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ON CONVERGENCE OF A DISCRETE AGGREGATE MODEL IN POLYCRYSTALLINE PLASTICITY

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Abstract—A discrete aggregate model, recently proposed by the author [1] as a basis for quantitative studies in polycrystalline plasticity, is extended and further analyzed herein. The discretized internal stress and strain increment fields, uniquely determined from the solution of a constrained quadratic programming problem, are proved to be strictly convergent to the solution of the corresponding continuum boundary value problem. Thus, the model is rigorously confirmed as a rational approximation well-suited for computational investigations of aggregate behavior.

1. INTRODUCTION

IN A recent paper [1], the author has presented a discrete polycrystalline aggregate model suitable for calculating macroscopic stress–strain relations and aggregate yield surfaces. The continuum boundary value problem (upon which the discretization is based) has been chosen with the objective of simulating quasi-static, small-deformation behavior of macroscopically homogeneous thin-walled metal tubes and flat sheet specimens. The discrete form incorporates approximating, piecewise linear infinitesimal displacement fields within crystal grains, but is otherwise general and includes cubic or hexagonal crystal anisotropy and broadly defined hardening laws over crystallographic slip systems. The solution is unique in internal stress and strain fields.

It is our purpose herein to extend the analytical foundation of the discrete model by proving strict convergence to the (incremental) solution of the corresponding continuum boundary value problem, which solution also is unique [2]. We thereby clearly establish the model as a well-defined, rational approximation in the theory of small-strain polycrystalline plasticity.

2. GENERAL SOLUTION OF THE DISCRETE MODEL

The boundary value problem is briefly described as follows. We introduce the mathematical model of an aggregate of identical "unit cubes", each containing a distribution of contiguous, polyhedral crystal grains of arbitrarily chosen orientations, and consider a "flat sheet" whose thickness is the linear dimension of the cube (1 mm, say). Then, by adopting crystal distributions symmetric about the two bisecting planes parallel to transverse cube faces, biaxial macroscopic straining of the sheet produces spatially uniform normal displacement fields (and zero tangential shearing stresses) over these faces. It also produces (generally) non-uniform normal stress distributions whose surface integrals and moments are the macroscopic stresses and couple-stresses due to the applied biaxial strains. (Equivalently, the macroscopic stress components can be calculated as volume averages of the corresponding internal stress fields [1].) Thus, our boundary value problem is one wherein either a particular infinitesimal displacement component is prescribed on a face A_i of the unit cube, or the associated traction is zero. (For a thorough discussion of the rationale for selecting this mathematical model, the reader is referred to [1].)

The crystal constitutive equations, in terms of increments, are

$$\delta\boldsymbol{\xi}^e = \mathbf{C}\delta\boldsymbol{\zeta} = \mathbf{A}^T\mathbf{C}_c\mathbf{A}\delta\boldsymbol{\zeta}. \tag{1}$$

$$\delta\boldsymbol{\xi}^p = \mathbf{N}^T\delta\boldsymbol{\gamma} = \mathbf{A}^T\mathbf{N}_c\delta\boldsymbol{\gamma} \tag{2}$$

$$\delta\boldsymbol{\tau}_{cr} = \mathbf{H}(\boldsymbol{\gamma})\delta\boldsymbol{\gamma} \tag{3}$$

and, for a critical (i.e. potentially active) slip system,

$$\tau_k = \mathbf{N}_k\boldsymbol{\zeta} = \tau_{cr}^k \tag{4}$$

$$\delta\tau_k = \mathbf{N}_k\delta\boldsymbol{\zeta} \leq \delta\tau_{cr}^k, \qquad \delta\gamma_k \geq 0. \tag{5a,b}$$

