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

KERRY S. HAVNER

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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 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.

ERRATA

Page	Correction
12	In (4.8) and (4.9), replace $\delta\boldsymbol{\sigma}$ and $\delta\boldsymbol{\varepsilon}$ by $\delta\boldsymbol{\sigma}^*$ and $\delta\boldsymbol{\varepsilon}^*$, respectively.
15	In the fifth line following the subheading, aggregate should be plural.
17	In (6.1), replace $\delta\boldsymbol{u}^M$ by $\delta\bar{\boldsymbol{u}}^M$.
17	In (6.3), replace $\delta\boldsymbol{\xi}_{(q)}$ by $\delta\bar{\boldsymbol{\xi}}_{(q)}$.
24	The first line following (7.14) should read: "The approximate static..."
24	In (7.16), replace $\delta\boldsymbol{\Delta}^o$ by $\delta\boldsymbol{U}^o$.
33	In (A.4), replace N_k by $\boldsymbol{N}_k$.

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1. INTRODUCTION

The first satisfactory theory for predicting the plastic deformation of polycrystalline aggregates from phenomenological laws of single crystal behavior was advanced by Sir. G. I. 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 and his associates [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 the response of thin-walled, polycrystalline tubes 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 crystal and aggregate behavior established by Hill [24, 25]. The paper is organized as follows. In Section 2, a continuum mathematical model of an aggregate of identical, polycrystalline "unit cubes" is introduced and macroscopically uniform fields are defined. The aggregate virtual work equation relating microscopic and macroscopic tensor variables then follows as a direct consequence. Several different internal stress and infinitesimal strain fields are presented in Section 3, and an inequality is established which leads to a proof in Section 4 of a macroscopic Bauschinger effect for the polycrystalline aggregate. In Section 5 a further specification of the continuum model is given appropriate to the formulation of aggregate boundary value problems. Sections 6 and 7 contain the general analysis of the discretized model for prescribed aggregate macrostrain, based upon approximating, piecewise linear infinitesimal displacement fields within crystal grains. Kinematic conditions are met identically; equilibrium between grains is satisfied in an average sense at each crystallite node; and both anisotropic crystal elasticity and fairly general crystal hardening matrices are included as constitutive behavior. Aggregate matrices to be inverted (or decomposed) are established as symmetric, positive-definite; and in Section 8 a strict uniqueness proof is presented for both incremental plastic shears in crystallographic slip systems and internal stress- and strain-increment fields (as determined from the discrete model). Lastly, in Section 9 the necessary steps for calculation of subsequent yield surfaces are given and a suggested model for quantitative studies is briefly discussed.

2. PRINCIPLE OF VIRTUAL WORK WITHIN THE POLYCRYSTALLINE AGGREGATE

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 $\underset{\sim}{T}^*$ on S, by $\underset{\sim}{\sigma}^*$ (with tensor components σ^*_{ij}) and any continuous, piecewise differentiable infinitesimal displacement field by $\delta\underset{\sim}{u}^o$. A straightforward application of Gauss' theorem then yields

$$\int_V (\underset{\sim}{\zeta}^* \cdot \delta\underset{\sim}{\xi}^o)dV = \int_S (\underset{\sim}{T}^* \cdot \delta\underset{\sim}{u}^o)dS \tag{2.1}$$

wherein

$$\delta\underset{\sim}{\xi}^o = \underset{\sim}{D}^T \delta\underset{\sim}{u}^o \tag{2.2}$$

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

$$\delta\underset{\sim}{u}^o(A_i^+) = \delta\underset{\sim}{u}^o(A_i^-) + \overset{i}{\underset{\sim}{c}}{}^o \tag{2.3}$$

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

(respectively kinematically and statically admissible). A_i^+ denotes the unit cube face corresponding to the positive coordinate axis x_i and $\overset{i}{\underset{\sim}{c}}{}^o$ is a constant vector independent of position over A_i^+. Macroscopic stress and incremental strain are evaluated in a natural way as

$$\sigma_{ij}^* = \int_{A_i^+} \overset{i}{T}{}_j^* \, dA_i \quad \text{(no summation)} \tag{2.5}$$

$$\delta\epsilon_{ij}^o = \frac{1}{2}(\overset{i}{c}{}_j^o + \overset{j}{c}{}_i^o) . \tag{2.6}$$

Upon substitution of (2.3), (2.4) and (2.5) into (2.1), we find

$$\int_S (\underset{\sim}{T}^* \cdot \delta \underset{\sim}{u}^o) dS = \sigma^*_{ij} \, c^{\,i\,o}_{j} \quad . \tag{2.7}$$

From considerations of moment equilibrium

$$\int_{A_i^+} \overset{i}{T}{}^*_j \, dA_i = \int_{A_j^+} \overset{j}{T}{}^*_i \, dA_j \quad . \tag{2.8}$$

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

$$\int_V (\underset{\sim}{\zeta}^* \cdot \delta \underset{\sim}{\xi}^o) dV = \underset{\sim}{\sigma}^* \cdot \delta \underset{\sim}{\varepsilon}^o \tag{2.9}$$

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

$$\delta \underset{\sim}{\varepsilon}^o = \int_V (\delta \underset{\sim}{\xi}^o) dV \tag{2.10}$$

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

$$\underset{\sim}{\sigma}^* = \int_V \underset{\sim}{\zeta}^* \, dV \ . \tag{2.11}$$

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

$$\int_{A_i} (\overset{i}{T}{}_j^* \, \delta u_k^o) dA_i = (\int_{A_i} \overset{i}{T}{}_j^* \, dA_i) \int_{A_i} (\delta u_k^o) dA_i \tag{2.12}$$

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

$$\overset{i}{\underset{\sim}{m}}{}^* = \int_{A_i^+} (\underset{\sim}{r} \times \overset{i}{\underset{\sim}{T}}{}^*) dA_i \tag{2.13}$$

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

3. SOME GENERAL INEQUALITIES AND INTERNAL FIELDS

Let $\underset{\sim}{\zeta}^{(e)}$ denote the local stress field within a crystal grain determined by assuming that the aggregate response to macrostress $\underset{\sim}{\sigma}$ is wholly elastic. As in [25], we take $\underset{\sim}{\zeta}^{(e)}$ to be expressible in terms of $\underset{\sim}{\sigma}$ and a tensor (matrix) function $\underset{\sim}{\Psi}$ of position within V (i.e., the influence of elastic inhomogeneity on the stress field):

$$\underset{\sim}{\zeta}^{(e)} = \underset{\sim}{\Psi}\,\underset{\sim}{\sigma} \quad . \tag{3.1}$$

Then, from (2.11)

$$\underset{\sim}{\sigma} = \int_V \underset{\sim}{\zeta}^{(e)} dV \tag{3.2}$$

so that $\int_V \underset{\sim}{\Psi}\, dV = \underset{\sim}{I}$ (the identity matrix). We further define a microstress field $\underset{\sim}{\zeta}^{S(\sigma)}$ due to internal slip and self-stressing,

$$\underset{\sim}{\zeta}^{S(\sigma)} = \underset{\sim}{\zeta} - \underset{\sim}{\zeta}^{(e)} \tag{3.3}$$

with (2.11 and 3.2)

$$\int \underset{\sim}{\zeta}^{S(\sigma)} dV = \underset{\sim}{0} \quad , \tag{3.4}$$

and introduce kinematically admissible, infinitesimal displacement and corresponding strain fields $\delta\underset{\sim}{u}^{S(\sigma)}$, $\delta\underset{\sim}{\xi}^{S(\sigma)}$ such that

$$\delta\underset{\sim}{\xi} = \underset{\sim}{C}\,\delta\underset{\sim}{\zeta}^{(e)} + \delta\underset{\sim}{\xi}^{S(\sigma)} \quad . \tag{3.5}$$

$\underset{\sim}{C}$ is the positive-definite, elastic compliance matrix of an individual grain and $\underset{\sim}{\zeta}$, $\underset{\sim}{\xi}$ are the actual local stress and strain fields. We also have

$$\delta\underset{\sim}{\xi} = \underset{\sim}{C}\,\delta\underset{\sim}{\zeta} + \delta\underset{\sim}{\xi}^{P} \tag{3.6}$$

where $\underset{\sim}{C}\,\delta\underset{\sim}{\zeta} = \delta\underset{\sim}{\xi}^{e}$ is the micro-elastic strain increment. The local micro-plastic strain increment $\delta\underset{\sim}{\xi}^{P}$ is determined from the incremental plastic shears $\delta\gamma_k$ on the N slip systems of the crystal through the transformation

$$\delta\underset{\sim}{\xi}^{P} = \underset{\sim}{N}^{T}\delta\underset{\sim}{\gamma} \quad , \tag{3.7}$$

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

$$\underset{\sim}{\tau} = \underset{\sim}{N}\,\underset{\sim}{\zeta} \quad . \tag{3.8}$$

The transformation matrix $\underset{\sim}{N}$ is defined in terms of its kth row vector $\underset{\sim}{N}_k$ 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).

