}^*) \, \mathrm{d}A_i^+ \tag{2.13}$$

where $\mathbf{r}$ is the position vector to a point on the face A_i^+.

3. SELECTION OF MODEL FOR POLYCRYSTALLINE AGGREGATE ANALYSIS

If we were to consider only (idealized) elastically isotropic crystals in defining an aggregate boundary value problem, elastic field solutions for point body forces could be introduced (as in [17, 18, 20]), thus permitting both non-uniform microstress and displacement fields over unit cube faces A_i while still satisfying the virtual work equation (2.9). To consider aggregates of anisotropic crystals, however, (thereby enabling investigation of the effects of texturing on macroscopic yield surfaces, for example), it is almost mandatory that a model with either uniform tractions or (at most) linearly varying displacements over the faces A_i be adopted. The latter is chosen herein as the preferred approximation on the basis of the following argument.

Consider a thin-walled tube subjected to, say, axial load and internal pressure. The wall thickness of specimens studied experimentally in combined stress tests is often in the range 1–2 mm, with from 10–30 grains through the thickness (see [27, 28]). Thus, as an idealization of the physical situation, we assume a thickness of 1 mm and define a unit cube $V = 1\ \mathrm{mm}^3$ containing on the order 1000 crystal grains in the corresponding "flat sheet" representation (i.e. a *macroscopic* plane stress problem). Then the longitudinal faces (Fig. 1) become planes of symmetry in our model of identically deforming cubes. We further assume the distribution of crystal orientations to be symmetric with respect to transverse planes. Hence, (2.3) and (2.4) are satisfied, with displacement components constant or corresponding stresses zero on the various faces. If uniform tractions had been imposed over the cube, the transverse and longitudinal faces would no longer be planes of symmetry and adjacent cubes could not deform identically. Thus, we select as a model for analysis a

unit cube (of generally anisotropic crystals) on each of whose faces A_i either infinitesimal displacements are prescribed, to give the appropriate macroscopic strain increment [through (2.6)], or tractions are zero (free face).

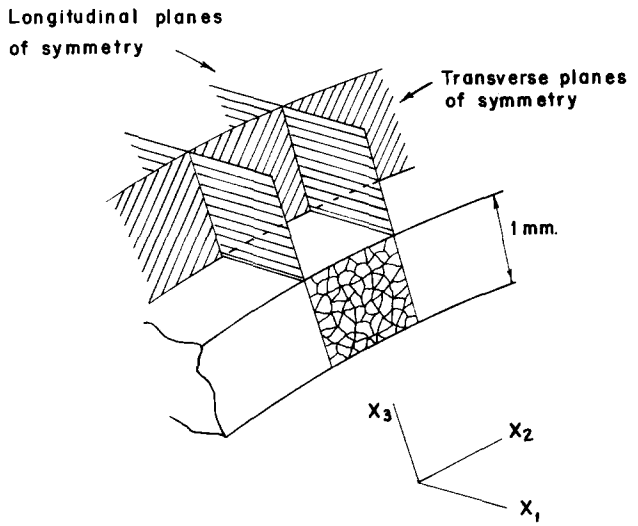

FIG. 1. Idealized unit cube in thin-walled polycrystalline specimen.

4. CONSTITUTIVE EQUATIONS AND RESOLUTION OF INTERNAL STRAIN FIELD

Let $\mathbf{C}_c$ denote the positive-definite crystal elastic compliance matrix referred to the geometric (lattice) axes and $\mathbf{C}$ denote the local elastic compliance referred to the unit cube axes x_i. Then

$$\mathbf{C} = \mathbf{A}^T\mathbf{C}_c\mathbf{A} \tag{4.1}$$

where $\mathbf{A}$ is the stress vector transformation matrix from the cube axes to the lattice axes (an orthogonal rotation in six-dimensional stress space, whence $\mathbf{A}^{-1} = \mathbf{A}^T$). We define $\delta\boldsymbol{\xi}^{(e)}$ as the infinitesimal strain field determined by assuming that the aggregate response to imposed macrostrain increment $\delta\boldsymbol{\varepsilon}$ is wholly elastic:

$$\delta\boldsymbol{\xi}^{(e)} = \boldsymbol{D}^T\delta\mathbf{u}^{(e)} = \boldsymbol{\Upsilon}\delta\boldsymbol{\varepsilon} \tag{4.2}$$

in which $\boldsymbol{\Upsilon}$ is a tensor (matrix) function of position within V, due to the elastic inhomogeneity. We further denote

$$\delta\boldsymbol{\xi}^s = \boldsymbol{D}^T\delta\mathbf{u}^s = \delta\boldsymbol{\xi} - \delta\boldsymbol{\xi}^{(e)} \tag{4.3}$$

as the infinitesimal strain due to internal slip and self-straining and define a related stress field

$$\delta\boldsymbol{\zeta}^s = \delta\boldsymbol{\zeta} - \mathbf{C}^{-1}\delta\boldsymbol{\xi}^{(e)}. \tag{4.4}$$

