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# CONTINUUM MICRO-MECHANICS OF ELASTOPLASTIC POLYCRYSTALS

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**THE** internal inhomogeneities of stress and strain in an arbitrarily deformed aggregate of elasto-plastic crystals are evaluated theoretically. A tensor constitutive law of a general kind is assumed for the individual crystals. The implied mechanical properties of the aggregate as a whole are estimated by means of a self-consistent model akin to one used by HERSHEY (1954), KRÖNER (1958, 1961) and BUDIANSKY and WU (1962), but differing in significant respects.

## 1. INTRODUCTION

IN CONTINUUM mechanics of solids a basic problem of long standing is to correlate polycrystal and monocrystal behaviour under plastic strain. Specifically, supposing the shapes, orientations, and mechanical states of all grains in an aggregate known at some stage, at least in a statistical sense, it is required to derive the isothermal constitutive relations for the aggregate as a whole. These are the tensor connexions between arbitrary differential increments of overall stress and quasi-static strain, formed as space averages of the field variables. Once the incremental fields have been determined somehow, the accompanying changes in the geometry and state of all grains follow from the given monocrystal properties. In this way the total effect of a continuing process of overall deformation can in principle be analysed step by step.

The incremental behaviour at a generic stage, however, is the sole object of interest here. Neither the preceding strain path nor the existing pattern of local stress and lattice orientation are particularized. Correspondingly, a constitutive relation of sufficiently general type is adopted for a typical grain, capable of representing any actual mechanism of plastic flow. The aim is to construct a broad theoretical framework for rationalizing observations on metal polycrystals at ordinary temperatures. Computations for particular aggregates are deferred and the present conclusions are mainly qualitative.

It is regarded as being of the essence of the problem to take due account of the inhomogeneity of the distortion within a polycrystal. In fact, the primary task of the analysis will be to determine the average strain concentration factor in grains with a given lattice orientation. For this purpose we follow in spirit the 'self-consistent' method originated independently by HERSHEY (1954) and KRÖNER (1958) for elastically deformed aggregates. However, it has been found necessary to re-appraise the method and to systematize its details. An extension to plastically

deformed aggregates is then formulated. This differs fundamentally from one also due to KRÖNER (1961), which was developed by BUDIANSKY and WU (1962) and HUTCHINSON (1964).

## 2. SYMBOLIC NOTATION

In order to let the essential structure of subsequent formulae appear more clearly, a familiar symbolic notation is adopted for curvilinear tensors.

Associated tensors of second order are denoted simply by their kernel letter,  $\mathbf{u}$  say, set in lower case boldface as if for a vector. Correspondingly, their tensor components in any representation are considered to be arranged in some definite sequence as a  $9 \times 1$  column. Associated tensors of fourth order are denoted by an ordinary capital,  $A$  say, and are regarded as  $9 \times 9$  matrices. More precisely, the leading pair of indices is set in correspondence with rows and the terminal pair with columns, both in the chosen sequence, so that the second-order inner product of tensors  $A$  and  $\mathbf{u}$  can be written as the matrix product  $A\mathbf{u}$ . Similarly,  $AB$  can stand for the fourth-order inner product of  $A$  and  $B$ . Subsequent formulae can be interpreted in terms of tensor components in any representation, so long as it be done consistently.

A special word is needed in regard to inverses of fourth-order tensors  $A$ , which are here always symmetric with respect to interchange of the leading pair of indices and also of the terminal pair. The representative matrices are thus singular, with rank  $\leq 6$ ; for instance,  $As$  vanishes identically when  $s$  is the column for any skew second-order tensor. Nevertheless, equations of type  $\mathbf{u} = A\mathbf{v}$  are compatible when  $\mathbf{u}$  and  $\mathbf{v}$  are any *symmetric* second-order tensors and matrix  $A$  has rank 6. In this sense we can define a unique inverse  $A^{-1}$  as the solution of

$$AA^{-1} = I \quad \text{or} \quad A^{-1}A = I,$$

where  $I$  is a 'unit' matrix with the symmetries of  $A$  and with mixed tensor components

$$\frac{1}{2} (\delta_{k^i} \delta_{l^j} + \delta_{l^i} \delta_{k^j})$$

in terms of the Kronecker delta. Then

$$A^{-1}\mathbf{u} = A^{-1}A\mathbf{v} = I\mathbf{v} = \mathbf{v}$$

as required, for any  $A$ ,  $\mathbf{u}$  and  $\mathbf{v}$  with the stated properties.

## 3. AN AUXILIARY PROBLEM

(i) A single crystal, arbitrarily ellipsoidal in shape, is imagined to be embedded in a finite homogeneous mass of some different material. Neither phase is necessarily elastic or isotropic, but in each the invariant relationship between an objective stress-rate  $\dot{\tau}$  and the strain-rate  $\epsilon$  is supposed to be one-one and linear. The tensors of instantaneous moduli are denoted by  $L_e$  and  $L$ , respectively, and their inverse compliances by  $M_e$  and  $M$ . In addition to the symmetries mentioned already, the representative matrices are required to have full diagonal symmetry so that the cross-moduli and compliances are pairwise equal. A further minimal restriction is that the respective quadratic forms,  $\mathbf{u}(L\mathbf{u})$  etc., in any second-order tensor  $\mathbf{u}$  of rank 1 are positive.