We now introduce the following scalar averages over the unit cube:

$$
\begin{aligned}
d_p &= \int_V (\delta\underset{\sim}{\zeta} \cdot \delta\underset{\sim}{\xi}^{P})dV \\
w_p &= \int_V (\delta\underset{\sim}{\zeta}^{(e)} \cdot \delta\underset{\sim}{\xi}^{S(\sigma)})dV \\
u_e &= \int_V (\delta\underset{\sim}{\zeta} \cdot \underset{\sim}{C}\,\delta\underset{\sim}{\zeta})dV \\
w_e &= \int_V (\delta\underset{\sim}{\zeta}^{(e)} \cdot \underset{\sim}{C}\,\delta\underset{\sim}{\zeta}^{(e)})dV \quad .
\end{aligned}
\tag{3.9}
$$

(Note that (2.9) applies <u>separately</u> only to w_p and w_e since $\delta\underset{\sim}{\xi}^{P}$ and $\underset{\sim}{C}\,\delta\underset{\sim}{\zeta}$ are not derivable from displacement fields, hence are not separately kinematically admissible.) From (2.9), (3.4-3.6), and (3.9)

$$d_p + u_e = \delta\underset{\sim}{\sigma} \cdot \delta\underset{\sim}{\varepsilon} = v_p + v_e \tag{3.10}$$

$$u_e - v_e = \int_V (\delta\underset{\sim}{\varepsilon}^{S(\sigma)} \cdot \underset{\sim}{C}\, \delta\underset{\sim}{\varepsilon}^{S(\sigma)})dV > 0. \tag{3.11}$$

Hence, combining (3.10, 3.11) with (2.9) and (3.3-3.6),

$$d_p - v_p = \int_V (\delta\underset{\sim}{\varepsilon}^{S(\sigma)} \cdot \delta\underset{\sim}{\varepsilon}^{P})dV < 0 \tag{3.12}$$

or (using 3.7 and 3.8)

$$\int_V (\delta\underset{\sim}{\tau}^{S(\sigma)} \cdot \delta\underset{\sim}{\gamma})dV < 0 \tag{3.13}$$

from which we conclude that the incremental shear stresses $\delta\tau_k^{S(\sigma)}$ due to slip and self-stressing oppose the incremental plastic shears $\delta\gamma_k$ in a majority (if not all) of the active slip systems of the aggregate. This result will be called upon in determining certain general characteristics of subsequent yield surfaces in Section 4.

In similar manner to the above, we denote $\underset{\sim}{\varepsilon}^{(e)}$ as the local strain field determined by assuming elastic aggregate response to macrostrain $\underset{\sim}{\varepsilon}$ and define a function $\underset{\sim}{T}$ of position within V such that

$$\underset{\sim}{\varepsilon}^{(e)} = \underset{\sim}{T}\,\underset{\sim}{\varepsilon} \tag{3.14}$$

and (2.10)

$$\underset{\sim}{\epsilon} = \int_V \underset{\sim}{\epsilon}^{(e)} dV \quad , \quad \int_V \underset{\sim}{T} \, dV = \underset{\sim}{I} \quad . \tag{3.15}$$

Introducing kinematically admissible, infinitesimal displacement and corresponding strain fields $\delta \underset{\sim}{u}^{S(\epsilon)}$, $\delta \underset{\sim}{\epsilon}^{S(\epsilon)}$ due to internal slip and self-straining,

$$\delta \underset{\sim}{\epsilon} = \delta \underset{\sim}{\epsilon}^{(e)} + \delta \underset{\sim}{\epsilon}^{S(\epsilon)} \quad , \tag{3.16}$$

and a related stress field $\underset{\sim}{\sigma}^{S(\epsilon)}$,

$$\underset{\sim}{\sigma}^{S(\epsilon)} = \underset{\sim}{\sigma} - \underset{\sim}{C}^{-1} \underset{\sim}{\epsilon}^{(e)} \quad , \tag{3.17}$$

we find, from (2.10), (2.11), (3.14) and (3.15)

$$\int_V \delta \underset{\sim}{\epsilon}^{S(\epsilon)} dV = \underset{\sim}{0} \quad , \tag{3.18}$$

and

$$\int_V \underset{\sim}{\sigma}^{S(\epsilon)} dV = \underset{\sim}{\sigma} - \left(\int_V \underset{\sim}{C}^{-1} \underset{\sim}{T} \, dV\right) \cdot \underset{\sim}{\epsilon} \quad . \tag{3.19}$$

The inverse elastic compliance matrix of the aggregate obviously is

$$\underset{\sim}{C}^{-1}_{Macro} = \int_V \underset{\sim}{C}^{-1} \underset{\sim}{T} \, dV \quad . \tag{3.20}$$

We also have, from (3.1) and (3.5),

$$\int_V \delta \underset{\sim}{\epsilon}^{S(\sigma)} dV = \delta \underset{\sim}{\epsilon} - \left(\int_V \underset{\sim}{C} \, \underset{\sim}{Y} \, dV\right) \cdot \delta \underset{\sim}{\sigma} \tag{3.21}$$

so that the aggregate compliance matrix can be alternately expressed

$$\underset{\sim}{C}_{Macro} = \int_V \underset{\sim}{C}\,\underset{\sim}{\Psi}\,dV \quad . \tag{3.22}$$

From (3.19-3.22), (apparent) macroscopic plastic strain and "plastic stress" increments are appropriately defined as

$$\delta\underset{\sim}{\varepsilon}^{P} = \int_V \delta\underset{\sim}{\zeta}^{S(\sigma)}dV = \delta\underset{\sim}{\varepsilon} - \int_V \underset{\sim}{C}\,\delta\underset{\sim}{\zeta}^{(e)}\,dV \tag{3.23}$$

$$\delta\underset{\sim}{\sigma}^{P} = -\int_V \delta\underset{\sim}{\zeta}^{S(\varepsilon)}dV = \int_V \underset{\sim}{C}^{-1}\delta\underset{\sim}{\zeta}^{(s)}dV - \delta\underset{\sim}{\sigma} \quad . \tag{3.24}$$

(For clarity, these various terms are interpreted for the uniaxial case in Figure 1.) Lastly, we relate the internal stress fields $\underset{\sim}{\zeta}^{S(\sigma)}$ and $\underset{\sim}{\zeta}^{S(\varepsilon)}$ from (3.3), (3.14), (3.17) and (3.22):

$$\underset{\sim}{\zeta}^{S(\sigma)} = \underset{\sim}{\zeta}^{S(\varepsilon)} + \underset{\sim}{C}^{-1}\,\underset{\sim}{T}(\underset{\sim}{\varepsilon} - \underset{\sim}{C}_{Macro}\,\underset{\sim}{\sigma}) \quad . \tag{3.25}$$

4. GENERAL CHARACTERISTICS OF SUBSEQUENT YIELD SURFACES

Hill's proof [25] of generalized normality for aggregates satisfying (2.9) is based upon postulated conditions which are equivalent to the requirement

$$\delta\tau^{k}_{cr}\,\delta\gamma_{k} > 0 \tag{4.1}$$

(i.e., crystal grains strain harden in active systems, with τ^{k}_{cr} denoting the critical shear stress in the kth crystallographic slip system). The final form of Hill's equation [25] can be written

$$\delta\underset{\sim}{\sigma}^{*} \cdot \delta\underset{\sim}{\varepsilon} - \delta\underset{\sim}{\varepsilon}^{*} \cdot \delta\underset{\sim}{\sigma} \leq 0 \tag{4.2}$$

in which $\delta\underset{\sim}{\sigma}$, $\delta\underset{\sim}{\varepsilon}$ are macro-stress and related strain increments which produce slip in one or more slip systems while $\delta\underset{\sim}{\sigma}^{*}$, $\delta\underset{\sim}{\varepsilon}^{*}$ correspond to purely elastic response of the aggregate (with $\delta\underset{\sim}{\varepsilon}^{*} = \underset{\sim}{C}_{Macro}\ \delta\underset{\sim}{\sigma}^{*}$). Thus, we have the following orthogonality conditions for the quantities defined in (3.23) and (3.24):

$$\delta\underset{\sim}{\sigma}^{*} \cdot \delta\underset{\sim}{\varepsilon}^{P} \leq 0 \tag{4.3}$$

$$\delta\underset{\sim}{\varepsilon}^{*} \cdot \delta\underset{\sim}{\sigma}^{P} \leq 0 \quad . \tag{4.4}$$

According to (4.3), the domain of all possible incremental plastic strain vectors $\delta\underset{\sim}{\varepsilon}^{P}$ from a stress point $\underset{\sim}{\sigma}$ in macrostress space is orthogonal to the domain of all stress increments $\delta\underset{\sim}{\sigma}^{*}$ producing purely elastic response (i.e., directed into the elastic region in stress space). According to (4.4), the domain of all possible incremental "plastic stress" vectors $\delta\underset{\sim}{\sigma}^{P}$ from a strain point $\underset{\sim}{\varepsilon}$ in macrostrain space is orthogonal to the domain of all strain increments $\delta\underset{\sim}{\varepsilon}^{*}$ producing purely elastic response (i.e., directed into the elastic region in strain space). The first of these interpretations is, of course, compatible with the customary manner of describing yield surfaces and is physically more appealing since $\underset{\sim}{\varepsilon}^{P}$ is the strain remaining upon mechanical unloading to zero stress (if the present yield surface encloses the origin of macrostress space).