Then, from (2.9), (2.10) and (4.2)–(4.4),

$$\int \delta\zeta^* \,.\, \delta\xi^{(e)}\, dV = \delta\sigma^* \,.\, \delta\varepsilon \tag{4.5}$$

$$\int \delta\zeta^* \,.\, \delta\xi^{s}\, dV = 0 \tag{4.6}$$

wherein ζ^* may be ζ, $\zeta^{(e)} = \mathbf{C}^{-1}\xi^{(e)}$, or ζ^s. Moreover, a symmetric, inverse elastic compliance matrix of the aggregate can be calculated as

$$\mathbf{C}^{-1}_{\text{macro}} = \int \Upsilon^T \mathbf{C}^{-1} \Upsilon \, dV. \tag{4.7}$$

The local micro-plastic strain increment $\delta\xi^p$ is determined by the incremental plastic shears $\delta\gamma_k$ on the N crystallographic slip systems of the crystal grain through the transformation

$$\delta\xi^p = \mathbf{N}^T \delta\gamma = \delta\xi - \mathbf{C}\,\delta\zeta \tag{4.8}$$

with the resolved shear stresses τ_k in these slip systems evaluated as

$$\tau = \mathbf{N}\zeta = \mathbf{N}_c\mathbf{A}\zeta, \tag{4.9}$$

in which $\mathbf{N}_c$ is referred to the crystal axes. The transformation matrix $\mathbf{N}$ is defined in terms of its kth row vector $\mathbf{N}_k$ in the Appendix. (Opposite senses of slip in the same crystallographic slip system are denoted by different k's so that $\delta\gamma_k$ is always non-negative.) From (4.3), (4.4) and (4.8), $\delta\zeta^s$ can also be expressed

$$\delta\zeta^s = \mathbf{C}^{-1}(\delta\xi^s - \delta\xi^p) \tag{4.10}$$

and, with the aid of (2.9), (4.5), (4.6), (4.9) and some additional algebra, we can establish the inequality

$$\int \delta\tau^s \,.\, \delta\gamma \, dV < 0, \tag{4.11}$$

which condition will prove of consequence in our investigation of a Bauschinger effect in Section 7. Lastly, we introduce a general crystal hardening matrix $\mathbf{H}$ [24, 29] relating increments in critical stresses $\delta\tau^k_{\text{cr}}$ in the various slip systems to the incremental shears $\delta\gamma_k$:

$$\delta\tau_{\text{cr}} = \mathbf{H}(\gamma)\,\delta\gamma. \tag{4.12}$$

For the present, we require only that $\mathbf{H}$ be positive-semidefinite. Yielding in a particular critical (potentially active) slip system occurs only when $\delta\tau_k = \delta\tau^k_{\text{cr}}$. A critical system is of course defined by $\tau_k = \int \delta\tau^k_{\text{cr}}$, where the latter is integrated over the plastic strain history from an initial critical stress τ_0.

5. DISCRETIZATION OF AGGREGATE MODEL AND GENERAL SOLUTION FOR CRYSTAL SHEARS

To discretize the above-defined aggregate model, we introduce a kinematically admissible, approximating infinitesimal displacement field which is continuous throughout the

aggregate and piecewise linear within each crystal grain. Correspondingly, a crystal subvolume with constant microstrain field is represented by a tetrahedral element, herein called a crystallite, with nodal points I, J, K, L (Fig. 2). The infinitesimal displacement $\delta\bar{\mathbf{u}}(\mathbf{x})$ within the crystallite q is readily expressed in terms of the nodal displacements $\delta\bar{\mathbf{u}}^M$ as (see [30], for example)

$$\delta\bar{\mathbf{u}}(\mathbf{x}) = \sum_{M(q)} \phi_M^q(\mathbf{x})\, \delta\bar{\mathbf{u}}^M \tag{5.1}$$