On the external surface the velocity is prescribed to correspond to a uniform overall strain-rate  $\bar{\epsilon}$ . Primarily, we seek the deformation induced within the crystal, given that the velocity and traction-rate are continuous across the interface. To be definite, stress-rate is taken to be the convected time-derivative of contravariant Kirchhoff stress, based on the current configuration. In the absence of body forces this satisfies the equilibrium equations

$$\frac{\partial}{\partial x^i} \left( \dot{\tau}^{ij} + \tau^{ik} \frac{\partial v^j}{\partial x^k} \right) = 0$$

where  $v^j$  is velocity,  $\partial \tau^{ik} / \partial x^i = 0$  since the existing stress is self-equilibrated, and  $x^i$  is a rectangular coordinate. The convective term would vanish identically in a field of uniform straining and will in any event be disregarded, presuming the existing stress to be a sufficiently small fraction of the dominant moduli. This approximation is permissible since Hadamard instability, which would involve local spins large compared with the strain-rates, is prevented by the minimal restrictions placed on the moduli (HILL 1962, § 4 (ii)). Moreover, these same restrictions also ensure a unique solution (*op. cit.* § 4 (iii)), which can therefore be expected to have the character of a uniform field locally perturbed in the neighbourhood of the crystal. In particular the overall, or macroscopic, stress-rate  $\dot{\bar{\tau}}$  is then equal to  $L\bar{\epsilon}$ , since the contribution from the crystal becomes vanishingly small when the outer phase is sufficiently extensive. Furthermore,  $\dot{\bar{\tau}}$  and  $\bar{\epsilon}$  are also approached asymptotically by the local field values at the external surface.

It is plain that the solution is formally identical with that of the analogous displacement problem in linearized elasticity when both materials are Green-elastic. In that context the solution is well known in outline when the outer phase can be treated as unbounded. Its principal feature is that the ellipsoid is strained uniformly, though not necessarily coaxially (ESHELBY 1957; 1961).

This property prompts the introduction of an 'overall constraint' tensor  $L^*$  for the outer phase, with inverse  $M^*$ , in respect of loading over the interface by any distribution of traction-rate compatible with a uniform field of stress-rate,  $\dot{\tau}^*$  say. That is, if  $\epsilon^*$  is the accompanying uniform rate of straining of the ellipsoid,

$$\dot{\tau}^* = -L^* \epsilon^*, \quad \epsilon^* = -M^* \dot{\tau}^*. \quad (1)$$

The corresponding matrices have of course diagonal symmetry, as may easily be shown by Betti's reciprocal theorem, and are functions of  $L$  or  $M$  and the aspect ratios of the ellipsoid. Once  $L^*$  and  $M^*$  have been determined, the solution of the auxiliary problem follows by superimposing the uniform fields  $\dot{\bar{\tau}}$  and  $\bar{\epsilon}$ , and identifying  $\dot{\tau}^*$  with  $\dot{\tau}_c - \dot{\bar{\tau}}$  and  $\epsilon^*$  with  $\epsilon_c - \bar{\epsilon}$ . Then

$$\begin{aligned} \dot{\tau}_c - \dot{\bar{\tau}} &= L^* (\bar{\epsilon} - \epsilon_c), & \epsilon_c - \bar{\epsilon} &= M^* (\dot{\bar{\tau}} - \dot{\tau}_c), \\ \text{or} & & & \\ L^* \epsilon_c + \dot{\tau}_c &= (L^* + L) \bar{\epsilon}, & M^* \dot{\tau}_c + \epsilon_c &= (M^* + M) \dot{\bar{\tau}}. \end{aligned} \quad \left. \vphantom{\begin{aligned} \dot{\tau}_c - \dot{\bar{\tau}} &= L^* (\bar{\epsilon} - \epsilon_c), \\ L^* \epsilon_c + \dot{\tau}_c &= (L^* + L) \bar{\epsilon}, \end{aligned}} \right\} \quad (2)$$

Finally,

$$(L^* + L_c) \epsilon_c = (L^* + L) \bar{\epsilon}, \quad (M^* + M_c) \dot{\tau}_c = (M^* + M) \dot{\bar{\tau}}, \quad (3)$$

which furnish the required fields in the crystal in terms of the macroscopic quantities. It seems that this attractively direct approach has not been adopted by other writers, with apparently the single exception of HERSHEY (1954), who, however, did not emphasize its advantages.

(ii) Instead, following ESHELBY (1957), it has become customary to focus attention on the entire two-phase system, starting from a certain transformation problem for an infinite homogeneous elastic continuum with stiffness tensor  $L^\dagger$ . In this, an ellipsoidal region would undergo an infinitesimal transformation strain  $e$  if free, but attains only the strain  $Se$  *in situ*. The tensor  $S$  is determinable uniquely, by virtue of the minimal restriction on  $L$ , and it obviously possesses an inverse  $S^{-1}$  since  $e$  vanishes with  $Se$  (no stress being then induced outside the transformed region nor therefore within it). The  $x^i$  components of  $S$ , being dimensionless, are functions of the moduli ratios and of the aspect ratios of the ellipsoid and its orientation in the frame of reference. When  $L$  is isotropic, explicit formulae for the components on the ellipsoid axes have been given by Eshelby (*op. cit.*). Formulae for the two-dimensional analogue have been given recently by BHARGAVA and RADHAKRISHNA (1964) when the medium is orthotropic and by WILLIS (1964) when it has cubic symmetry. For general anisotropy the basis for a three-dimensional solution was sketched by ESHELBY (1951, p. 105)†.