A particular yield hyperplane in stress space is defined as (3.1, 3.3 and 3.8)

$$f_k = \underset{\sim}{N}_k \underset{\sim}{\Psi} \underset{\sim}{\sigma} + \tau_k^{S(\sigma)} - \tau_{cr}^k = 0 \tag{4.5}$$

with the corresponding hyperplane in strain space given by (3.8, 3.14 and 3.17)

$$g_k = \underset{\sim}{N}_k \underset{\sim}{C}^{-1} \underset{\sim}{T} \underset{\sim}{\varepsilon} + \tau_k^{S(\varepsilon)} - \tau_{cr}^k = 0 \ . \tag{4.6}$$

The shear stresses $\tau_k^{S(\sigma)}$ and $\tau_k^{S(\varepsilon)}$ are related through (3.8) and (3.25):

$$\tau_k^{S(\sigma)} = \tau_k^{S(\varepsilon)} + \underset{\sim}{N}_k \underset{\sim}{C}^{-1} \underset{\sim}{T} (\underset{\sim}{\varepsilon} - \underset{\sim}{C}_{Macro} \underset{\sim}{\sigma}) \ . \tag{4.7}$$

Admissible stress and strain increments $\delta\underset{\sim}{\sigma}^*$, $\delta\underset{\sim}{\varepsilon}^*$ corresponding to unloading from all potentially active systems must satisfy

$$\underset{\sim}{N}_k \underset{\sim}{\Psi} \delta\underset{\sim}{\sigma} \leq 0 \tag{4.8}$$

and

$$\underset{\sim}{N}_k \underset{\sim}{C}^{-1} \underset{\sim}{T} \delta\underset{\sim}{\varepsilon} \leq 0 \tag{4.9}$$

which are equivalent statements since, from (3.1), (3.14) and (3.22)

$$\underset{\sim}{C} \underset{\sim}{\Psi} = \underset{\sim}{T} \underset{\sim}{C}_{Macro} \ . \tag{4.10}$$

In stress space the local elastic region lies within the pyramid of inner bounding hyperplanes f_k whose unit normal vectors are

$$\underset{\sim}{n}_k = (\underset{\sim}{N}_k \underset{\sim}{\nu})^T / \| \underset{\sim}{N}_k \underset{\sim}{\nu} \| \quad . \tag{4.11}$$

The distance to the kth hyperplane is (4.5 and 4.11)

$$\overset{\sigma}{D}_k = (\tau^k_{cr} - \tau^{S(\sigma)}_k) / \| \underset{\sim}{N}_k \underset{\sim}{\nu} \| \tag{4.12}$$

which for isotropic aggregates simplifies to (see Appendix)

$$\overset{\sigma}{D}_k = \sqrt{2}\, (\tau^k_{cr} - \tau^{S(\sigma)}_k) \quad . \tag{4.13}$$

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

$$\delta \overset{\sigma}{D}_{(k+)} = (\delta\tau^{(k+)}_{cr} - \delta\tau^{S(\sigma)}_k) / \| \underset{\sim}{N}_k \underset{\sim}{\nu} \| \quad . \tag{4.14}$$

From (3.13)

$$\int_V \left(\sum_k \delta\tau^{S(\sigma)}_k \, \delta\gamma_k\right) dV < 0 \quad . \tag{4.15}$$

As this inequality must hold locally for the majority of active systems, we can assume it holds for the particular k of interest. Thus

$$\delta\tau_k^{S(\sigma)}\,\delta\gamma_k < 0 \qquad (4.16)$$

and (4.1 and 4.16)

$$\delta\overset{\sigma}{D}_{(k+)} = (\delta\tau_{cr}^{(k+)} + |\delta\tau_k^{S(\sigma)}|)/\|\underset{\sim}{M}_k\,\underset{\sim}{\nu}\| > 0 \ . \qquad (4.17)$$

Similarly, the distance (in the opposite direction in stress space) to the parallel hyperplane corresponding to the negative sense of slip (k-) in this crystallographic system is

$$\overset{\sigma}{D}_{(k-)} = (\tau_{cr}^{(k-)} + \tau_k^{S(\sigma)})/\|\underset{\sim}{M}_k\,\underset{\sim}{\nu}\| \qquad (4.18)$$

and its change is

$$\delta\overset{\sigma}{D}_{(k-)} = (\delta\tau_{cr}^{(k-)} - |\delta\tau_k^{S(\sigma)}|)/\|\underset{\sim}{M}_k\,\underset{\sim}{\nu}\| \ . \qquad (4.19)$$

Thus, if the change in crystal hardening $\delta\tau_{cr}^{(k-)}$ in reverse slip is less than the change in the resolved shear stress due to internal slip and self-stressing, $\delta\overset{\sigma}{D}_{(k-)} < 0$ and the two hyperplanes move in the same direction. This is certainly the case when the crystal strain-<u>softens</u> in reverse slip (as is suggested by the experimental work of Paterson [27] on copper), and there will be a corresponding strong Bauschinger effect in macrostress space. There will be at least a weak Bauschinger effect if only $\delta\tau_{cr}^{(k-)} \leq \delta\tau_{cr}^{(k+)}$, hence $\delta\overset{\sigma}{D}_{(k-)} < \delta\overset{\sigma}{D}_{(k+)}$. Introducing the generalized Schmid-Taylor law [24, 28]

$$\delta\underset{\sim}{\tau}_{cr} = \underset{\sim}{H}(\underset{\sim}{\gamma})\,\delta\underset{\sim}{\gamma} \qquad (4.20)$$

(in which $\underset{\sim}{H}(\underset{\sim}{\gamma})$ is the crystal hardening matrix), this inequality is met for both Taylor hardening [1, 29] and the translational hardening adopted by Budiansky and Wu [10] and Tung and Lin [19], as well as for any positive combination [30]

$$\underset{\sim}{H} = h(\underset{\sim}{\gamma})\underset{\sim}{1} + c(\underset{\sim}{\gamma})\underset{\sim}{N}\,\underset{\sim}{N}^T \quad . \tag{4.21}$$

($\underset{\sim}{1}$ 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, $\underset{\sim}{H}$ of (4.21) is at least positive semi-definite ($\underset{\sim}{H} \geq 0$), and if $c \neq 0$, $\underset{\sim}{H} > 0$ over active systems [24, 30]. The property $\underset{\sim}{H} \geq 0$ will be of importance in establishing uniqueness of solution for the discrete model in Section 8.

5. 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 aggregate 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 [31] and [32]). Thus, as an idealization of the physical situation, we assume a thickness of 1 mm and define a unit cube $V = 1\ mm^3$ containing on the order 1000 crystal grains in the corresponding "flat sheet" representation (i.e., a macroscopic plane stress problem). Then the longitudinal feces (Figure 2) 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 the displacements either constant or (for other combined loadings) linearly varying over the appropriate 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).