In the above, $\boldsymbol{\zeta}$ and $\delta\boldsymbol{\xi}$ are vector representations of internal stress and infinitesimal strain. $\mathbf{C}_c$ denotes the crystal elastic compliance matrix referred to the geometric (lattice) axes and $\mathbf{A}$ (determined by the grain orientation) is the stress vector transformation matrix from the cube axes x_i to the lattice axes (an orthogonal rotation in six-dimensional stress space). $\mathbf{N}$ is the N by 6 transformation matrix from the cube axes to the local crystallographic slip systems and $\mathbf{N}_k$ is its kth row vector. The $\delta\boldsymbol{\gamma}$ are incremental plastic shears, τ_{cr}^k is a critical shear stress and $\mathbf{H}(\boldsymbol{\gamma})$ is a general crystal hardening matrix [2, 3]. (Opposite senses of slip in the same crystallographic slip system are denoted by distinct k's so that $\delta\gamma_k$ is always non-negative.) We require $\mathbf{C}_c$ (hence $\mathbf{C}$) to be positive-definite and $\mathbf{H}$ to be at least positive-semidefinite (including the null matrix—i.e. an elastic–perfectly plastic crystal model). Every critical slip system must satisfy (4) and (5a, b). An active system satisfies the equality in (5a) and the inequality in (5b).

Corresponding to these general constitutive equations, the boundary value problem of *incremental* response of the unit cube to an increment in aggregate macrostrain yields unique internal stress and strain increment fields [2]. Introducing the approximation of kinematically admissible, piecewise linear infinitesimal displacement functions, the formal solution to the discrete model of the continuum problem can be expressed in terms of the general matrix equation (from [1])

$$(\overline{\mathbf{H}}+\overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T)\delta\overline{\boldsymbol{\Gamma}}-\overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 \geq \mathbf{0} \tag{6}$$

with the equality satisfied for each active system ($\delta\bar{\gamma}_k > 0$). (In [1], the crystal tetrahedral sub-volumes V_q of (spatially) constant microstrain fields, called crystallites, are required to be of equal volume. We relax that requirement herein and so define certain of the symbols from (6) somewhat differently than in the preceding paper.) $\delta\mathbf{U}^0$ is the vector of prescribed surface displacement increments corresponding to incremental macroscopic strain $\delta\boldsymbol{\varepsilon}$, $\delta\overline{\boldsymbol{\Gamma}}^T = (\ldots, \delta\bar{\boldsymbol{\gamma}}_{(q)}^T\sqrt{V_q}, \ldots)$, $\overline{\mathbf{H}} = \lceil \mathbf{H}_{(q)} \rfloor$, $\overline{\mathbf{N}} = \lceil \mathbf{N}_c \rfloor$ and

$$\mathbf{Q} = \mathbf{S}[\mathbf{I}-\mathbf{B}_i\mathbf{K}^{-1}\mathbf{B}_i^T\mathbf{S}] \tag{7}$$

wherein $\mathbf{I}$ is an identity matrix, $\mathbf{S} = \lceil \mathbf{C}_c^{-1} \rfloor$ and $\mathbf{K} = \mathbf{B}_i^T\mathbf{S}\mathbf{B}_i$ (the symmetric, positive-definite, aggregate elastic "stiffness" matrix). 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

$$\mathbf{B}_{qJ} = \begin{cases} \mathbf{A}_{(q)}\boldsymbol{\beta}_q^J\sqrt{V_q} & \text{if } J \text{ is a node of } q \\ \mathbf{0} & \text{if } J \text{ is not a node of } q. \end{cases} \tag{8}$$

The $\boldsymbol{\beta}_q^J$ in (8) are determined from the geometry of the crystallite q. Thus [1]

$$\boldsymbol{\beta}_q^M = \mathscr{D}^T \phi_M^q(\mathbf{x}), \tag{9}$$

in which $\mathscr{D}$ is a matrix representation of the spatial gradient corresponding to the vector representations of stress and strain (whence, $\mathscr{D}^T \delta\mathbf{u} = \delta\boldsymbol{\xi}$ and $\mathscr{D}\delta\boldsymbol{\zeta} = \mathbf{0}$ in the continuum model) and

$$\phi_M^q(\mathbf{x}) = \alpha_M^q + \beta_{Mj}^q x_j. \tag{10}$$

The repeated index indicates summation and 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. [In (6), $\overline{\mathbf{H}}$, $\overline{\mathbf{N}}$ and $\delta\overline{\boldsymbol{\Gamma}}$ are defined only over those crystallites q containing potentially active slip systems.]