The general connexion with  $L^*$  or  $M^*$  is most easily obtained by imagining the transformation problem solved from the viewpoint of (1), interpreted in an elastic context. That is, we substitute

$$e^* = Se, \quad \tau^* = L(e^* - e) \text{ in } \tau^* = -L^* e^*.$$

Then, since these hold for all  $e$ ,

$$L^* S = L(I - S), \quad (I - S) M^* = SM, \quad (4)$$

where  $I$  is the unit tensor defined in § 2. These are equivalent formulae for  $L^*$  or  $M^*$  in terms of  $S$ . Or they can be put inversely as

$$S = (L^* + L)^{-1} L = M^* (M^* + M)^{-1}$$

for  $S$  in terms of  $L^*$  or  $M^*$ .

Another dimensionless tensor  $T$ , the dual of  $S$ , could just as well be admitted on this footing. Set

$$\left. \begin{aligned} M^* T &= SM = P, \text{ say,} \\ TL &= L^* S = Q, \text{ say,} \end{aligned} \right\} \quad (5)$$

so that

$$\left. \begin{aligned} M^* T &= M(I - T), \quad (I - T) L^* = TL, \\ T &= L^* (L^* + L)^{-1} = (M^* + M)^{-1} M. \end{aligned} \right\} \quad (6)$$

The significance of  $T$  is that the stress  $\tau^*$  in the transformed region can be written as  $T\tau$ , where  $\tau$  is the stress that would remove the strain  $e$ . Separate symbols  $P$  and  $Q$  have been introduced for the products in (5) since these appear frequently in the sequel. We note the further connexions

†Pre-occupation with this standpoint can lead to needlessly devious derivations. An extreme example is to be found in several papers by BHARGAVA and RADHAKRISHNA (1963a, b; 1964) on the two-dimensional auxiliary problem. The elastic field outside the ellipse is actually obtained by exact analysis at the outset, from which  $L^*$ ,  $M^*$  and the compatible internal field could forthwith be read off, but are not. Instead, the total potential energy of both phases is laboriously computed for any final internal strain, and afterwards minimized as a means of satisfying the remaining requirement of traction continuity at the interface.

‡WILLIS (1964, private communication) has developed this into a feasible numerical procedure by reducing the integrals.

$$\left. \begin{aligned} PL + MQ &= I, \\ P &= M(I - T), \quad Q = L(I - S), \\ \text{and } P^{-1} &= L^* + L, \quad Q^{-1} = M^* + M. \end{aligned} \right\} \quad (7)$$

From the latter pair one sees that matrices  $P$  and  $Q$  have the diagonal symmetry stipulated for the moduli and compliances (while  $S$  and  $T$  generally do not). This can of course also be established purely within the context of the transformation problem by means of Betti's reciprocal theorem.

(iii) We return to the original auxiliary problem. As in a related situation (HILL 1963) it is advantageous to define 'concentration-factor tensors'  $A_c$  and  $B_c$  such that

$$\epsilon_c = A_c \bar{\epsilon}, \quad \dot{\tau}_c = B_c \dot{\bar{\tau}}, \quad (8)$$

with the consequent inter-relations

$$L_c A_c = B_c L, \quad M_c B_c = A_c M. \quad (9)$$

From (8),

$$A_c = (L^* + L_c)^{-1} (L^* + L), \quad B_c = (M^* + M_c)^{-1} (M^* + M), \quad (10)$$

in terms of the overall constraint of the outer phase. Eliminating this with the help of (7), we have the variants

$$A_c^{-1} = I + P(L_c - L), \quad B_c^{-1} = I + Q(M_c - M), \quad (11)$$

in terms of the explicit differences between the phase properties, and involving quantities directly to do with the transformation problem.

#### 4. POLYCRYSTAL ELASTICITY

(i) We consider polycrystals whose geometry is such that the grains can be treated, on average, either as variously-sized spheres or as similar ellipsoids (in particular elliptic cylinders) with their corresponding axes aligned. On the other hand, the lattice orientation in the cartesian frame of reference may vary from grain to grain, not necessarily randomly.

Tensors  $L_c$  and  $M_c$  will now denote the stiffness and compliance of a typical crystal, in respect of incremental 'elastic' strain (not an essential interpretation, as remarked in §3 (i)). In the auxiliary problem  $L$  and  $M$  become the overall tensors for the polycrystal itself, while  $L^*$ ,  $M^*$ ,  $S$  and  $T$  specifically relate to the sphere or ellipsoid representing the average grain shape. Consequently, in a common frame of reference, the components of  $L$ ,  $M$ ,  $L^*$ ,  $M^*$ ,  $S$ ,  $T$ ,  $P$ ,  $Q$  are constants, whereas the components of  $L_c$ ,  $M_c$ ,  $A_c$ ,  $B_c$  depend on local lattice orientation.