6. DISCRETIZATION OF BOUNDARY VALUE PROBLEMS OF PRESCRIBED AGGREGATE MACROSTRAIN

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 sub-volume with constant microstrain field is represented by a tetrahedral element, herein called a crystallite, with nodal points I, J, K, L (Figure 3). The infinitesimal displacement $\delta\bar{\underset{\sim}{u}}(\underset{\sim}{x})$ within the crystallite q is readily expressed in terms of the nodal displacements $\delta \bar{\underset{\sim}{u}}^M$ as (see [33], for example)

$$\delta \bar{\underset{\sim}{u}}(\underset{\sim}{x}) = \sum_{M(q)} \phi_M(\underset{\sim}{x}) \, \delta \underset{\sim}{u}^M \qquad (6.1)$$

wherein

$$\phi_M(\underset{\sim}{x}) = \alpha_M + \beta_{Mj} x_j \qquad (6.2)$$

with the general expressions for α_M, β_{Mj} in terms of nodal coordinates x_i^J given in the Appendix. From (2.2), the local strain field is

$$\delta \underset{\sim}{\xi}_{(q)} = \sum_{M(q)} \underset{\sim}{\beta}_q^M \, \delta \bar{\underset{\sim}{u}}^M \qquad (6.3)$$

in which

$$\underset{\sim}{\beta}_q^M = \underset{\sim}{D}^T \phi_M(\underset{\sim}{x}) \quad . \qquad (6.4)$$

Then, from (2.10),

$$\int_V \delta \bar{\underset{\sim}{\xi}} \, dV = \sum_q \delta \bar{\underset{\sim}{\xi}}_{(q)} V_q = \delta \underset{\sim}{\varepsilon} \qquad (6.5)$$

exactly if the infinitesimal nodal displacements on the faces A_i of the unit cube are prescribed consistent with (2.3) and (2.6). Denoting incremental tractions on the crystallite faces by $\delta \bar{\underset{\sim}{t}}$, the virtual work equation for the element is (from 2.1)

$$\int_{V_q} \delta\bar{\zeta} \cdot \delta\bar{\xi}\, dV - \int_{S_q} \delta\bar{t} \cdot \delta\bar{u}\, dS = 0 \tag{6.6}$$

so that, from (6.3) and (6.4), the element equilibrium equation can be expressed

$$\sum_{M(q)} (\beta_q^M)^T \int_{V_q} \delta\bar{\zeta}\, dV = \sum_{M(q)} \int_{S_q} \phi_M\, \delta\bar{t}\, dS \quad . \tag{6.7}$$

Since an approximating displacement field has been adopted, tractions cannot be matched exactly between adjacent crystals. Rather, we introduce from (6.7) the equivalent nodal force increments

$$\delta F^J_{(q)} = \int_{S_q} \phi_J\, \delta\bar{t}\, dS \tag{6.8}$$

and require that

$$\sum_{q(J)} \delta F^J_{(q)} = 0 \tag{6.9}$$

over the q elements having the common node J. Equilibrium between crystallites is then satisfied in an average sense, and the discontinuous microstress field $\delta\bar{\zeta}$ through the aggregate is only approximately statically admissible. Hence, defining macroscopic stress according to (2.11), the aggregate virtual work equation (2.9) will not be exactly satisfied, and a measure of the discretization error is (from 6.5)

$$e = \int_V \delta\bar{\zeta} \cdot \delta\bar{\xi}\, dV - \left(\int_V \delta\bar{\zeta}\, dV\right) \cdot \delta\varepsilon \tag{6.10}$$

which can be written

$$\varepsilon = \sum_q \delta\bar{\xi}_{(q)} \cdot \delta\bar{\xi}_{(q)} V_q - (\sum_q \delta\bar{\xi}_{(q)} V_q) \cdot \delta\varepsilon \quad . \tag{6.11}$$

Upon substitution of (6.7) and (6.8) into (6.9), the nodal equilibrium equation becomes

$$\sum_{q(J)} (\beta_q^J)^T \int_{V_q} \delta\bar{\zeta}\, dV = 0 \quad . \tag{6.12}$$

Since our boundary value problem is one of prescribed macrostrain, we seperate the stress field as in (3.17) and write (using 6.3 and 6.4 and deleting the superscript (ε) for simplicity)

$$\int_{V_q} \delta\bar{\zeta}\, dV = C_{(q)}^{-1} \sum_{M(q)} \beta_q^M \delta\bar{u}^{(e)M} V_q + \int_{V_q} \delta\bar{\zeta}^S\, dV \tag{6.13}$$

wherein $C_{(q)}$ is the crystal compliance matrix referred to the unit cube axes and $\delta\bar{u}^{(e)}$ is the (kinematically admissible) infinitesimal displacement field determined by assuming elastic aggregate response to $\delta\varepsilon$. Substituting (6.13) into (6.12), the nodal equilibrium equation is seperable into two equations by definition of the field $\delta\bar{u}^{(e)}$:

$$\sum_{q(J)} (\beta_q^J)^T C_{(q)}^{-1} \sum_{M(q)} \beta_q^M \delta\bar{u}^{(e)M} V_q = 0 \tag{6.14}$$

$$\sum_{q(J)} (\beta_q^J)^T \int_{V_q} \delta\bar{\xi}^S\, dV = 0 \quad . \tag{6.15}$$

Assembling the first of these equations into a general matrix equilibrium equation for the overall vector $\delta\bar{U}^{(e)} = (\ldots, \delta\bar{u}^{(e)M}, \ldots)^T$ of elastic nodal displacements and noting that

$$\underset{\sim}{C}^{-1}_{(q)} = \underset{\sim}{A}^{T}_{(q)} \underset{\sim}{C}^{-1}_{c} \underset{\sim}{A}_{(q)} \tag{6.16}$$

(where $\underset{\sim}{C}_c$ is the crystal compliance matrix referred to the crystal axes and $\underset{\sim}{A}_{(q)}$ is a transformation matrix given in the Appendix), we have

$$\underset{\sim}{B}^T \underset{\sim}{S} \underset{\sim}{B} V_c \, \delta \bar{\underset{\sim}{U}}^{(e)} = \underset{\sim}{0} \tag{6.17}$$

in which all crystallites have been chosen of equal volume $V_c << 1$ for convenience in subsequent analysis. (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-cubes as desired.) The matrix $\underset{\sim}{B}$ is composed of 6 by 3 elements $\underset{\sim}{B}_{qJ}$ defined as

$$\underset{\sim}{B}_{qJ} = \begin{cases} \underset{\sim}{A}_{(q)} \underset{\sim}{E}^J_q = \underset{\sim}{A}_{(q)} \underset{\sim}{D}^T \phi_J & \text{if } J \text{ is a node of } (q) \\ \underset{\sim}{0} & \text{if } J \text{ is not a node of } (q) \; . \end{cases} \tag{6.18}$$

The matrix $\underset{\sim}{S}$ is a diagonal matrix of positive-definite submatrices $\underset{\sim}{C}^{-1}_c$:

$$\underset{\sim}{S} = \lceil \underset{\sim}{C}^{-1}_c \rfloor \quad . \tag{6.19}$$

The overall matrix $\underset{\sim}{B}^T \underset{\sim}{S} \underset{\sim}{B}$ is positive-semidefinite since a piecewise linear displacement field admits infinitesimal rigid body motion with no change in strain energy. In terms of the unknown interior displacements $\delta \underset{\sim}{\Delta}^{(e)}$ and the prescribed exterior displacements $\delta \underset{\sim}{U}^{o}$, (6.17) can be written

$$\underset{\sim}{B}_i^T \underset{\sim}{S} \underset{\sim}{B}_i V_c \, \delta\underset{\sim}{u}^{(e)} + \underset{\sim}{K} \, \delta\underset{\sim}{u}^{(e)} = - \underset{\sim}{B}_i^T \underset{\sim}{S} \underset{\sim}{B}_o V_c \, \delta\underset{\sim}{U}^o \qquad (6.20)$$

wherein $\underset{\sim}{B}_i$ is obtained from $\underset{\sim}{B}$ by deleting all vector columns corresponding to exterior nodes J^o. The matrix $\underset{\sim}{B}_o$ is similarly determined by deleting all vector columns corresponding to interior nodes J. The aggregate elastic "stiffness" matrix $\underset{\sim}{K}$ is symmetric and positive-definite, an arbitrary rigid body motion in the solution having been eliminated by prescribing $\delta\underset{\sim}{U}^o$ on the surface of the unit cube. Thus, the internal strain field $\delta\bar{\underset{\sim}{\zeta}}^{(e)} = \underset{\sim}{D}^T \delta\bar{\underset{\sim}{u}}^{(e)}$ is determined as

$$\delta\bar{\underset{\sim}{\zeta}}_q^{(e)} = \sum_{M(q)} \left(\underset{\sim}{B}_q^{M^o} \, \delta\underset{\sim}{u}_o^{M^o} - \underset{\sim}{B}_q^{M} \underset{\sim}{K}_M^{-1} \underset{\sim}{B}_i^T \underset{\sim}{S} \underset{\sim}{B}_o V_c \, \delta\underset{\sim}{U}^o \right) \qquad (6.21)$$

in which $\underset{\sim}{K}_M^{-1}$ denotes a row vector of 3 by 3 submatrices of $\underset{\sim}{K}^{-1}$ and the separate contributions of interior and exterior nodes of (q) are as indicated. The overall vector of infinitesimal strains $\delta\underset{\sim}{E}^{(e)} = (\ldots, \delta\bar{\underset{\sim}{\zeta}}_{(q)}^{(e)}, \ldots)^T$ can be expressed

$$\delta\underset{\sim}{E}^{(e)} = \underset{\sim}{A}^T \left[\underset{\sim}{I} - \underset{\sim}{B}_i \left(\underset{\sim}{B}_i^T \underset{\sim}{S} \underset{\sim}{B}_i \right)^{-1} \underset{\sim}{B}_i^T \underset{\sim}{S} \right] \underset{\sim}{B}_o \, \delta\underset{\sim}{U}^o \qquad (6.22)$$

wherein $\underset{\sim}{I}$ is an identity matrix and $\underset{\sim}{A}^T$ is a diagonal matrix of elements $\underset{\sim}{A}_{(q)}^T$.