It is shown in [1] that the solution evaluation of (6) and (5b) can be defined as a quadratic programming problem with linear constraints and is unique (assuming no geometric dependence among critical slip systems within crystallites). We minimize the convex functional

$$I(\delta\overline{\boldsymbol{\Gamma}}) = \tfrac{1}{2}\delta\overline{\boldsymbol{\Gamma}}^T \mathbf{P}\delta\overline{\boldsymbol{\Gamma}} - \delta\overline{\boldsymbol{\Gamma}}\overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 \tag{11}$$

subject to $\delta\overline{\boldsymbol{\Gamma}} \geq \mathbf{0}$, where $\mathbf{P} = \overline{\mathbf{H}} + \overline{\mathbf{N}}\mathbf{Q}\overline{\mathbf{N}}^T$ is positive-definite over critical systems [1]. If there is such geometric dependence, $\mathbf{P}$ is positive-*semi*definite. The quadratic programming problem remains well-posed, although no longer strictly convex. The incremental stress and strain fields are still unique, but there now can be more than one set of incremental shears within a particular grain minimizing $I(\delta\overline{\boldsymbol{\Gamma}})$ and producing the same $\delta\bar{\boldsymbol{\xi}}^p$. (For a discussion of this point in relation to the continuum problem, see [2].) Since geometric dependence among critical systems is immaterial in the minimization of $I(\delta\overline{\boldsymbol{\Gamma}})$, we disregard it in the sequel.

In closing this review of the discrete model, we list the following general results (somewhat modified from [1]) which will be required in proving convergence:

$$\mathbf{K}\delta\overline{\mathbf{U}}^{(e)} = -\mathbf{B}_i^T\mathbf{S}\mathbf{B}_0\delta\mathbf{U}^0 \tag{12}$$

$$\mathbf{K}\delta\overline{\mathbf{U}}^s = \mathbf{B}_i^T\mathbf{S}\overline{\mathbf{N}}^T\delta\overline{\boldsymbol{\Gamma}} \tag{13}$$

$$\delta\overline{\mathbf{E}}^{(e)} = \overline{\mathbf{A}}^T\mathbf{S}^{-1}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 \tag{14}$$

$$\delta\overline{\boldsymbol{\Sigma}}^{(e)} = \overline{\mathbf{A}}^T\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 \tag{15}$$

$$\delta\overline{\mathbf{E}}^s = \overline{\mathbf{A}}^T\mathbf{B}_i\mathbf{K}^{-1}\mathbf{B}_i^T\mathbf{S}\overline{\mathbf{N}}^T\delta\overline{\boldsymbol{\Gamma}} \tag{16}$$

$$\delta\overline{\boldsymbol{\Sigma}}^s = -\overline{\mathbf{A}}^T\mathbf{Q}\overline{\mathbf{N}}^T\delta\overline{\boldsymbol{\Gamma}}. \tag{17}$$

$\delta\overline{\mathbf{U}}^{(e)} = (\ldots, \delta\bar{\mathbf{u}}^{(e)M}, \ldots)$ is the overall vector of unknown nodal displacements corresponding to assumed elastic response of the aggregate; $\delta\overline{\mathbf{U}}^s = (\ldots, \delta\bar{\mathbf{u}}^{(s)M}, \ldots)$ is the overall vector of "slip" displacements; $\delta\bar{\boldsymbol{\zeta}}^{(e)}$, $\delta\bar{\boldsymbol{\xi}}^{(e)}$ and $\delta\bar{\boldsymbol{\zeta}}^s$, $\delta\bar{\boldsymbol{\xi}}^s$ are the associated stress and strain increments; $\delta\overline{\boldsymbol{\Sigma}}^{(e)} = (\ldots, \delta\bar{\boldsymbol{\zeta}}_{(q)}^{(e)}\sqrt{V_q}, \ldots)$; $\delta\overline{\mathbf{E}}^{(e)} = (\ldots, \delta\bar{\boldsymbol{\xi}}_{(q)}^{(e)}\sqrt{V_q}, \ldots)$; $\delta\overline{\boldsymbol{\Sigma}}^s = (\ldots, \delta\bar{\boldsymbol{\zeta}}_{(q)}^s\sqrt{V_q}, \ldots)$; and $\delta\overline{\mathbf{E}}^s = (\ldots, \delta\bar{\boldsymbol{\xi}}_{(q)}^s\sqrt{V_q}, \ldots)$.

