Bounds and self-consistent estimates for creep of polycrystalline materials

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A study of steady creep of face centred cubic (f.c.c.) and ionic polycrystals as it relates to single crystal creep behaviour is made by using an upper bound technique and a self-consistent method. Creep on a crystallographic slip system is assumed to occur in proportion to the resolved shear stress to a power. For the identical systems of an f.c.c. crystal the slip-rate on any system is taken as $\gamma = \alpha(\tau/\tau_0)^n$ where α is a reference strain-rate, τ is the resolved shear stress and τ_0 is the reference shear stress. The tensile behaviour of a polycrystal of randomly orientated single crystals can be expressed as $\bar{\epsilon} = \alpha(\bar{\sigma}/\bar{\sigma}_0)^n$ where $\bar{\epsilon}$ and $\bar{\sigma}$ are the overall uniaxial strain-rate and stress and $\bar{\sigma}_0$ is the uniaxial reference stress. The central result for an f.c.c. polycrystal in tension can be expressed as $\bar{\sigma}_0 = h(n)\,\tau_0$. Calculated bounds to $h(n)$ coincide at one extreme ($n = \infty$) with the Taylor result for rigid/perfectly plastic behaviour and at the other ($n = 1$) with the Voigt bound for linear viscoelastic behaviour. The self-consistent results, which are shown to be highly accurate for $n = 1$, agree closely with the upper bound for $n \geqslant 3$. Two types of glide systems are considered for ionic crystals: A-systems, $\{110\}\langle110\rangle$, with $\gamma = \alpha(\tau/\tau_A)^n$; and B-systems, $\{100\}\langle110\rangle$, with $\gamma = \alpha(\tau/\tau_B)^n$. The upper bound to the tensile reference stress $\bar{\sigma}_0$ is shown to have the simple form $\bar{\sigma}_0 \leqslant A(n)\,\tau_A + B(n)\,\tau_B$; $A(n)$ and $B(n)$ are computed for the entire range of n, including the limit $n = \infty$. Self-consistent predictions are again in good agreement with the bounds for high n. Upper bounds in pure shear are also calculated for both f.c.c. and ionic polycrystals. These results, together with those for tension, provide a basis for assessing the most commonly used stress creep potentials. The simplest potential based on the single effective stress invariant is found to give a reasonably accurate characterization of multiaxial stress dependence.

1. Introduction

A pure power relation between strain-rate and stress is often used to characterize steady creep of metals and other materials at temperatures above, typically, one third the absolute melting temperature in the stress range lying one or two orders of magnitude below the stress at which the creep-rate (s^{-1}) becomes of order unity (Ashby & Frost 1975). The connection between single crystal creep properties and those of a polycrystal are studied in this paper for such power law materials. We confine attention to the steady creep of polycrystals comprised of randomly

orientated single crystals. Single crystal slip is taken to be the sole source of inelastic behaviour; additional sources such as grain boundary sliding, void growth and micro-cracking are not considered. The rate of sliding across a grain boundary is thought to depend essentially linearly on stress. Since power law creep usually involves stress to the third power or greater, increasing the overall stress tends to decrease the importance of grain boundary sliding relative to single crystal creep. Thus, for most materials, grain boundary sliding should be negligible in at least the upper portion of the stress range of power law creep. Void growth and micro-cracking are non-steady processes which bring about the breakdown of steady creep. During much of the steady state lifetime their contribution to the overall strain-rate is small.

Two methods are used to calculate the overall steady creep properties of face centred cubic (f.c.c.) and ionic polycrystals in terms of the properties of their single crystal constituents. The simplest is the uniform strain-rate upper bound. An attractive feature of the present formulation is that, by considering all degrees of power law nonlinearity, we connect up the Taylor–Bishop–Hill-type bound for rigid/perfectly plastic behaviour and the Voigt-type bound for linear viscoelastic behaviour. Calculations are made for overall tension and shear. Based on these results it is possible to draw some conclusions with regard to potentials for steady creep.

Hill's (1965) self-consistent scheme is shown to apply in a form which is simpler than might be expected for such highly nonlinear material behaviour. At the limit corresponding to linear viscoelasticity the self-consistent method gives highly accurate results, as will be established using the relatively tight bounding techniques of Hashin & Shtrikman (1962). The only available bounding technique which continues to apply in the nonlinear range is the uniform strain-rate upper bound (and the less interesting uniform stress lower bound). Thus the self-consistent method is a welcome additional procedure for the analysis of these nonlinear materials, particularly so given its physical plausibility and its known success in linear applications.