7. GENERAL SOLUTION FOR INCREMENTAL CRYSTAL SHEARS

From (3.6), (3.7), (3.16) and (3.17)

$$\int_{V_q} \delta\bar{\underset{\sim}{\zeta}}^S \, dV = \underset{\sim}{C}_{(q)}^{-1} \int_{V_q} \left(\delta\bar{\underset{\sim}{\zeta}}^S - \underset{\sim}{N}_{(q)}^T \, \delta\bar{\underset{\sim}{\gamma}} \right) dV \qquad (7.1)$$

or, using (6.3),

$$\int_{V_q} \delta\bar{\xi}^S \, dV = C_{(q)}^{-1} \sum_{M(q)} \beta_q^M \, \delta\bar{u}^{(S)M} \, V_q - C_{(q)}^{-1} \, N_{(q)}^T \int_{V_q} \delta\bar{\gamma} \, dV \tag{7.2}$$

in which $\delta\bar{u}^S$ is the previously defined (Section 3) infinitesimal displacement field due to internal slip and self-straining (i.e., $\delta\bar{\xi}^S = D^T \, \delta\bar{u}^S$). Thus, substituting into the second nodal equilibrium equation (6.15),

$$\sum_{q(J)} (\beta_q^J)^T \, C_{(q)}^{-1} \sum_{M(q)} \beta_q^M \, \delta\bar{u}^{(S)M} \, V_q = \sum_{q(J)} (\beta_q^J)^T \, C_{(q)}^{-1} \, N_{(q)}^T \int_{V_q} \delta\bar{\gamma} \, dV \ . \tag{7.3}$$

Since, from (3.18), $\delta\bar{u}^{(S)M^o} \equiv 0$ for exterior nodes on the cube faces, we have (proceeding as before)

$$B_1^T \, S \, B_1 \, V_c \, \delta\Delta^S = B_1^T \, S \, N^T \, \delta\bar{\gamma} \, V_c \tag{7.4}$$

in which $\delta\Delta^S = (\ldots, \delta\bar{u}^{(S)M}, \ldots)^T$, $\delta\bar{\gamma} = (\ldots, \delta\bar{\gamma}_{(q)}, \ldots)^T$, and

$$N = \lceil N_{(q)} A_{(q)}^T \rfloor = \lceil N^c \rfloor \tag{7.5}$$

where N^c is the transformation matrix from the local crystal axes to the crystallographic slip systems. Hence

$$\delta\Delta^S = K^{-1} \, B_1^T \, S \, N^T \, \delta\bar{\gamma} \, V_c \tag{7.6}$$

and

$$\delta\bar{\xi}_{(q)}^S = \sum_{M(q)} \beta_q^M \, K_M^{-1} \, B_1^T \, S \, N^T \, \delta\bar{\gamma} \, V_c \ . \tag{7.7}$$

Upon substitution of (7.7) into (7.2), the internal stress field due to crystal slip and self-straining becomes

$$\delta\bar{\zeta}^S_{(q)} = C^{-1}_{(q)} \sum_{M(q)} \beta^M_q K^{-1}_M B^T_1 S N^T \delta\bar{\gamma} V_c - C^{-1}_{(q)} N^T_{(q)} \delta\bar{\gamma}_{(q)} \; . \tag{7.8}$$

Thus, the overall vector of incremental stresses $\delta\bar{\Sigma}^S = (\ldots, \delta\bar{\zeta}^S_{(q)}, \ldots)^T$ can be expressed (from 6.18, 7.4, 7.5 and 7.8)

$$\delta\bar{\Sigma}^S = -A^T [S - S B_1 (B_1^T S B_1)^{-1} B_1^T S] N^T \delta\bar{\gamma} \tag{7.9}$$

with

$$A^T = \lceil A^T_{(q)} \rfloor \tag{7.10}$$

as previously defined. Then, from (3.8), (7.5), and (7.9-7.10), the overall vector of incremental shear stresses $\delta\bar{\tau}^S = (\ldots, \delta\bar{\tau}^S_{(q)}, \ldots)$ due to internal slip is given in terms of the vector of infinitesimal crystal shears by

$$\delta\bar{\tau}^S = - N Q N^T \delta\bar{\gamma} = - P^S \delta\bar{\gamma} \tag{7.11}$$

wherein

$$Q = S [I - B_1 (B_1^T S B_1)^{-1} B_1^T S] \; . \tag{7.12}$$

The symmetric matrix $P^S = N Q N^T$ will be called the self-straining matrix. In Section 8 it is proved that this matrix is positive-definite over critical (potentially active) slip systems, hence it has a unique decomposition (or inverse).

Substituting (7.9) and (6.22) into (6.13) (or 3.17) and denoting $\delta\bar{\Sigma} = (\ldots, \delta\bar{\xi}_{(q)}, \ldots)^T$, we have

$$\delta\bar{\Sigma} = A^T S \, [I - B_1(B_1^T S B_1)^{-1} B_1^T S][B_o \, \delta U^o - N^T \delta\bar{\gamma}] \tag{7.13}$$

or (from 7.12)

$$\delta\bar{\Sigma} = A^T Q \, [B_o \, \delta U^o - N^T \delta\bar{\gamma}] \; . \tag{7.14}$$

The appropriate static admissibility of this stress field for arbitrary surface displacements and internal shears is, of course, confirmed by substitution of (7.14) into the nodal equilibrium equations (6.12), expressed in general matrix form, whence

$$B_1^T A \, \delta\bar{\Sigma} = B_1^T Q \, [B_o \, \delta U^o - N^T \delta\bar{\gamma}] \equiv 0 \tag{7.15}$$

since $B_1^T Q \equiv 0$ from (7.12). (The influence matrix Q is analogous to the integrodifferential operators on $\delta\xi^P(x)$ in [20] and [34].) The overall vector $\delta\bar{\tau} = (\ldots, \delta\bar{\tau}_{(q)}, \ldots)^T$ of incremental resolved shear stresses in the various crystallographic slip systems within the cube is (3.8, 7.5, 7.10 and 7.14)

$$\delta\bar{\tau} = N Q \, [B_o \, \delta\Delta^o - N^T \delta\bar{\gamma}] \; . \tag{7.16}$$

Therefore, the equation for the incremental stress in the kth critical slip system of crystallite (q) becomes

$$\delta\bar{\tau}_{k(q)} = \underset{\sim}{N}_k^c \underset{\sim}{C}_c^{-1} \sum_{M(q)} A_{(q)} (\underset{\sim}{E}_q^{M^o} \delta\underset{\sim}{\psi}_o^{M^o} - \underset{\sim}{E}_q^M \underset{\sim}{K}_M^{-1} \underset{\sim}{B}_1^T \underset{\sim}{S} [\underset{\sim}{B}_o \delta\underset{\sim}{\psi}^o$$

$$- \underset{\sim}{N}^T \delta\bar{\underset{\sim}{\gamma}}] V_c) - \underset{\sim}{N}_k^c \underset{\sim}{C}_c^{-1} (\underset{\sim}{N}^c)^T \delta\bar{\underset{\sim}{\gamma}}_{(q)}. \qquad (7.17)$$