3. A MINIMUM PRINCIPLE AND ITS CONSEQUENCES

In [2], attention is directed to positive-definite (hence, invertible) hardening matrices, and two extremum principles are developed. As a necessary adjunct to our proof of convergence herein, we modify and slightly extend one of these principles, continuing to require only that **H** be positive-semidefinite. Thus, defining the following scalar averages over the unit cube

$$u_e = \int \delta\boldsymbol{\zeta} \,.\, \mathbf{C}\delta\boldsymbol{\zeta} \,\mathrm{d}V > 0 \tag{18}$$

$$d_p = \int \delta\boldsymbol{\zeta} \,.\, \delta\boldsymbol{\xi}^p \,\mathrm{d}V = \int \delta\boldsymbol{\gamma}^T \mathbf{H}\delta\boldsymbol{\gamma} \,\mathrm{d}V \geq 0, \tag{19}$$

and introducing the functional

$$I_1 = \tfrac{1}{2}(u_e + d_p) = \frac{1}{2}\int \delta\boldsymbol{\zeta} \,.\, \delta\boldsymbol{\xi} \,\mathrm{d}V > 0, \tag{20}$$

we establish that I_1 is an absolute minimum corresponding to the continuum solution. Let I_1^0 denote the value determined from any kinematically admissible, infinitesimal displacement field $\delta\mathbf{u}^0$. Then, as $\int \delta\boldsymbol{\zeta} \,.\, \Delta\delta\boldsymbol{\xi} \,\mathrm{d}V = 0$ (since surface tractions **T** are identically zero on S_T), we have

$$I_1^0 - I_1 = \Delta I_1 = \frac{1}{2}\int (\Delta\delta\boldsymbol{\zeta} \,.\, \delta\boldsymbol{\xi}^0 - \delta\boldsymbol{\zeta} \,.\, \Delta\delta\boldsymbol{\xi}) \,\mathrm{d}V \tag{21}$$

and, after some algebra [substituting the constitutive equations (1)–(5)],

$$I_1^0 - I_1 = \frac{1}{2}\int \{\Delta\delta\boldsymbol{\zeta} \,.\, \mathbf{C}\Delta\delta\boldsymbol{\zeta} + \Delta\delta\boldsymbol{\gamma} \,.\, \mathbf{H}\Delta\delta\boldsymbol{\gamma} + 2(\delta\boldsymbol{\tau}_{\mathrm{cr}} - \delta\boldsymbol{\tau}) \,.\, \delta\boldsymbol{\gamma}^0\} \,\mathrm{d}V. \tag{22}$$

The last term in the integrand is non-negative if the *critical* (but not necessarily the active) slip systems coincide, since the negative of the product of (5a) and (5b) is positive or zero. Whence, $I_1^0 > I_1$ (unless $\delta\mathbf{u}^0 \equiv \delta\mathbf{u}$) and we conclude that a correct basis for analytical determination of convergence of kinematically admissible approximations is the investigation of convergence *in the incremental sense*. That is, does the incremental solution of a discrete model, which proceeds from an assumed known state of stress and strain within the aggregate, converge to the incremental response of the continuum problem as we reduce element sizes within crystal grains?

Consider the functional $\bar{I}_1 = \frac{1}{2}(\bar{u}_e + \bar{d}_p)$ for the discrete model presented herein, where [from (2) and (14)–(17)]

$$\begin{aligned}\bar{u}_e &= \sum_q \delta\bar{\boldsymbol{\zeta}}_{(q)} \,.\, \mathbf{C}_{(q)}\delta\bar{\boldsymbol{\zeta}}_{(q)} V_q \\ &= (\mathbf{B}_0\delta\mathbf{U}^0 - \overline{\mathbf{N}}^T\delta\overline{\boldsymbol{\Gamma}})^T\mathbf{Q}(\mathbf{B}_0\delta\mathbf{U}^0 - \overline{\mathbf{N}}^T\delta\overline{\boldsymbol{\Gamma}}) > 0 \end{aligned} \tag{23}$$

$$\bar{d}_p = \delta\overline{\boldsymbol{\Gamma}}^T\overline{\mathbf{N}}\mathbf{Q}(\mathbf{B}_0\delta\mathbf{U}^0 - \overline{\mathbf{N}}^T\delta\overline{\boldsymbol{\Gamma}}). \tag{24}$$