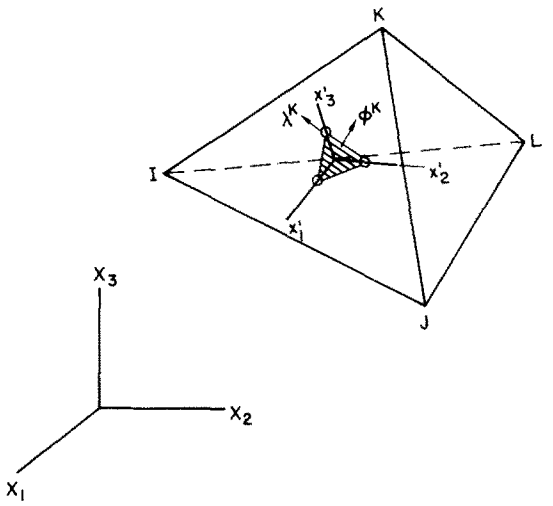

FIG. 2. Tetrahedral crystallite showing orientation of crystal axes and kth slip system.

wherein

$$\phi_M^q(\mathbf{x}) = \alpha_M^q + \beta_{Mj}^q x_j. \tag{5.2}$$

The constants α_M^q, β_{Mj}^q are determined from the nodal coordinates of q through the equations $\phi_M^q(\mathbf{x}^J) = \delta_M^J$, $J, M = 1, \ldots, 4$ (where δ_M^J is the Kronecker delta). The local incremental strain field is

$$\delta\bar{\boldsymbol{\xi}}_{(q)} = \sum_{M(q)} \boldsymbol{\beta}_q^M\, \delta\bar{\mathbf{u}}^M \tag{5.3}$$

in which

$$\boldsymbol{\beta}_q^M = \boldsymbol{D}^T \phi_M^q(\mathbf{x}). \tag{5.4}$$

From virtual work considerations (see [31] for additional details), the incremental differential field equation $\boldsymbol{D}\,\delta\boldsymbol{\zeta} = \mathbf{0}$ within the unit cube is replaced by the set of discrete equations

$$\sum_{q(J)} \boldsymbol{D}\phi_J^q \int \delta\bar{\boldsymbol{\zeta}}_{(q)}\, \mathrm{d}V_q = \mathbf{0} \tag{5.5}$$

over the crystallite nodes J at which displacements are to be determined. Resolving the infinitesimal strain field as in (4.2), (4.3), then, from (4.4), (4.8), (5.3) and (5.4), equations

(5.5) are separable into two sets, the first of which can be solved independently of the second. These equations are written in general matrix form as

$$\mathbf{B}_i^T \mathbf{S} \mathbf{B}_i \, \delta\bar{\mathbf{U}}^{(e)} \equiv \mathbf{K} \, \delta\bar{\mathbf{U}}^{(e)} = -\mathbf{B}_i^T \mathbf{S} \mathbf{B}_0 \, \delta\mathbf{U}^0 \tag{5.6}$$

$$\mathbf{K} \, \delta\bar{\mathbf{U}}^s = \mathbf{B}_i^T \mathbf{S} \bar{\mathbf{N}}^T \, \delta\bar{\boldsymbol{\Gamma}} \tag{5.7}$$

in which $\delta\bar{\mathbf{U}}^{(e)} = (\ldots, \delta\bar{\mathbf{u}}^{(e)M}, \ldots)$ is the overall vector of unknown elastic nodal displacements, $\delta\mathbf{U}^0$ is the vector of prescribed displacements corresponding to $\delta\boldsymbol{\varepsilon}$ through (2.3) and (2.6), $\delta\bar{\mathbf{U}}^s = (\ldots, \delta\bar{\mathbf{u}}^{s(M)}, \ldots)$ is the overall vector of "slip" displacements, and $\delta\bar{\boldsymbol{\Gamma}} = (\ldots, \delta\bar{\gamma}_{(q)}, \ldots)$ is the overall vector of incremental shears. The matrices $\mathbf{B}_i$ (defined over nodes J of unknown displacements) and $\mathbf{B}_0$ (defined over nodes J^0 of prescribed displacements) are composed of 6 by 3 elements $\mathbf{B}_{qJ}$ given as

$$\mathbf{B}_{qJ} = \begin{cases} \mathbf{A}_{(q)} \boldsymbol{\beta}_q^J = \mathbf{A}_{(q)} \boldsymbol{D}^T \phi_J^q \text{ if } J \text{ is a node of } (q) \\ \mathbf{0} \text{ if } J \text{ is not a node of } (q). \end{cases} \tag{5.8}$$