In the 'self-consistent' method due to HERSHEY (1954), and independently to KRÖNER (1958), the stress field around a grain in the auxiliary problem is taken to be representative of the actual neighbouring field in the polycrystal, averaged for all grains of that orientation. Further, and more explicitly, it is postulated that a certain macroscopic tensor quantity should be obtained as the average, over the relevant range of lattice orientations, of the corresponding local tensor for a grain in the auxiliary problem. But which quantity should be singled out

for this treatment has perhaps seemed arbitrary hitherto : Kröner examined two possibilities, only one of which was tried by Hershey, while ESHELBY (1961, § 6) proposed yet a third. Still other choices are equally natural. By means of (2), however, it is a simple matter to establish their equivalence, thus finally justifying the description 'self-consistent.'

To begin with, suppose that the macroscopic strain-rate is taken as the average of the crystal strain-rate in the family of auxiliary problems. Then, from (8) and afterwards (9),

$$\{A_c\} = I \rightarrow M = \{M_c B_c\} \quad (12)$$

where orientation averages are indicated by enclosure within curly brackets. Alternatively, dual operations with stress-rate give

$$\{B_c\} = I \rightarrow L = \{L_c A_c\}. \quad (13)$$

That such dual approaches are equivalent can be seen at a glance from (2) : the leading equation states an invariant linear relation between deviations from the respective means, and so the average deviations necessarily vanish together.

If, now, one wished to transform equations (12) by means of (10), they could first be put as

$$\{(A_c^{-1} - I) A_c\} = 0, \quad \{(M_c - M B_c^{-1}) B_c\} = 0,$$

from which

$$P\{(L_c - L) A_c\} = 0, \quad S\{(M_c - M) B_c\} = 0.$$

Treating (13) similarly,

$$Q\{(M_c - M) B_c\} = 0, \quad T\{(L_c - L) A_c\} = 0.$$

The matrix factors  $P$ ,  $Q$ ,  $S$ ,  $T$  are non-singular and can be dropped. It is then apparent that not only are (12) and (13) equivalent to one another but also to each of

$$\{(L_c - L) A_c\} = 0, \quad \{(M_c - M) B_c\} = 0. \quad (14)$$

In fact, as they stand, these are just the averages of the dual 'polarization tensors' :

$$\begin{aligned} \{\dot{\epsilon}_c - L \epsilon_c\} &= (L^* + L) \{\bar{\epsilon} - \epsilon_c\} = 0, \\ \{\epsilon_c - M \dot{\epsilon}_c\} &= (M^* + M) \{\dot{\bar{\epsilon}} - \dot{\epsilon}_c\} = 0, \end{aligned}$$

obtained directly from (2).

Returning again to (12) and (13), and combining them in turn with (11) :

$$\{[I + P(L_c - L)]^{-1}\} = I, \quad \{[I + Q(M_c - M)]^{-1}\} = I. \quad (15)$$

Alternatively, by combining (14) and (11),

$$\{[P + (L_c - L)^{-1}]^{-1}\} = 0, \quad \{[Q + (M_c - M)^{-1}]^{-1}\} = 0. \quad (16)$$

While these four variants are equivalent, as already proved, it may in practice be slightly more convenient to proceed from one in preference to the others. In any event the final result of carrying out the appropriate averaging is a set of algebraic equations just sufficient to determine the separate components of  $L$  or  $M$ , in terms of matrices  $P$  and  $Q$  furnished by the solution of the transformation problem.

On the other hand, if the primary datum is the constraint tensor of the outer phase in the auxiliary problem, a possible starting-point would be either of

$$\{(L_c - L)(L^* + L_c)^{-1}\} = 0, \quad \{(M_c - M)(M^* + M_c)^{-1}\} = 0, \quad (17)$$

from (10) with (14). The equivalence with (16) can be checked at once by means of (7). More attractive variants are

$$(L^* + L)^{-1} = \{(L^* + L_c)^{-1}\}, \quad (M^* + M)^{-1} = \{(M^* + M_c)^{-1}\}, \quad (18)$$

from (10) with (12) and (13) respectively. Or these can be 'solved' as

$$L = \{(L^* + L_c)^{-1}\}^{-1} - L^*, \quad M = \{(M^* + M_c)^{-1}\}^{-1} - M^*.$$

(ii) It appears that the self-consistent method has so far been applied numerically only when the grains are spheres and the lattice orientation is random. Tensors  $L$  and  $M$  are then isotropic and can be written in the symbolic notation as

$$L = 3\kappa \mathbf{i} \mathbf{i}' + 2\mu (I - \mathbf{i} \mathbf{i}'),$$

$$M = \frac{1}{3\kappa} \mathbf{i} \mathbf{i}' + \frac{1}{2\mu} (I - \mathbf{i} \mathbf{i}'),$$

or still more shortly as

$$L \equiv (3\kappa, 2\mu), \quad M \equiv \left(\frac{1}{3\kappa}, \frac{1}{2\mu}\right), \quad (19)$$

where  $\kappa$  and  $\mu$  are the usual bulk and shear moduli. Column  $\mathbf{i}$  is the 'unit vector' representing  $\delta_{ij}/\sqrt{3}$ , and the row  $\mathbf{i}'$  is its transpose, so that  $\mathbf{i}' \mathbf{i} = 1$ . Clearly, matrices  $\mathbf{i} \mathbf{i}'$  and  $I - \mathbf{i} \mathbf{i}'$  represent isotropic operators that decompose a second-order tensor, such as stress or strain, into its hydrostatic and deviatoric parts. They also have the properties

$$(\mathbf{i} \mathbf{i}')^2 = \mathbf{i} \mathbf{i}', \quad \mathbf{i} \mathbf{i}' (I - \mathbf{i} \mathbf{i}') = 0, \quad (I - \mathbf{i} \mathbf{i}')^2 = I - \mathbf{i} \mathbf{i}'.$$