From (6), (12) (14)–(17) and the above, $\bar{I}_1$ can be written

$$\bar{I}_1 = \tfrac{1}{2}\delta\overline{\mathbf{U}}^{(e)} \,.\, \mathbf{K}\delta\overline{\mathbf{U}}^{(e)} + \delta\overline{\mathbf{U}}^{(e)} \,.\, \mathbf{B}_1^T\mathbf{S}\mathbf{B}_0\delta\mathbf{U}^0 + D + \tfrac{1}{2}\delta\overline{\boldsymbol{\Gamma}}^T\mathbf{P}\delta\overline{\boldsymbol{\Gamma}} - \delta\overline{\boldsymbol{\Gamma}}^T\overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 \tag{25}$$

with $D = \frac{1}{2}(\mathbf{B}_0\delta\mathbf{U}^0)^T\mathbf{S}(\mathbf{B}_0\delta\mathbf{U}^0)$, a constant. Since the displacement fields leading to the solution equation (6) are kinematically admissible, $\bar{I}_1 > I_1$. Let I_1^* denote the functional obtained by substituting into (25) the actual displacement values at the nodes and the average values $\delta\boldsymbol{\gamma}_{(q)}$ of the actual incremental plastic shear fields within the crystallite regions (i.e. $\delta\boldsymbol{\gamma}_{(q)}V_{(q)} = \int \delta\boldsymbol{\gamma}\,\mathrm{d}V_q$ for each q). Thus

$$I_1^* = \tfrac{1}{2}\delta\mathbf{U}^{(e)} \,.\, \mathbf{K}\delta\mathbf{U}^{(e)} + \delta\mathbf{U}^{(e)} \,.\, \mathbf{B}_1^T\mathbf{S}\mathbf{B}_0\delta\mathbf{U}^0 + D + \tfrac{1}{2}\delta\boldsymbol{\Gamma}^T\mathbf{P}\delta\boldsymbol{\Gamma} - \delta\boldsymbol{\Gamma}^T\overline{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0. \tag{26}$$

From (5b) and (6),

$$\delta\bar{\mathbf{\Gamma}}^T\mathbf{P}\delta\bar{\mathbf{\Gamma}} = \delta\bar{\mathbf{\Gamma}}^T\bar{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 \tag{27}$$

$$\delta\mathbf{\Gamma}\,.\,(\mathbf{P}\delta\bar{\mathbf{\Gamma}}-\bar{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0) \geq 0. \tag{28}$$

Therefore, with the aid of (12) and the above,

$$\begin{aligned} I_1^* - \bar{I}_1 = {} & \tfrac{1}{2}(\delta\mathbf{U}^{(e)}-\delta\bar{\mathbf{U}}^{(e)})^T\mathbf{K}(\delta\mathbf{U}^{(e)}-\delta\bar{\mathbf{U}}^{(e)})+\tfrac{1}{2}(\delta\mathbf{\Gamma}-\delta\bar{\mathbf{\Gamma}})^T\mathbf{P}(\delta\mathbf{\Gamma}-\delta\bar{\mathbf{\Gamma}}) \\ & +\delta\mathbf{\Gamma}\,.\,(\mathbf{P}\delta\bar{\mathbf{\Gamma}}-\bar{\mathbf{N}}\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0) > 0 \end{aligned} \tag{29}$$

so that

$$I_1^* > \bar{I}_1 > I_1 > 0. \tag{30}$$

To establish convergence it is sufficient to prove that I_1^*, hence $\bar{I}_1$, converges to I_1.