The matrices $\mathbf{S}$ and $\bar{\mathbf{N}}$ are diagonal in the sub-matrices $\mathbf{C}_c^{-1}$ and $\mathbf{N}_c$,

$$\mathbf{S} = \lceil \mathbf{C}_c^{-1} \rfloor, \qquad \bar{\mathbf{N}} = \lceil \mathbf{N}_c \rfloor, \tag{5.9}$$

and the aggregate elastic "stiffness" matrix $\mathbf{K}$ is symmetric and positive-definite, arbitrary rigid body motion having been eliminated from the solution by prescribing $\delta\mathbf{U}^0$. (In the above, all crystallites have been chosen of equal volume $V_c \ll 1$ for convenience. This is easily realized geometrically since a cubic volume can be separated into six equal volume tetrahedrons, and the unit cube can be divided into as many sub-cubic grains as desired.)

From (5.3), (5.6) and (5.7), the overall vectors of strains $\delta\bar{\mathbf{E}}^{(e)} = (\ldots, \delta\bar{\boldsymbol{\xi}}_{(q)}^{(e)}, \ldots)$ and $\delta\bar{\mathbf{E}}^s = (\ldots, \delta\bar{\boldsymbol{\xi}}_{(q)}^s, \ldots)$ are

$$\delta\bar{\mathbf{E}}^{(e)} = \bar{\mathbf{A}}^T [\mathbf{I} - \mathbf{B}_i \mathbf{K}^{-1} \mathbf{B}_i^T \mathbf{S}] \mathbf{B}_0 \, \delta\mathbf{U}^0 \tag{5.10}$$

$$\delta\bar{\mathbf{E}}^s = \bar{\mathbf{A}}^T \mathbf{B}_i \mathbf{K}^{-1} \mathbf{B}_i^T \mathbf{S} \bar{\mathbf{N}} \, \delta\bar{\boldsymbol{\Gamma}} \tag{5.11}$$

with $\bar{\mathbf{A}} = \lceil \mathbf{A}_{(q)} \rfloor$. (It is understood that $\bar{\mathbf{N}}$ and $\delta\bar{\boldsymbol{\Gamma}}$ are defined only over those crystallites q containing potentially active slip systems.) The overall vector of incremental, resolved shear stresses $\delta\bar{\mathbf{T}}^s = (\ldots, \delta\bar{\tau}_{(q)}^s, \ldots)$ due to internal slip follows from (4.8)–(4.10) and (5.11):

$$\delta\bar{\mathbf{T}}^s = -\bar{\mathbf{N}} \mathbf{Q} \bar{\mathbf{N}}^T \, \delta\bar{\boldsymbol{\Gamma}} = -\mathbf{P}^s \, \delta\bar{\boldsymbol{\Gamma}} \tag{5.12}$$

wherein

$$\mathbf{Q} = \mathbf{S}[\mathbf{I} - \mathbf{B}_i \mathbf{K}^{-1} \mathbf{B}_i^T \mathbf{S}]. \tag{5.13}$$

In Section 6 it is proved that the symmetric matrix $\mathbf{P}^s$ is positive-definite, whence, forming the scalar product of (5.12) with $\delta\bar{\boldsymbol{\Gamma}}$, we have a discrete counterpart of (4.11). The influence (or interaction) matrix $\mathbf{Q}$ is analogous to the integrodifferential operators on $\delta\boldsymbol{\xi}^p(\mathbf{x})$ in [20, 32].

From (4.4), (4.9), (5.10) and (5.12), denoting $\delta\bar{\mathbf{T}} = (\ldots, \delta\bar{\tau}_{(q)}, \ldots)$, we have

$$\delta\bar{\mathbf{T}} = \bar{\mathbf{N}} \mathbf{Q} [\mathbf{B}_0 \, \delta\mathbf{U}^0 - \bar{\mathbf{N}}^T \, \delta\bar{\boldsymbol{\Gamma}}]. \tag{5.14}$$

Since, in each critical system,

$$\delta\bar{\tau}_k \leq \delta\bar{\tau}_{cr}^k = \mathbf{H}_k(\bar{\gamma}_q) \, \delta\bar{\gamma}_{(q)}, \tag{5.15}$$

the final matrix equation for the incremental crystal shears can be expressed (denoting $\overline{\mathbf{H}} = \lceil \mathbf{H}_{(q)} \rfloor$)

$$(\overline{\mathbf{H}} + \overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T)\,\delta\overline{\Gamma} - \overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\,\delta\mathbf{U}^0 \geq \mathbf{0} \tag{5.16}$$

with the equality satisfied for each active system ($\delta\bar{\gamma}_k > 0$). The matrix $\mathbf{P} = \overline{\mathbf{H}} + \overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T$ is positive-definite over critical (hence, active) slip systems, and (5.16) yields a unique solution for $\delta\overline{\Gamma}$, as proved in the following section.