For an active system,

$$\delta\bar{\tau}_{k(q)} = \delta\tau_{cr}^{k(q)} = \underset{\sim}{H}_k(\bar{\underset{\sim}{\gamma}}_q)\delta\bar{\underset{\sim}{\gamma}}_{(q)} \qquad (7.18)$$

with the hardening matrix of the crystallite depending only upon the local plastic deformation ($\underset{\sim}{H}_k$ denoting the kth row vector). Thus, from (7.17) and (7.18)

$$[\underset{\sim}{H}_k(\bar{\underset{\sim}{\gamma}}_q) + \underset{\sim}{N}_k^c \underset{\sim}{C}_c^{-1}(\underset{\sim}{N}^c)^T]\delta\bar{\underset{\sim}{\gamma}}_{(q)} - \underset{\sim}{N}_k^c \underset{\sim}{C}_c^{-1} \sum_{M(q)} A_{(q)} \underset{\sim}{E}_q^M \underset{\sim}{K}_M^{-1} \underset{\sim}{B}_1^T \underset{\sim}{S} V_c \underset{\sim}{N}^T \delta\bar{\underset{\sim}{\gamma}}$$

$$= \underset{\sim}{N}_k^c \underset{\sim}{C}_c^{-1} \sum_{M(q)} A_{(q)} (\underset{\sim}{E}_q^{M^o} \delta\underset{\sim}{\psi}_o^{M^o} - \underset{\sim}{E}_q^M \underset{\sim}{K}_M^{-1} \underset{\sim}{B}_1^T \underset{\sim}{S} V_c \underset{\sim}{B}_o \delta\underset{\sim}{\psi}^o) \qquad (7.19)$$

in which the only unknowns are the incremental shears $\delta\bar{\gamma}_{k(q)}$ in the various active slip systems. Writing the equality (7.18) for all the active systems, equations (7.19) can be expressed in general matrix form as

$$[\underset{\sim}{H}_A + \underset{\sim}{N}_A \underset{\sim}{Q}_A \underset{\sim}{N}_A^T] \delta\bar{\underset{\sim}{\gamma}}_A = \underset{\sim}{N}_A \underset{\sim}{Q}_A (\underset{\sim}{B}_o)_A \delta\underset{\sim}{\psi}^o \qquad (7.20)$$

wherein $\underset{\sim}{H}_A$ is a diagonal matrix whose elements are the individual crystallite hardening matrices. The subscript A denotes the respective vector or matrix reduced to include only those crystallites (q) containing one or more active critical systems. The symmetric matrix

$$\underset{\sim}{P}_A = \underset{\sim}{H}_A + \underset{\sim}{N}_A \, \underset{\sim}{Q}_A \, \underset{\sim}{N}_A^T \tag{7.21}$$

is positive-definite for all crystal hardening matrices of type (4.21), as proved in the following section, and (7.20) (or 7.19) yields a unique solution for $\delta\bar{\underset{\sim}{\gamma}}_A$.

8. UNIQUENESS OF INTERNAL FIELDS IN THE DISCRETIZED AGGREGATE MODEL

From (6.16), (6.19) and (7.10), the overall vector of infinitesimal elastic strains $\delta\bar{\underset{\sim}{E}}^e = (\ldots, \underset{\sim}{C}_{(q)}\delta\bar{\underset{\sim}{\xi}}_{(q)}, \ldots)^T$ is

$$\delta\bar{\underset{\sim}{E}}^e = \underset{\sim}{A}^T \underset{\sim}{S}^{-1} \underset{\sim}{Q} \, [\underset{\sim}{B}_o \, \delta\underset{\sim}{U}^o - \underset{\sim}{N}^T \delta\bar{\underset{\sim}{\gamma}}] \quad . \tag{8.1}$$

Reintroducing the scalar average u_e of (3.9), we write

$$\bar{u}_e = \sum_q \delta\bar{\underset{\sim}{\xi}}_{(q)} \cdot \underset{\sim}{C}_{(q)}\delta\bar{\underset{\sim}{\xi}}_{(q)} \, V_c = \delta\bar{\underset{\sim}{\xi}} \cdot \delta\bar{\underset{\sim}{E}}^e \, V_c > 0 \ . \tag{8.2}$$

Hence, from (7.14) and (8.1),

$$\bar{u}_e = (\underset{\sim}{B}_o \, \delta\underset{\sim}{U}^o - \underset{\sim}{N}^T\delta\bar{\underset{\sim}{\gamma}})^T \underset{\sim}{Q}(\underset{\sim}{B}_o \, \delta\underset{\sim}{U}^o - \underset{\sim}{N}^T\delta\bar{\underset{\sim}{\gamma}}) \, V_c > 0 \quad . \tag{8.3}$$

Assume now two distinct sets of internal fields $\delta\bar{\underset{\sim}{\xi}}_{(q)}$, $\delta\bar{\underset{\sim}{\xi}}_{(q)}$, $\delta\bar{\underset{\sim}{\gamma}}_{(q)}$ and

$\delta\bar{\boldsymbol{\xi}}^*_{(q)}$, $\delta\bar{\boldsymbol{\xi}}^*_{(q)}$, $\delta\bar{\boldsymbol{\gamma}}^*_{(q)}$, both of which satisfy all appropriate equations of the discretized model for an infinitesimal macrostrain $\delta\boldsymbol{\varepsilon}$ (i.e., uniquely prescribed $\delta\boldsymbol{U}^o$). Denoting their differences by $\langle\delta\bar{\boldsymbol{\xi}}_{(q)}\rangle = \delta\bar{\boldsymbol{\xi}}_{(q)} - \delta\bar{\boldsymbol{\xi}}^*_{(q)}$, etc., then from the above

$$\langle\delta\bar{\boldsymbol{\gamma}}\rangle^T \boldsymbol{N}\,\boldsymbol{Q}\,\boldsymbol{N}^T \langle\delta\bar{\boldsymbol{\gamma}}\rangle > 0 \quad . \tag{8.4}$$

This equation is written only over <u>potentially</u> 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. Therefore, $\boldsymbol{P}^S = \boldsymbol{N}\,\boldsymbol{Q}\,\boldsymbol{N}^T$ is positive definite over critical systems; consequently, it is also positive definite over active systems ($\boldsymbol{P}^S_A > 0$). We also find, from (3.7), (7.5), and (7.14),

$$\sum_q \langle\delta\bar{\boldsymbol{\xi}}_{(q)}\rangle \cdot \langle\delta\bar{\boldsymbol{\xi}}_{(q)}\rangle + \langle\delta\bar{\boldsymbol{\gamma}}\rangle^T \boldsymbol{N}\,\boldsymbol{Q}\,\boldsymbol{N}^T \langle\delta\bar{\boldsymbol{\gamma}}\rangle = 0 \ . \tag{8.5}$$

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

$$\langle\delta\bar{\boldsymbol{\xi}}_{(q)}\rangle \cdot \langle\delta\bar{\boldsymbol{\xi}}^p_{(q)}\rangle \geq \langle\delta\bar{\boldsymbol{\gamma}}_{(q)}\rangle^T \boldsymbol{H}_{(q)} \langle\delta\bar{\boldsymbol{\gamma}}_{(q)}\rangle \quad , \tag{8.6}$$

and substituting into (8.5), we have

$$0 \geq \langle\delta\bar{\boldsymbol{\gamma}}\rangle^T \lceil \boldsymbol{H}_{(q)} \rfloor \langle\delta\bar{\boldsymbol{\gamma}}\rangle + \langle\delta\bar{\boldsymbol{\gamma}}\rangle^T \boldsymbol{N}\,\boldsymbol{Q}\,\boldsymbol{N}^T \langle\delta\bar{\boldsymbol{\gamma}}\rangle \ . \tag{8.7}$$

From (8.4) the second term is positive, and for $\underset{\sim}{H} \geq 0$ (as in 4.21) the first term is non-negative. Hence, the inequality is violated for non-zero $\langle \delta \bar{\underset{\sim}{\gamma}} \rangle$, from which we conclude that the incremental shears are unique. It follows from (7.14) that the incremental stress field is unique. Consequently, the infinitesimal total strain field is also unique, and the proof is complete. The matrix $\underset{\sim}{P}_A$ of (7.21) is obviously positive-definite from (8.4) and the above.

A final comment is necessary pertaining to determination of the unique aggregate response from a particular deformed state, since an admissible solution of (7.20) is constrained by the physical requirement $\delta \bar{\gamma}_k \geq 0$ for all k (which is implicit in 8.6). If, for example, (7.20) is solved for $\delta \bar{\underset{\sim}{\gamma}}$ based upon the expectation that all critical slip systems will be active in a macrostrain increment $\delta \underset{\sim}{\varepsilon}$, certain of the $\delta \bar{\gamma}_{k(q)}$ may be calculated as negative. In this event (7.20) must again be solved, after eliminating the appropriate slip systems, until all incremental plastic shears are positive.