It follows that the product of any pair of isotropic fourth-order tensors is isotropic and commutative, and that the coefficients in its decomposition are just the respective products of the original components. For instance, the order of factors in any product in (4), (5) and (6) can be reversed, with the consequence that  $T = I - S$  and

$$\left. \begin{aligned} S &\equiv (\alpha, \beta) \text{ say } \dagger, & T &\equiv (1 - \alpha, 1 - \beta), \\ P &\equiv \left(\frac{\alpha}{3\kappa}, \frac{\beta}{2\mu}\right), & Q &\equiv (3\kappa(1 - \alpha), 2\mu(1 - \beta)), \\ L^* &\equiv \left(\frac{3\kappa}{\alpha}(1 - \alpha), \frac{2\mu}{\beta}(1 - \beta)\right), & M^* &\equiv \left(\frac{\alpha}{3\kappa(1 - \alpha)}, \frac{\beta}{2\mu(1 - \beta)}\right), \\ &\equiv 2\mu \left(2, \frac{1 - \beta}{\beta}\right), & &\equiv \frac{1}{2\mu} \left(\frac{1}{2}, \frac{\beta}{1 - \beta}\right). \end{aligned} \right\} \quad (20)$$

Equally, the average of any orientation-dependent fourth-order quantity, with matrix  $Z$  say, is isotropic and can be similarly decomposed :

$$\{Z\} \equiv (\xi, \eta) \text{ where } \xi = \text{tr}(Z \mathbf{i} \mathbf{i}'), \quad \xi + 5\eta = \text{tr} Z,$$

$\dagger$ The actual values are  $\alpha = 3 - 5\beta = \kappa/(\kappa + \frac{4}{3}\mu)$  [see, for example, ESHELBY (1957)].



where 'tr' stands for trace (i.e. sum of elements in the principal diagonal). Coefficients  $\xi$ ,  $\eta$  are invariants and can therefore be evaluated from the cartesian components of  $\mathbf{Z}$  for *any* convenient lattice orientation. In this way each of the equivalent relations (15), (16), (17) or (18), when averaged in form  $\{\mathbf{Z}\} = 0$ , is reduced to a pair of simultaneous algebraic equations  $\xi = 0 = \eta$  in the overall moduli  $\kappa$  and  $\mu$ .

Kröner and Hershey, starting in effect from the second of (13), arrived respectively at the second of (15) and (18), both of which yield a quartic equation  $\eta = 0$  for  $\mu$  alone when the lattice has cubic symmetry (in which case  $\xi = 0$  states the obvious fact that  $\kappa$  is just the single crystal bulk modulus). The quartic contains a non-vanishing factor  $9\kappa + 8\mu$ , the numerator of the fraction  $1 - \beta$  corresponding precisely to the factor  $T$  noticed above, and so can be reduced at sight to a cubic†. The cubic, as such, was also obtained by Kröner essentially from the first of (12), which leads to the first of (16), and again by Eshelby from the first of (14) phrased in terms of energies‡. But the final coincidence of these approaches, here shown to be inevitable, went unexplained.

## 5. AUXILIARY PROBLEM WITH PLASTIC FLOW

The previous formulation and analysis of the auxiliary problem already covers certain inelastic behaviour (for instance hypoelastic), but not elastic/plastic behaviour as typified by the common metals at not too high temperatures. This is characterized by a *non-linear* relation between stress-rate and strain-rate (still homogeneous of degree one). With polycrystalline metals mainly in mind, we therefore attempt an appropriate extension of the analysis in § 3.

(i) Suppose, first, that only the crystal is elastic/plastic. Then equations (2) still hold and the connexion between local and overall quantities, replacing (3), is clearly determinable in principle. To derive it explicitly, suppose the operator  $M_c$  for a crystal *in situ* to be *piecewise linear*. If necessary, this can always be assumed as an approximation that can be made as close as one wishes. Then

$$M_c - \mathcal{M}_c = \eta \frac{m_c m_c'}{h_c} + \dots \quad (21)$$

where  $\mathcal{M}_c$  is the elastic compliance tensor of a crystal, and each  $\eta$  is 1 or 0 according as its associated  $m_c' \cdot m_c$  is positive or negative. Succeeding terms, up to any finite number, are similar in type to the one displayed. This law is recognizably akin to what is often premissed for multislip in a metal cubic crystal. Without necessarily intending this interpretation, one may say that the strain-rate tensor in a contributory 'mode of plastic deformation' always has a representative vector in a specific direction, typically  $m_c$  where  $m_c' \cdot m_c = 1$ ; furthermore, 'workhardening' in this mode is controlled by a modulus  $h_c$ , whose value may conceivably depend both on the mode in question and on which others are simultaneously activated. Naturally, every  $m_c$  and  $h_c$  is a function also of the current stress in

†Namely

$$8\mu^3 + (5c_{11} + 4c_{12})\mu^2 - c_{44}(7c_{11} - 4c_{12})\mu - c_{44}(c_{11} - c_{12})(c_{11} + 2c_{12}) = 0$$

with the usual notation for crystal moduli. The version given by Eshelby (1961) contains some misprints.