4. A CONVERGENCE PROOF FOR THE DISCRETE AGGREGATE MODEL

Utilizing (8), (15), (19), (23) and the element strain–displacement relation [1]

$$\delta\bar{\boldsymbol{\xi}}_{(q)} \equiv \mathscr{D}^T\delta\bar{\mathbf{u}}_{(q)}(\mathbf{x}) = \sum_{M(q)} \boldsymbol{\beta}_q^M\delta\bar{\mathbf{u}}^M, \tag{31}$$

we define the following scalar averages:

$$\omega_e^* = \int\delta\boldsymbol{\xi}^{*(e)}\,.\,\mathbf{C}^{-1}\delta\boldsymbol{\xi}^{*(e)}\,\mathrm{d}V = (\mathbf{B}_i\delta\mathbf{U}^{(e)}+\mathbf{B}_0\delta\mathbf{U}^0)^T\mathbf{S}(\mathbf{B}_i\delta\mathbf{U}^{(e)}+\mathbf{B}_0\delta\mathbf{U}^0) > 0 \tag{32}$$

$$\bar{\omega}_e = \int\delta\bar{\boldsymbol{\xi}}^{(e)}\,.\,\mathbf{C}^{-1}\delta\bar{\boldsymbol{\xi}}^{(e)}\,\mathrm{d}V = (\mathbf{B}_0\delta\mathbf{U}^0)^T\mathbf{Q}\mathbf{B}_0\delta\mathbf{U}^0 > 0 \tag{33}$$

$$u_e^* = (\mathbf{B}_0\delta\mathbf{U}^0-\bar{\mathbf{N}}^T\delta\mathbf{\Gamma})^T\mathbf{Q}(\mathbf{B}_0\delta\mathbf{U}^0-\bar{\mathbf{N}}^T\delta\mathbf{\Gamma}) > 0 \tag{34}$$

$$d_p^* = \sum_q \delta\boldsymbol{\gamma}_{(q)}^T\mathbf{H}_{(q)}\delta\boldsymbol{\gamma}_{(q)}V_q = \delta\mathbf{\Gamma}^T\bar{\mathbf{H}}\delta\mathbf{\Gamma} \geq 0 \tag{35}$$

in which

$$\delta\boldsymbol{\xi}^{*(e)}_{(q)} \equiv \mathscr{D}^T\delta\mathbf{u}^{*(e)}_{(q)} = \sum_{M(q)} \boldsymbol{\beta}_q^M\delta\mathbf{u}^{(e)M}$$

such that

$$\delta\boldsymbol{\xi}^{*(e)} = \delta\boldsymbol{\xi}^{(e)}+\mathbf{O}(h), \tag{36}$$

where h is a typical crystallite dimension and $\mathbf{O}(h)$ indicates the truncation error in the Taylor series expansion. Then, from (26) and (32–35), I_1^* can be equivalently expressed

$$I_1^* = \tfrac{1}{2}(\omega_e^*-\bar{\omega}_e)+\tfrac{1}{2}(u_e^*+d_p^*). \tag{37}$$

We first investigate convergence to zero of the first term, corresponding to solutions assuming elastic response of the aggregate. Denoting

$$\omega_e = \int\delta\boldsymbol{\xi}^{(e)}\,.\,\mathbf{C}^{-1}\delta\boldsymbol{\xi}^{(e)}\,\mathrm{d}V, \tag{38}$$

it is obvious from (32), (36) and (38) that $\omega_e^* = \omega_e + 0(h)$. Also, from (29),

$$\omega_e^* - \bar{\omega}_e = (\delta\mathbf{U}^{(e)} - \delta\bar{\mathbf{U}}^{(e)})^T\mathbf{K}(\delta\mathbf{U}^{(e)} - \delta\bar{\mathbf{U}}^{(e)}) > 0 \tag{39}$$

and, from (12), (33) and (38), $\bar{\omega}_e > \omega_e$ (the ordinary elasticity minimum principle). Therefore, $\omega_e + 0(h) = \omega_e^* > \bar{\omega}_e > \omega_e > 0$ and [(12), (33), (39)]

$$0(h) > \bar{\omega}_e - \omega_e > \int \Delta\delta\boldsymbol{\zeta}^{(e)} . \mathbf{C}\Delta\delta\boldsymbol{\zeta}^{(e)} \,\mathrm{d}V > 0 \tag{40}$$

from which ω_e^* and $\bar{\omega}_e$ converge to ω_e with decreasing h and $\delta\bar{\boldsymbol{\zeta}}^{(e)}$ converges to $\delta\boldsymbol{\zeta}^{(e)}$. (This is analogous to the proof of convergence of the "finite element method" for linear elasticity problems given in [4].)