9. REMARKS ON QUANTITATIVE MODELS AND THE CALCULATION OF AGGREGATE YIELD SURFACES

At a particular stage of aggregate straining, a subsequent yield surface is obtained by determining the positions of yield hyperplanes in stress space, as follows. Consider the case of applied biaxial strain $\underset{\sim}{\varepsilon} = (\varepsilon_{11}, \varepsilon_{22})^T$ corresponding to the biaxial macrostress state $\bar{\underset{\sim}{\sigma}} = (\bar{\sigma}_{11}, \bar{\sigma}_{22})^T$ discussed in Section 5. From the elastic solution of (6.21) (or 6.22) we define, according to (3.14),

$$\bar{\underset{\sim}{\xi}}^e_{(q)} = \bar{\underset{\sim}{T}}_{(q)} \underset{\sim}{\varepsilon} \tag{9.1}$$

in which $\bar{T}_{(q)}$ is a 6 by 2 matrix whose columns are determined from separate evaluations of (6.21) for the states $(\varepsilon_{11}, \varepsilon_{22} = 0)$ and $(\varepsilon_{11} = 0, \varepsilon_{22})$ respectively. Hence, from (3.20)

$$\bar{C}^{-1}_{Macro} = \sum_q C^{-1}_{(q)} \bar{T}_{(q)} V_c \quad , \tag{9.2}$$

a 2 by 2 matrix (using only the first two rows of each $C^{-1}_{(q)}$). Adopting the volume average definition of macroscopic stress (2.11), we have

$$\bar{\sigma} = \sum_q \bar{\zeta}_{(q)} V_c \quad , \tag{9.3}$$

where again only the two leading elements are chosen. Introducing the notation ζ^R for $\zeta^{S(\sigma)}$ (since from (3.1) and (3.3) $\zeta^{S(\sigma)}$ is the residual microstress field remaining in the aggregate upon unloading to zero macrostress), then, from (4.7), (6.16) and (7.5),

$$\bar{\tau}^R_{k(q)} = \bar{\tau}^S_{k(q)} + N^c_k C^{-1}_c A_{(q)} \bar{T}_{(q)} (\varepsilon - \bar{C}_{Macro} \bar{\sigma}) \tag{9.4}$$

wherein $\bar{\tau}^S_{k(q)}$ is the sum of increments $\delta\bar{\tau}^S_{k(q)}$ determined from (7.11) over the strain history and $\bar{C}_{Macro}$ and $\bar{\sigma}$ are as calculated above. The distance to the kth hyperplane in macrostress space then is determined from (4.12) as

$$\overset{\sigma}{D}_{k(q)} = (\bar{\tau}^{k(q)}_{cr} - \bar{\tau}^R_{k(q)}) / \| N_{k(q)} \bar{\Psi}_{(q)} \| \tag{9.5}$$

in which, from (4.10), (6.16) and (7.5)

$$N_{k(q)} \bar{\Psi}_{(q)} = N_k^c C_c^{-1} A_{(q)} \bar{T}_{(q)} C_{Macro} \quad . \tag{9.6}$$

The direction, as given by (4.11), remains fixed. The elastic domain is the inner bound of all such hyperplanes in $\bar{\sigma}_{11}$, $\bar{\sigma}_{22}$ space.

A quantitative model which should prove suitable for such evaluations (corresponding to thin-walled tubes) is an aggregate cube of 1296 crystallites arranged within 216 sub-cubic volumes. From the symmetry conditions of Section 5, the discrete boundary value problem can be reduced to a consideration of 324 crystallites with 112 distinct interior and exterior nodes and 223 unknown nodal displacements. The symmetric, positive-definite matrix K is then of order 223 with a half-band width of approximately 43. Thus, its accurate inversion is a relatively modest task for a triangular decomposition routine. Concerning the solution of (7.20) for incremental shears, the order of P_A should be small (less than 100) during the early stages of aggregate straining as only a relatively few slip systems will be critical. With increasing plastic deformation, numerical studies could feasibly be continued until several systems become active within each of the majority of the crystallites, at which stage the order of P_A would still be less than 1000. A digital computer program for studying the quantitative effects of aggregate texturing, crystal structure and anisotropy, and crystal hardening laws on theoretical macroscopic response 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

$$\underset{\sim}{\zeta} = (\zeta_{11}, \sqrt{2}\,\zeta_{12}, \sqrt{2}\,\zeta_{13}, \zeta_{22}, \sqrt{2}\,\zeta_{23}, \zeta_{33})^T \qquad (A.1)$$

$$\delta\underset{\sim}{\xi} = (\delta\xi_{11}, \sqrt{2}\,\delta\xi_{12}, \sqrt{2}\,\delta\xi_{13}, \delta\xi_{22}, \sqrt{2}\,\delta\xi_{23}, \delta\xi_{33})^T \qquad (A.2)$$

from which the equilibrium and kinematic equations can be written $\underset{\sim}{D}\,\underset{\sim}{\zeta} = \underset{\sim}{0}$ and $\underset{\sim}{D}^T\delta\underset{\sim}{\xi} = \delta\underset{\sim}{u} \equiv (\delta u_1, \delta u_2, \delta u_3)^T$, with

$$D = \begin{bmatrix} \partial_1 & \frac{1}{\sqrt{2}}\partial_2 & \frac{1}{\sqrt{2}}\partial_3 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}\partial_1 & 0 & \partial_2 & \frac{1}{\sqrt{2}}\partial_3 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}\partial_1 & 0 & \frac{1}{\sqrt{2}}\partial_2 & \partial_3 \end{bmatrix} \tag{A.3}$$

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

The kth row vector of the crystal transformation matrix N is given in terms of unit vectors ϕ^k, λ^k in the normal and glide directions, respectively, of the kth crystallographic slip system:

$$N_k = [\phi_1^k\lambda_1^k, \ \frac{1}{\sqrt{2}}(\phi_1^k\lambda_2^k + \phi_2^k\lambda_1^k), \ \frac{1}{\sqrt{2}}(\phi_1^k\lambda_3^k + \phi_3^k\lambda_1^k), \ \phi_2^k\lambda_2^k, \ \frac{1}{\sqrt{2}}(\phi_2^k\lambda_3^k + \phi_3^k\lambda_2^k), \ \phi_3^k\lambda_3^k] \, . \tag{A.4}$$

Consequently

$$\| N_k \| = (N_k N_k^T)^{\frac{1}{2}} = \frac{1}{\sqrt{2}} \, . \tag{A.5}$$

For the tetrahedral crystallite (Figure 3),the configuration parameters α_M, β_{Mj} are determined as (introducing the permutation tensor ε_{ijk} and summing on repeated indices)

$$\alpha_I = \frac{1}{6V_q} \epsilon_{ijk} x_i^J x_j^K x_k^L$$

$$\alpha_J = \frac{1}{6V_q} \epsilon_{ijk} x_i^K x_j^I x_k^L$$

$$\alpha_K = \frac{1}{6V_q} \epsilon_{ijk} x_i^I x_j^J x_k^L \tag{A.6}$$

$$\alpha_L = \frac{1}{6V_q} \epsilon_{ijk} x_i^I x_j^K x_k^L$$

and

$$\beta_{Mj} = \frac{1}{6V_q} (\text{cofactor})_j^M \begin{bmatrix} 1 & x_1^I & x_2^I & x_3^I \\ 1 & x_1^J & x_2^J & x_3^J \\ 1 & x_1^K & x_2^K & x_3^K \\ 1 & x_1^L & x_2^L & x_3^L \end{bmatrix} \tag{A.7}$$

where $6V_q$ is the determinant of the matrix.