‡Kröner's second method, essentially in the form of the first of (15), has recently been adopted by Kneer (1965) to compute the bulk and shear moduli when the lattice is hexagonal.

the crystal and of its mechanical state, while the cartesian components of any  $\mathbf{m}_c$  depend as well on lattice orientation.

It can now be seen that  $M_c$  is constant in each of the pyramidal regions created by the dissection of stress-rate space by the set of hyperplanes  $\mathbf{m}_c' \dot{\boldsymbol{\tau}}_c = 0$ , etc. In particular, it is equal to  $\mathcal{M}_c$  in the region whose boundary corresponds to the local vertex on the yield surface of the crystal. Within any pair of adjoining regions the families of active modes differ by just one member whose 'direction' is *normal* to the mutual interface. Moreover, this member is not activated by any stress-rate lying in the mutual surface; consequently, strain-rate varies continuously with stress-rate through the entire space. Finally, because of the assumed normality, matrix  $M_c$  automatically has the required diagonal symmetry when this is stipulated for  $\mathcal{M}_c$ . A linear equation, identical with the second of (8), is therefore valid in respect of each pyramidal region in  $\dot{\boldsymbol{\tau}}_c$  space or its equivalent in  $\dot{\boldsymbol{\tau}}$  space.

When the yield surface is locally regular, its unique normal defines the direction of the possible plastic strain-rate. Expression (21) terminates with the mode shown and inverts to

$$\left. \begin{aligned} \mathcal{L}_c - L_c &= \eta \frac{l_c l_c'}{g_c} \\ \text{where } l_c &= \mathcal{L}_c \mathbf{m}_c, \quad g_c - h_c = \mathbf{m}_c' \mathcal{L}_c \mathbf{m}_c = l_c' \mathcal{M}_c l_c. \end{aligned} \right\} \quad (22)$$

$\mathcal{L}_c$  is the tensor of elastic moduli, reciprocal to  $\mathcal{M}_c$ , and we assume that  $g_c > 0$ . By evaluating in analogous fashion the matrix reciprocals in (10), the concentration factors are obtained as

$$A_c = \left[ I + \eta \frac{(L^* + \mathcal{L}_c)^{-1} l_c l_c'}{g_c - l_c' (L^* + \mathcal{L}_c)^{-1} l_c} \right] (L^* + \mathcal{L}_c)^{-1} (L^* + L) \quad (23)$$

where  $\eta$  is 1 or 0 according as  $l_c' (L^* + \mathcal{L}_c)^{-1} (L^* + L) \bar{\epsilon}$  is positive or negative, and

$$B_c = \left[ I - \eta \frac{(M^* + \mathcal{M}_c)^{-1} \mathbf{m}_c \mathbf{m}_c'}{h_c + \mathbf{m}_c' (M^* + \mathcal{M}_c)^{-1} \mathbf{m}_c} \right] (M^* + \mathcal{M}_c)^{-1} (M^* + M) \quad (24)$$

where  $\eta$  is 1 or 0 according as  $\mathbf{m}_c' (M^* + \mathcal{M}_c)^{-1} (M^* + M) \dot{\boldsymbol{\tau}}$  is positive or negative. Denominators of the quotients here are identically equal and are assumed positive (for which an amply sufficient condition would be that the various matrices are positive definite). The plastic part of the crystal strain-rate is

$$\epsilon_c^p = (M_c - \mathcal{M}_c) B_c \dot{\boldsymbol{\tau}} = \eta \mathbf{m}_c \frac{\mathbf{m}_c' (M^* + \mathcal{M}_c)^{-1} (M^* + M) \dot{\boldsymbol{\tau}}}{h_c + \mathbf{m}_c' (M^* + \mathcal{M}_c)^{-1} \mathbf{m}_c},$$

in the direction of the yield surface normal.

In the event that both phases have the same elastic moduli, so that  $\mathcal{L}_c = L$ ,  $\mathcal{M}_c = M$ , these formulae reduce to

$$\begin{aligned} A_c &= I + \eta \frac{Pl_c l_c'}{g_c - l_c' Pl_c}, \\ B_c &= I - \eta \frac{Q \mathbf{m}_c \mathbf{m}_c'}{h_c + \mathbf{m}_c' Q \mathbf{m}_c}, \\ \epsilon_c^p &= \eta \mathbf{m}_c \frac{\mathbf{m}_c' \dot{\boldsymbol{\tau}}}{h_c + \mathbf{m}_c' Q \mathbf{m}_c}, \end{aligned}$$

where  $P$  and  $Q$  are as in (7). When, in addition, the phases are elastically isotropic the decomposition (20) is available. Thus, supposing also that the plastic mode involves no dilatation, as is appropriate for metals,

$$\dot{\tau}_c = B_c \dot{\tau} = \dot{\tau} - 2\mu(1 - \beta) \epsilon_c^p$$

with

$$\epsilon_c^p = \eta m_c \frac{m_c' \dot{\tau}}{h_c + 2\mu(1 - \beta) m_c' m_c}.$$

If, further, the mode is a simple shear without hardening, we recover the prototype formulae of BUDIANSKY, HASHIN and SANDERS [1960, (12) and (13), obtained via the transformation problem outlined in § 3 (ii) here].