Returning to (37), it is evident from (35) and the definition of $\delta\boldsymbol{\gamma}_{(q)}$ that d_p^* converges to d_p, since the integrand converges locally over each crystallite. [We take $\mathbf{H}_{(q)} = \mathbf{H}(\boldsymbol{\gamma}_{(q)})$, where $\boldsymbol{\gamma}_{(q)}$ is similarly defined as the volume average of $\boldsymbol{\gamma}(\mathbf{x})$ over the crystallite.] It remains to prove that u_e^* converges to u_e. From (7), (15) and (34),

$$u_e^* = (\delta\bar{\boldsymbol{\Sigma}}^{(e)} + \delta\hat{\boldsymbol{\Sigma}}^s)^T\bar{\mathbf{A}}^T\mathbf{S}^{-1}\bar{\mathbf{A}}(\delta\bar{\boldsymbol{\Sigma}}^{(e)} + \delta\hat{\boldsymbol{\Sigma}}^s) = \sum_q(\delta\bar{\boldsymbol{\zeta}}_{(q)}^{(e)} + \delta\hat{\boldsymbol{\zeta}}_{(q)}^s)^T\mathbf{C}_{(q)}(\delta\bar{\boldsymbol{\zeta}}_{(q)}^{(e)} + \delta\hat{\boldsymbol{\zeta}}_{(q)}^s)V_q > 0 \tag{41}$$

where

$$\delta\hat{\boldsymbol{\Sigma}}^s = -\bar{\mathbf{A}}^T\mathbf{Q}\bar{\mathbf{N}}^T\delta\boldsymbol{\Gamma} = -\bar{\mathbf{A}}^T\mathbf{Q}\bar{\mathbf{A}}\delta\mathbf{E}^p. \tag{42}$$

Since, from the preceding analysis, $\delta\bar{\boldsymbol{\zeta}}^{(e)} \to \delta\boldsymbol{\zeta}^{(e)}$ with decreasing h, we focus attention on $\delta\hat{\boldsymbol{\zeta}}_{(q)}^s$. The continuum fields $\delta\boldsymbol{\zeta}^s$, $\delta\boldsymbol{\xi}^s$ correspond to the incremental elastic response of the *constrained* cube due to the plastic "residual" microstrain field $\delta\boldsymbol{\xi}^p = \mathbf{N}^T\delta\boldsymbol{\gamma}$ (with $\int\delta\boldsymbol{\zeta}^s . \delta\boldsymbol{\xi}^s \,\mathrm{d}V = 0$). Denoting the strain field determined from the solution of the piecewise linear displacement model by $\delta\hat{\boldsymbol{\xi}}^s$, we have, analogous to (13) and consistent with (42),

$$\mathbf{K}\delta\hat{\mathbf{U}}^s = \mathbf{B}_1^T\mathbf{S}\bar{\mathbf{N}}^T\delta\boldsymbol{\Gamma} \tag{43}$$

so that, locally, $\delta\hat{\boldsymbol{\zeta}}_{(q)}^s = \mathbf{C}_{(q)}^{-1}(\delta\hat{\boldsymbol{\xi}}_{(q)}^s - \mathbf{N}_{(q)}^T\delta\boldsymbol{\gamma}_{(q)})$, as can be confirmed by substituting (7) into (42). The corresponding potential energy functional of the discrete solution is

$$\hat{I}_2 = \frac{1}{2}\int \delta\hat{\boldsymbol{\xi}}^s . \mathbf{C}^{-1}\delta\hat{\boldsymbol{\xi}}^s \,\mathrm{d}V - \int \delta\hat{\boldsymbol{\xi}}^s . \mathbf{C}^{-1}\delta\boldsymbol{\xi}^p \,\mathrm{d}V = \frac{1}{2}\delta\hat{\mathbf{U}}^s . \mathbf{K}\delta\hat{\mathbf{U}}^s - \delta\hat{\mathbf{U}}^s . \mathbf{B}_1^T\mathbf{S}\bar{\mathbf{N}}^T\delta\boldsymbol{\Gamma}, \tag{44}$$