The transformation matrix $\mathcal{A}_{(q)}$ relating the stress or infinitesimal strain components referred to the unit cube axes with those referred to the crystal axes (Figure 3) is

$$\mathcal{A}_{(q)} = \begin{bmatrix} a_{11}^2 & \sqrt{2}\, a_{11}a_{12} & \sqrt{2}\, a_{11}a_{13} & a_{12}^2 & \sqrt{2}\, a_{12}a_{13} & a_{13}^2 \\ \sqrt{2}\, a_{11}a_{21} & a_{11}a_{22}+a_{12}a_{21} & a_{11}a_{23}+a_{13}a_{21} & \sqrt{2}\, a_{12}a_{22} & a_{12}a_{23}+a_{13}a_{22} & \sqrt{2}\, a_{13}a_{23} \\ \sqrt{2}\, a_{11}a_{31} & a_{11}a_{32}+a_{12}a_{31} & a_{11}a_{33}+a_{13}a_{31} & \sqrt{2}\, a_{12}a_{32} & a_{12}a_{33}+a_{13}a_{32} & \sqrt{2}\, a_{13}a_{33} \\ a_{21}^2 & \sqrt{2}\, a_{21}a_{22} & \sqrt{2}\, a_{21}a_{23} & a_{22}^2 & \sqrt{2}\, a_{22}a_{23} & a_{23}^2 \\ \sqrt{2}\, a_{21}a_{31} & a_{21}a_{32}+a_{22}a_{31} & a_{21}a_{33}+a_{23}a_{31} & \sqrt{2}\, a_{22}a_{32} & a_{22}a_{33}+a_{23}a_{32} & \sqrt{2}\, a_{23}a_{33} \\ a_{31}^2 & \sqrt{2}\, a_{31}a_{32} & \sqrt{2}\, a_{31}a_{33} & a_{32}^2 & \sqrt{2}\, a_{32}a_{33} & a_{33}^2 \end{bmatrix}$$

(A.8)

in which $a_{ij} = \cos (x_i^{'}, x_j)$. Thus

$$\underset{\sim}{\zeta}^{'}(q) = \underset{\sim}{A}(q)\underset{\sim}{\zeta}(q) \quad , \quad \delta\underset{\sim}{\xi}^{'}(q) = \underset{\sim}{A}(q) \; \delta\underset{\sim}{\xi}(q) \quad . \tag{A.9}$$

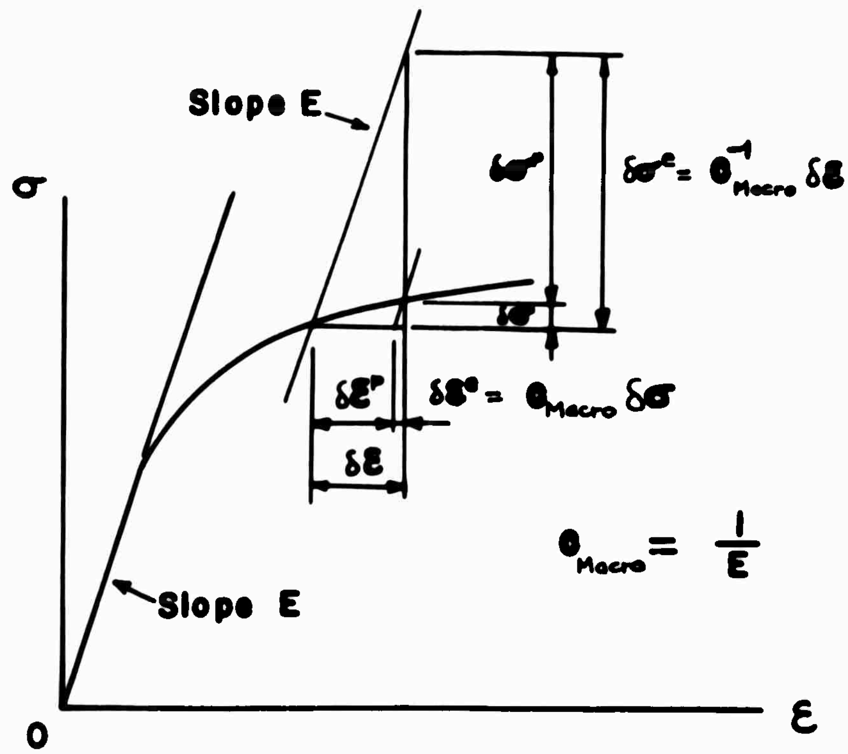

Fig. 1 Incremental Macroscopic Variables for the Uniaxial Case

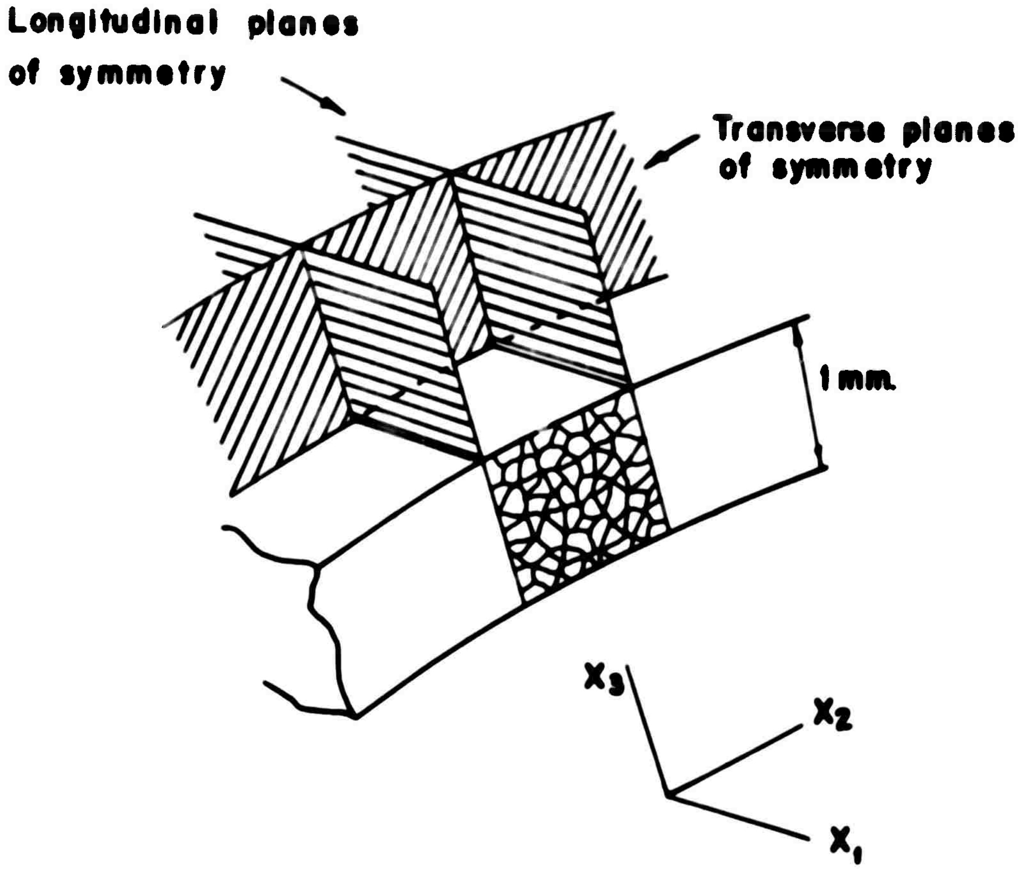

Fig. 2 Idealized Unit Cube in Thin-Walled Polycrystalline Specimen

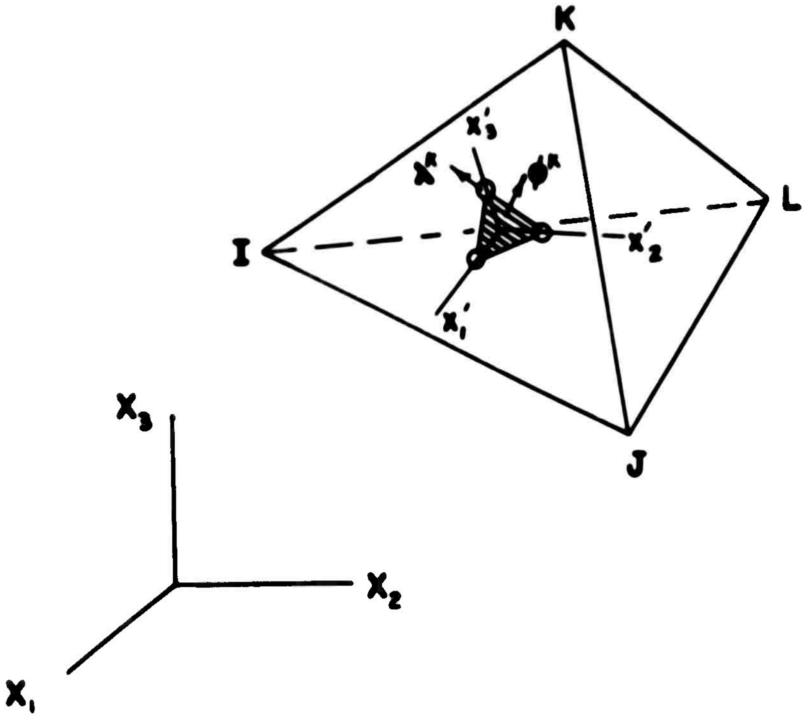

Fig. 3 Tetrahedral Crystallite Showing Orientation of Crystal Axes and K$^{\underline{th}}$ Slip System

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13 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 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.

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