6. UNIQUENESS OF INTERNAL FIELDS AND A QUADRATIC PROGRAMMING PROBLEM

Introducing the positive-definite scalar average

$$\bar{u}_e = \sum_q \delta\bar{\boldsymbol{\zeta}}_{(q)} \cdot \mathbf{C}_{(q)}\,\delta\bar{\boldsymbol{\zeta}}_{(q)} V_c > 0 \tag{6.1}$$

we have, from (4.1), (4.9) and (5.13)–(5.14),

$$\bar{u}_e = (\mathbf{B}_0\,\delta\mathbf{U}^0 - \overline{\mathbf{N}}^T\,\delta\overline{\Gamma})^T\mathbf{Q}(\mathbf{B}_0\,\delta\mathbf{U}^0 - \overline{\mathbf{N}}^T\,\delta\overline{\Gamma})V_c > 0. \tag{6.2}$$

Assume two distinct sets of internal fields $\delta\bar{\boldsymbol{\zeta}}_{(q)}$, $\delta\bar{\boldsymbol{\xi}}_{(q)}$, $\delta\bar{\gamma}_{(q)}$ and $\delta\bar{\boldsymbol{\zeta}}^*_{(q)}$, $\delta\bar{\boldsymbol{\xi}}^*_{(q)}$, $\delta\bar{\gamma}^*_{(q)}$, both of which satisfy all appropriate equations of the discretized model for an infinitesimal macrostrain $\delta\boldsymbol{\varepsilon}$ (i.e. uniquely prescribed $\delta\mathbf{U}^0$). Denoting their differences by $\Delta\delta\bar{\boldsymbol{\zeta}}_{(q)} = \delta\bar{\boldsymbol{\zeta}}_{(q)} - \delta\bar{\boldsymbol{\zeta}}^*_{(q)}$, etc., then from the above

$$\Delta\,\delta\overline{\Gamma}^T\overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T\,\Delta\,\delta\overline{\Gamma} > 0. \tag{6.3}$$

This equation is written only over *potentially* active slip systems corresponding to the current states of internal stress and strain, since the active systems for either set of incremental shears will belong to this critical group. Thus, $\mathbf{P}^s = \overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T$ is positive-definite over critical systems. We also find, from (4.10), (5.11) and (6.2),

$$\sum_q \Delta\delta\bar{\boldsymbol{\zeta}}_{(q)} \cdot \Delta\delta\bar{\boldsymbol{\xi}}^p_{(q)} + \Delta\delta\overline{\Gamma}^T\overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T\,\Delta\delta\overline{\Gamma} = 0. \tag{6.4}$$

Introducing an inequality due to Hill [24] written over critical systems of a crystal grain,

$$\Delta\delta\bar{\boldsymbol{\zeta}}_{(q)} \cdot \Delta\delta\bar{\boldsymbol{\xi}}^p_{(q)} \geq \Delta\delta\bar{\gamma}^T_{(q)}\mathbf{H}_{(q)}\Delta\delta\bar{\gamma}_{(q)}, \tag{6.5}$$

we conclude from the above that, for $\mathbf{H} \geq 0$, the incremental shears are unique. It follows from (5.14) that the incremental stress field is unique. Consequently, the infinitesimal total strain field is unique, and the proof is complete. The matrix $\mathbf{P} = \overline{\mathbf{H}} + \overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T$ in (5.16) is obviously positive-definite.

Since an admissible solution of (5.16) is constrained by the physical requirement $\delta\bar{\gamma}_k \geq 0$ for all k (which is implicit in 6.5), determination of the unique aggregate response from a particular deformed state is not necessarily a straightforward calculation. If, for example, (5.16) is solved for $\delta\overline{\Gamma}$ on the expectation that all critical slip systems will be active in a macrostrain increment $\delta\boldsymbol{\varepsilon}$, certain of the $\delta\bar{\gamma}_k$ may be computed as negative. In this event (5.16) must again be solved, after eliminating the appropriate slip systems (thereby changing $\mathbf{P}$), until all incremental plastic shears are positive. This could prove to be a rather lengthy procedure for a large number of critical systems. Alternatively, evaluation of the $\delta\bar{\gamma}_k$ may be posed as a quadratic programming problem, as follows. We form the