More to the present purpose, suppose that the crystal is rigid/plastic, without specializing in other directions. Then, by putting  $\mathcal{M}_c = 0$  in (24), and using (4),

$$B_c S' = I - \eta \frac{L^* m_c m_c'}{h_c + m_c' L^* m_c} \quad (25)$$

where  $\eta$  is 1 or 0 according as  $(S^{-1} m_c)' \dot{\tau}$  is positive or negative, and

$$S^{-1} = I + ML^*, \quad S' = (I + L^* M)^{-1},$$

as in (4), a prime signifying the transpose. Equally, by a limiting operation on (23) or directly from  $A_c P = M_c B_c S'$  [which is the second of (9) with the first of (5) in the form  $S' = LP$ ],

$$A_c P = \eta \frac{m_c m_c'}{h_c + m_c' L^* m_c} \quad (26)$$

where  $\eta$  is 1 or 0 according as  $(P^{-1} m_c)' \dot{\epsilon}$  is positive or negative, and

$$P = SM = MS' = (L^* + L)^{-1}$$

as in (7).

(ii) Suppose, now, that the macroscopic constitutive law of an elastoplastic polycrystal is known and can be approximated piecewise linearly :

$$M - \mathcal{M} = \eta \frac{m m'}{h} + \dots, \quad (27)$$

where each  $\eta$  is 1 or 0 according as its associated  $m' \dot{\tau}$  is locally positive or negative. Consider the corresponding auxiliary problem where the crystal has the constitutive law (21). If the stress-rate at all points in the outer phase induces one and the same branch of  $M$ , the material behaviour is quasi-elastic and the previous analysis remains rigorously valid for the particular overall loading. It would be possible in principle to determine the loading ranges for which this happened, in respect of any given branch and any lattice orientation.

A more practicable course is to take as the representative outer phase a truly elastic material whose properties coincide with the actual branch of  $M$  associated with whatever *overall* stress-rate may be in question. Naturally, for certain loadings, the resulting solution of the auxiliary problem will sometimes violate the original (27) locally in the outer phase, but we can reasonably hope that the net error in the overall constraint will be negligible.

Expressed formally, our hypothesis means that (27) is modified to the extent

that each  $\gamma$  is taken as 1 or 0 according as its associated  $m' \dot{\tau}$  is positive or negative. The analysis in (i) above is then rigorously valid within each region of the space of overall stress-rate given by this dissection. In the formulae it is only necessary to insert the appropriate branch of  $L$  and  $M$  from the modified (27), together with the associated  $L^*$ ,  $M^*$ ,  $S$ ,  $T$ ,  $P$  and  $Q$ .

(iii) KRÖNER (1961) has suggested a different scheme. In BUDIANSKY and WU's elaboration of this (1962), adopted also by HUTCHINSON (1964), the representative outer phase is given the constitutive law

$$\epsilon - \bar{\epsilon} = \mathcal{N} (\dot{\tau} - \dot{\bar{\tau}})$$

where  $\mathcal{N}$  is the elastic compliance (assumed isotropic) of the aggregate and of the individual crystals. This is an artificial relation, patently not quasi-elastic; nevertheless Eshelby's analysis is still presumed to apply. The writer has not understood the subsequent line of argument, but the eventual formulae imply that

$$\epsilon_c - \bar{\epsilon} = -\mathcal{N}^* (\dot{\tau}_c - \dot{\bar{\tau}})$$

and so, in particular, that the aggregate deforms homogeneously when the crystals are rigid/plastic ( $\mathcal{N}$ ,  $\mathcal{N}^* = 0$ ). Thus, in effect if not by expressed intention, KRÖNER *et al.* assign to the outer phase the overall isotropic constraint that the aggregate would in fact exert if its incremental deformation were always purely elastic. This disregards the pronounced directional weaknesses in the constraint of an already yielded aggregate.

If used with the present formulae in (i) above, Kröner's proposal would entail replacing  $L^*$ ,  $M^*$ ,  $S$ ,  $T$ ,  $P$  and  $Q$  by their elastic counterparts. Neither Budiansky and Wu nor Hutchinson obtain such formulae, but calculate instead the rate of hardening of typical crystals in a random aggregate loaded either by uniaxial tension or pure shear. At the same time the overall hardening of the aggregate itself is computed by the self-consistent method.

## 6. SELF-CONSISTENT MODEL WITH PLASTIC FLOW

It is proposed to combine the hypothesis of § 5 (ii) with the self-consistent method of averaging. The object of calculation is now the macroscopic constitutive law itself. The unknown matrix  $M$  will certainly have the structure (27), since not only are its piecewise linearity and diagonal symmetry intrinsic to this theory but they are also clearly compatible with the law (21) assumed for the individual crystals. Of course the branches of  $M$  will not normally be foreseeable at the outset. They are determinable in principle with the help of the requirement that the overall stress-rate should always depend continuously on strain-rate.