and of the continuum solution

$$I_2 = \frac{1}{2}\int \delta\boldsymbol{\xi}^s . \mathbf{C}^{-1}\delta\boldsymbol{\xi}^s \,\mathrm{d}V - \int \delta\boldsymbol{\xi}^s . \mathbf{C}^{-1}\delta\boldsymbol{\xi}^p \,\mathrm{d}V = -\frac{1}{2}\int \delta\boldsymbol{\xi}^s . \mathbf{C}^{-1}\delta\boldsymbol{\xi}^s \,\mathrm{d}V, \tag{45}$$

whence [(43)–(45)],

$$\hat{I}_2 - I_2 = \frac{1}{2}\int (\delta\hat{\boldsymbol{\xi}}^s - \delta\boldsymbol{\xi}^s) . \mathbf{C}^{-1}(\delta\hat{\boldsymbol{\xi}}^s - \delta\boldsymbol{\xi}^s) \,\mathrm{d}V > 0. \tag{46}$$

Defining

$$I_2^* = \frac{1}{2}\int \delta\boldsymbol{\xi}^{*s} . \mathbf{C}^{-1}\delta\boldsymbol{\xi}^{*s} \,\mathrm{d}V - \int \delta\boldsymbol{\xi}^{*s} . \mathbf{C}^{-1}\delta\boldsymbol{\xi}^p \,\mathrm{d}V \tag{47}$$

in which, similarly as in (36), $\delta\xi^{*s} = \delta\xi^s + 0(h)$, with $\delta\xi^{*s}_{(q)} = \sum_{M(q)} \beta_q^M \delta u^{(s)M}$, then $I_2^* = I_2 + 0(h)$. I_2^* also can be expressed, analogous to (44),

$$I_2^* = \tfrac{1}{2}\delta U^s . K\delta U^s - \delta U^s . B_1^T S \bar{N}^T \delta\Gamma. \tag{48}$$

Therefore [(43), (44), (48)],

$$I_2^* - \hat{I}_2 = \tfrac{1}{2}(\delta U^s - \delta\hat{U}^s)^T K(\delta U^s - \delta\hat{U}^s) > 0. \tag{49}$$

Hence, $I_2 + 0(h) = I_2^* > \hat{I}_2 > I_2$ and $\hat{I}_2 \to I_2$ as $h \to 0$. Moreover, substituting (46),

$$0(h) > \frac{1}{2}\int (\delta\hat{\xi}^s - \delta\xi^s) . C^{-1}(\delta\hat{\xi}^s - \delta\xi^s)\, dV > 0. \tag{50}$$

It follows that $\delta\hat{\xi}^s \to \delta\xi^s$, $\delta\hat{\zeta}^s \to \delta\zeta^s$ and, with the results from (40), u_e^* converges to u_e. Thus, from (30), I_1^* and $\bar{I}_1$ converge to I_1 and, from (29), since $\mathbf{P}$ is positive-definite, $\delta\bar{\gamma}_{(q)} \to \delta\gamma_{(q)}$. Finally, from (22), reading $\bar{I}_1$ in place of the more general I_1^0, $\delta\bar{\zeta} \to \delta\zeta$ and the volume average converges to the incremental macrostress $\delta\sigma$, the desired result. (Q.E.D.)

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Абстракт—Расширается и аналиризуется далее дискретная аггрегатная модель, недавно предложенная автором [1], в смысле основы для качественных исследований в поликристаллической пластичности. Поля дискретизованных внутренних напряжений и приращений деформации, однозначно определенные ие решения задачи ограниченного квадратичного программирования, оказываются точно сходимыми к решению соответствующей краевой задачи сплошной среды. Затем, эта модель точно подтверждена как рациональное приближение пригодное для расчетных исследований поведения аггрегатной модели.