functional

$$I(\delta\hat{\boldsymbol{\Gamma}}) = \tfrac{1}{2}\,\delta\hat{\boldsymbol{\Gamma}}^T\mathbf{P}\,\delta\hat{\boldsymbol{\Gamma}} - \delta\hat{\boldsymbol{\Gamma}}^T\overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\,\delta\mathbf{U}^0 \tag{6.6}$$

wherein $\delta\hat{\boldsymbol{\Gamma}}$ is any set of incremental shears, defined over the critical slip systems, which satisfies the inequality $\delta\hat{\boldsymbol{\Gamma}} \geq \mathbf{0}$. Then, from (5.16) and (6.6),

$$I(\delta\hat{\boldsymbol{\Gamma}}) - I(\delta\overline{\boldsymbol{\Gamma}}) = \tfrac{1}{2}(\delta\hat{\boldsymbol{\Gamma}} - \delta\overline{\boldsymbol{\Gamma}})^T\mathbf{P}(\delta\hat{\boldsymbol{\Gamma}} - \delta\overline{\boldsymbol{\Gamma}}) + \delta\hat{\boldsymbol{\Gamma}}^T(\mathbf{P}\,\delta\overline{\boldsymbol{\Gamma}} - \overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\,\delta\mathbf{U}^0) > 0 \tag{6.7}$$

unless $\delta\hat{\boldsymbol{\Gamma}} \equiv \delta\overline{\boldsymbol{\Gamma}}$. Hence, the unique solution $\delta\overline{\boldsymbol{\Gamma}}$ of the discrete model minimizes the quadratic functional $I(\delta\hat{\boldsymbol{\Gamma}})$ subject to the linear constraints $\delta\hat{\gamma}_k \geq 0$. For a discussion of the application of nonlinear programming techniques in classical (macroscopic) plasticity theory, see [33].

7. GENERAL CHARACTERISTICS OF SUBSEQUENT YIELD SURFACES

At a particular stage of aggregate straining, a subsequent yield surface is defined (in stress or strain space) by determining the positions of the various yield hyperplanes. Consider the case of applied biaxial strain $\boldsymbol{\varepsilon} = (\varepsilon_{11}, \varepsilon_{22})$. From (4.2)

$$\overline{\boldsymbol{\xi}}^{(e)}_{(q)} = \overline{\boldsymbol{\Upsilon}}_{(q)}\boldsymbol{\varepsilon} \tag{7.1}$$

in which the columns of the matrix $\overline{\boldsymbol{\Upsilon}}_{(q)}$ are found from separate evaluations of the elastic solution (5.10) for the states $\varepsilon_{11}, \varepsilon_{22} = 0$ and $\varepsilon_{22}, \varepsilon_{11} = 0$, respectively. The distance to the kth yield plane $\overset{\varepsilon}{f}_k = 0$ in macrostrain space is then determined from (4.4), (4.9), (7.1) and the equality $\bar{\tau}_k = \bar{\tau}^k_{\mathrm{cr}}$ as

$$\overset{\varepsilon}{D}_k = (\bar{\tau}^k_{\mathrm{cr}} - \bar{\tau}^s_k)/\|\mathbf{N}_k\mathbf{C}^{-1}_{(q)}\overline{\boldsymbol{\Upsilon}}_{(q)}\|, \tag{7.2}$$

and, in macrostress space, the distance to the yield hyperplane $\overset{\sigma}{f}_k = 0$ is found to be

$$\overset{\sigma}{D}_k = (\bar{\tau}^k_{\mathrm{cr}} - \bar{\tau}^r_k)/\|\mathbf{N}_k\mathbf{C}^{-1}_{(q)}\overline{\boldsymbol{\Upsilon}}_{(q)}\overline{\mathbf{C}}_{\mathrm{macro}}\|, \tag{7.3}$$

in which

$$\bar{\tau}^r_k = \bar{\tau}^s_k + \mathbf{N}_k\mathbf{C}^{-1}_{(q)}\overline{\boldsymbol{\Upsilon}}_{(q)}(\boldsymbol{\varepsilon} - \overline{\mathbf{C}}_{\mathrm{macro}}\bar{\boldsymbol{\sigma}}) \tag{7.4}$$

is the residual microstress that would remain upon unloading to zero macrostress (if the subsequent yield surface contains the origin in stress space). In the above, $\overline{\mathbf{C}}_{\mathrm{macro}}$ is calculated from (4.7) and $\bar{\boldsymbol{\sigma}} = (\sigma_{11}, \sigma_{22})$ is computed using (2.11). The aggregate yield surface is, of course, the inner bounding set of all such hyperplanes (7.2) [or (7.3)] in the respective strain (or stress) space. Apparent macroscopic plastic strain and "plastic stress" increments are appropriately defined as