Fortunately, the elastic branch at least can be located already. It is associated with the pyramidal region defined by the inequalities

$$m_c' (\mathcal{N}^* + \mathcal{N}_c)^{-1} (\mathcal{N}^* + \mathcal{N}) \dot{\tau} < 0, \dots, ,$$

for all crystals and modes.  $\mathcal{N}^*$  is the reciprocal constraint tensor associated with the overall elastic compliance  $\mathcal{N}$  satisfying

$$(\mathcal{N}^* + \mathcal{N})^{-1} = \{(\mathcal{N}^* + \mathcal{N}_c)^{-1}\}$$

as in (18). The hyperplanes bounding this elastic region in overall stress-rate space correspond of course to the tangent planes at the currently given stress-point on the yield surface of the aggregate. The vertex is more or less pronounced according to whether the directions

$$(I + \mathcal{M}_c \mathcal{L}^*)^{-1} \mathbf{m}_c, \dots, ,$$

span a large or small solid angle.

Without resort to computation, the analysis can be carried farther only in particular cases. Suppose, for example, that the crystals are elastically isotropic and that the current internal stress is such as to activate just one mode  $\mathbf{m}$ , whose direction in strain-rate space is moreover the same for all grains. The typical crystal compliance can then be written as

$$M_c = \mathcal{M} + \eta \frac{\mathbf{m} \mathbf{m}'}{h_c}$$

where only the hardening parameter varies from grain to grain. Then, in the family of auxiliary problems for the various orientations,  $\eta$  is simultaneously 1 or 0 according as  $\mathbf{m}' (M^* + \mathcal{M})^{-1} (M^* + M) \dot{\bar{\tau}}$  is positive or negative; in particular, for the elastic branch  $\mathcal{M}$  this criterion expression becomes  $\mathbf{m}' \dot{\bar{\tau}}$ . By solving  $\{B_c\} = I$  for  $M$ , when the concentration factor  $B_c$  is the indicated specialization of (24), one finds that

$$M = \mathcal{M} + \eta \frac{\mathbf{m} \mathbf{m}'}{h},$$

regardless of what  $M^*$  might be, where

$$[h + \mathbf{m}' (M^* + \mathcal{M})^{-1} \mathbf{m}]^{-1} = \{[h_c + \mathbf{m}' (M^* + \mathcal{M})^{-1} \mathbf{m}]^{-1}\}. \quad (28)$$

Finally, by virtue of the *a posteriori* reduction

$$\begin{aligned} \mathbf{m}' (M^* + \mathcal{M})^{-1} (M^* + M) \dot{\bar{\tau}} &= \mathbf{m}' \left[ I + \eta (M^* + \mathcal{M})^{-1} \frac{\mathbf{m} \mathbf{m}'}{h} \right] \dot{\bar{\tau}} \\ &= \left[ 1 + \eta \frac{\mathbf{m}' (M^* + \mathcal{M})^{-1} \mathbf{m}}{h} \right] \mathbf{m}' \dot{\bar{\tau}}, \end{aligned}$$

it is confirmed that the criterion expression is essentially the same for both branches (the factor in square brackets being positive). The conclusion is, therefore, that the aggregate also deforms by the one plastic mode, for the overall stress, and that its overall rate of hardening is implicitly given by (28). Since  $M^*$  depends on  $M$ , which is itself a function of  $h$ , this equation is quite complicated. Leaving it and returning to (24), we obtain the following expression for the inhomogeneity of the internal fields :

$$\left. \begin{aligned} \dot{\bar{\tau}} - \dot{\bar{\tau}}_c &= L^* (\epsilon_c - \bar{\epsilon}) \\ &= \eta \left( 1 - \frac{h_c}{h} \right) \frac{\mathbf{m}' \dot{\bar{\tau}}}{h_c + \mathbf{m}' (M^* + \mathcal{M})^{-1} \mathbf{m}} (M^* + \mathcal{M})^{-1} \mathbf{m}. \end{aligned} \right\} \quad (29)$$

The inhomogeneity in strain-rate is seen to be of the same type in all grains, though deflected from direction  $\mathbf{m}$ .

The latter effect is purely elastic and would vanish if the crystals and aggregate were rigid/plastic, i.e. if  $\mathcal{M} = 0$ . In that event the strain-rate would necessarily always be homogeneous in the auxiliary problem, and so  $M^* = 0$  while  $m' \dot{\tau}_c = h_c$  and  $m' \dot{\tau} = h$ . Thus  $h = \{h_c\}$  is the limiting form of (28). To determine the stress-rate field uniquely, the auxiliary problem must naturally be re-set in the manner appropriate to rigid/plastic solids with a (piecewise) linear constitutive law (HILL 1956). When the direction of the only activated mode is *not* the same in all grains, combining  $\{B_c\} = I$  with (25) or  $\{A_c\} = I$  with (26) leads to the implicit equation

$$P = \left\{ \eta \frac{m_c m_c'}{h_c + m_c' L^* m_c} \right\} \quad (30)$$

for  $L$  or  $M$ . The accompanying conditions on  $\eta$  define a pyramidal dissection of the space of the overall stress-rate by hyperplanes with normals  $S^{-1} m_c$ , for the various branches of  $S$ .

Further consequences are left for future investigation.

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