$$\delta\bar{\boldsymbol{\varepsilon}}^p = \delta\boldsymbol{\varepsilon} - \overline{\mathbf{C}}_{\mathrm{macro}}\,\delta\bar{\boldsymbol{\sigma}} \tag{7.5}$$

$$\delta\bar{\boldsymbol{\sigma}}^p = \overline{\mathbf{C}}^{-1}_{\mathrm{macro}}\,\delta\boldsymbol{\varepsilon} - \delta\bar{\boldsymbol{\sigma}}. \tag{7.6}$$

From a general inequality established by Hill [25], the following orthogonality conditions apply to the aggregate continuum model:

$$\delta\boldsymbol{\sigma}_e \,.\, \delta\boldsymbol{\varepsilon}^p \leq 0 \tag{7.7}$$

$$\delta\boldsymbol{\varepsilon}_e \,.\, \delta\boldsymbol{\sigma}^p \leq 0 \tag{7.8}$$

in which $\delta\boldsymbol{\varepsilon}_e$ is any macrostrain increment which produces purely elastic response of the aggregate, and $\delta\boldsymbol{\sigma}_e = \mathbf{C}^{-1}_{\text{macro}}\,\delta\boldsymbol{\varepsilon}_e$. The orthogonality relations can be interpreted as generalized normality conditions on plastic strain and plastic stress increments in stress and strain space, respectively. These inequalities also hold for $\delta\bar{\boldsymbol{\varepsilon}}^p$ and $\delta\bar{\boldsymbol{\sigma}}^p$ of the discrete model (7.5), (7.6), save for a possible $0(h)$ discretization error, where h is an average crystallite dimension. (A strict proof of convergence of the discrete model solution, with decreasing element size, to that of the corresponding aggregate continuum is included within a forthcoming paper [34].)

Consider now the change in position of an active plane with increasing plastic deformation. Since k corresponds to the active sense of slip in a particular crystallographic system, we redefine it as $(k+)$ and write

$$\delta\overset{\varepsilon}{D}_{(k+)} = (\delta\bar{\tau}^{(k+)}_{\text{cr}} - \delta\bar{\tau}^s_k)/\|\mathbf{N}_k\mathbf{C}^{-1}_{(q)}\bar{\boldsymbol{\Upsilon}}_{(q)}\|. \tag{7.9}$$

From (5.12) [or (4.11) for the continuum]

$$\sum_q \left(\sum_k \delta\bar{\tau}^s_k\,\delta\gamma_k\right)_{(q)} V_c = -\delta\bar{\boldsymbol{\Gamma}}\,.\,\mathbf{P}^s\,\delta\bar{\boldsymbol{\Gamma}}\,V_c < 0. \tag{7.10}$$

As this inequality must hold locally for the majority of active systems, we can assume it holds for the particular k of interest. Thus $\delta\bar{\tau}^s_k < 0$ and (7.9)

$$\delta\overset{\varepsilon}{D}_{(k+)} = (\delta\bar{\tau}^{(k+)}_{\text{cr}} + |\delta\bar{\tau}^s_k|)/\|\mathbf{N}_k\mathbf{C}^{-1}_{(q)}\bar{\boldsymbol{\Upsilon}}_{(q)}\|. \tag{7.11}$$

Similarly, the change in the distance (in the opposite direction in strain space) to the parallel plane corresponding to the negative sense of slip $(k-)$ in this crystallographic system is

$$\delta\overset{\varepsilon}{D}_{(k-)} = (\delta\bar{\tau}^{(k-)}_{\text{cr}} - |\delta\bar{\tau}^s_k|)/\|\mathbf{N}_k\mathbf{C}^{-1}_{(q)}\bar{\boldsymbol{\Upsilon}}_{(q)}\|\,. \tag{7.12}$$

Thus, if the change in crystal hardening $\delta\tau^{(k-)}_{\text{cr}}$ in reverse slip is less than the change in the resolved shear stress due to internal slip and self-straining, $\delta\overset{\varepsilon}{D}_{(k-)} < 0$ and the two hyperplanes move in the same direction. This is certainly the case when the crystal strain-*softens* in reverse slip (as is suggested by the experimental work of Paterson [35] on copper), and there will be a corresponding strong Bauschinger effect in macrostrain space. There will be at least a weak Bauschinger effect if only $\delta\tau^{(k-)}_{\text{cr}} \leq \delta\tau^{(k+)}_{\text{cr}}$, hence $\delta\overset{\varepsilon}{D}_{(k-)} < \delta\overset{\varepsilon}{D}_{(k+)}$. This inequality is satisfied for both Taylor hardening [1, 36] and the translational hardening adopted by Budiansky and Wu [10] and Tung and Lin [19], as well as for any positive combination [32]

$$\mathbf{H} = h(\gamma)\mathbf{I} + c(\gamma)\mathbf{N}\mathbf{N}^T. \tag{7.13}$$

($\mathbf{I}$ is an N by N matrix all of whose elements are unity and h and c are scalar hardening functions determined from single crystal tests.) In addition, $\mathbf{H}$ of (7.13) is at least positive-

semidefinite, and if $c > 0$, $\mathbf{H} > 0$ over critical systems [24, 32]. It can also be shown that

$$\int \delta\tau^r \cdot \delta\gamma \, dV < 0. \tag{7.14}$$

(See [31] for details.) Thus, from (7.3) and the above, the Bauschinger effect also obtains in macrostress space. A digital computer program for studying the quantitative effects of aggregate texturing, crystal structure and anisotropy, and crystal hardening laws on macroscopic yield surfaces is in preparation, with numerical results to be presented in subsequent papers.

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APPENDIX

Internal stress and infinitesimal strain tensors are expressed in vector form as

$$\boldsymbol{\zeta} = (\zeta_{11}, \sqrt{(2)}\zeta_{12}, \sqrt{(2)}\zeta_{13}, \zeta_{22}, \sqrt{(2)}\zeta_{23}, \zeta_{33})^T \tag{A1}$$

$$\delta\boldsymbol{\xi} = (\delta\xi_{11}, \sqrt{(2)}\,\delta\xi_{12}, \sqrt{(2)}\,\delta\xi_{13}, \delta\xi_{22}, \sqrt{(2)}\,\delta\xi_{23}, \delta\xi_{33})^T \tag{A2}$$

from which the equilibrium and kinematic equations can be written $\boldsymbol{D}\boldsymbol{\zeta} = \mathbf{0}$ and $\boldsymbol{D}^T\,\delta\mathbf{u} = \delta\boldsymbol{\xi}$, with

$$\boldsymbol{D} = \begin{bmatrix} \partial_1 & \frac{1}{\sqrt{2}}\partial_2 & \frac{1}{\sqrt{2}}\partial_3 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}\partial_1 & 0 & \partial_2 & \frac{1}{\sqrt{2}}\partial_3 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}\partial_1 & 0 & \frac{1}{\sqrt{2}}\partial_2 & \partial_3 \end{bmatrix} \tag{A3}$$

(wherein ∂_i denotes partial differentiation with respect to the corresponding spatial coordinate).

The kth row vector of the crystal transformation matrix $\mathbf{N}$ is given in terms of unit vectors $\boldsymbol{\phi}^k$, $\boldsymbol{\lambda}^k$ in the normal and glide directions, respectively, of the kth crystallographic slip system:

$$\mathbf{N}_k = \left[\phi_1^k\lambda_1^k, \frac{1}{\sqrt{2}}(\phi_1^k\lambda_2^k + \phi_2^k\lambda_1^k), \frac{1}{\sqrt{2}}(\phi_1^k\lambda_3^k + \phi_3^k\lambda_1^k), \right.$$
$$\left. \phi_2^k\lambda_2^k, \frac{1}{\sqrt{2}}(\phi_2^k\lambda_3^k + \phi_3^k\lambda_2^k), \phi_3^k\lambda_3^k \right]. \tag{A4}$$

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Абстракт—Определяется дискретная модель, пригодная для анадиза поведения поликристаллического заполнителя под влиянием макроскопически однородной, квазистамической нагрузки, со специальным учетом характеристик поверхностей течения в пространстве напряжений и деформации. Внутренние напряжения и деформации определяются путем приближения кусочных, линейных, инфинитезимальных полей деформаций с кристаллическими зернами, на основе широко определенного констцтутивного поведения, которое дает возможность включить кубическую или гексагональную кристаллическую анизотропию и соотвественно обшие законы упрочнения для кристаллических систем скольженмя. Выводятся соотвествующие матрицц заполнителя в качестве симметрическцх и положительно определенных. Внутренние поля, соотвествующие решению дискретной модели, оказываются единственными. Далее указано, что остаточное решение для приращения сдвигов кристаллов можно рассматривать в качестве задачи квадратачеокэио программирования.