Throughout the paper we will use a combination of Cartesian tensor notation and a standard tensor/matrix notation. Bold-face lower case letters denote symmetric second order tensors; bold-face upper case letters represent fourth order tensors. The contracted product $a_{ij}b_{ij}$ is denoted by ab, $A_{ijkl}a_{kl}$ by Aa, $a_{ij}A_{ijkl}b_{kl}$ by aAb and $A_{ijkl}B_{klmn}$ by AB. All fourth order tensors in this paper have the indicial symmetries $A_{ijkl} = A_{jikl} = A_{ijlk}$; if in addition $A_{ijkl} = A_{klij}$, then A will be said to have diagonal symmetry. The inverse of a positive definite, diagonally symmetric fourth order tensor A is denoted by A^{-1}; it shares the same indicial symmetries as A and satisfies $A^{-1}A = AA^{-1} = I$ where the identity tensor is given in terms of the Kronecker delta by

$$I_{ijkl} = \tfrac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{1.1}$$

The notation permits a straightforward conversion to vector/matrix operations for numerical calculations.

2. Constitutive behaviour of single crystals and polycrystals in steady creep at constant temperature

Denote the unit normal to the slip plane of the kth system by $\boldsymbol{n}^{(k)}$ and the slip direction in the plane by $\boldsymbol{m}^{(k)}$. The fundamental tensor characterizing this system is defined as

$$\mu_{ij}^{(k)} = \tfrac{1}{2}(m_i^{(k)} n_j^{(k)} + m_j^{(k)} n_i^{(k)}). \tag{2.1}$$

With $\boldsymbol{\sigma}$ denoting the stress, the resolved shear stress on the kth system is

$$\tau^{(k)} = \boldsymbol{\sigma} \boldsymbol{\mu}^{(k)}. \tag{2.2}$$

Let $\gamma^{(k)}$ denote the shear strain-rate (engineering definition) on the kth system. Then $\gamma^{(k)}\boldsymbol{\mu}^{(k)}$ is the contribution of this system to the total strain-rate $\boldsymbol{\varepsilon}$. Since $\mu_{ii} = 0$, the creep strain-rate is volume preserving and the hydrostatic component of stress has no influence on τ.

The connection between the shear-rate and resolved shear stress on the kth system is taken as

$$\gamma^{(k)} = \alpha(\tau^{(k)}/\tau_0^{(k)})^n, \tag{2.3}$$

if $\tau^{(k)}$ is positive or, for arbitrary sign, as

$$\gamma^{(k)} = \alpha \left| \tau^{(k)}/\tau_0^{(k)} \right|^{n-1} \tau^{(k)}/\tau_0^{(k)}. \tag{2.4}$$

Here, α is any convenient reference creep-rate which could, without loss in mathematical generality, be taken to be unity (s^{-1}) but will be carried along explicitly for ease of application of the subsequent results. The reference stress $\tau_0^{(k)}$ for the kth system is a strong function of temperature, but our concern will be with isothermal deformations and therefore $\tau_0^{(k)}$ is regarded as known for each system. The exponent n also depends on temperature, although somewhat less strongly, and usually falls between 3 and 8 for metals. Ashby & Frost (1975) have broadly surveyed polycrystal and single crystal data for many metals to determine the range of temperature and stress over which steady creep can be reasonably approximated by a power law stress dependence. For many materials this range can cover, typically, from one to two orders of magnitude of stress and four to eight orders of magnitude of strain-rate.

The creep rule for the kth system (2.4) embodies the assumption that $\gamma^{(k)}$ depends on the stress only through $\tau^{(k)}$ and otherwise not on creep activity on the other systems. There is relatively little experimental creep data available to subject this independency assumption to critical examination. Most single crystal creep data is obtained with one system more highly stressed than all the others. In timeindependent plasticity the strain hardening characteristics of a crystal are significantly affected by the interactions between active systems. For f.c.c. metals Kocks (1970) has shown that polycrystal strain hardening data can be correlated with single crystal data, via Taylor's (1938) well known formula, if the single crystal data is obtained from a test in which multiple systems are active. This is consistent

with occurrence of multiple slip in nearly all grains of a polycrystal. In the present context, (2.4) cannot be expected to represent both predominantly single system creep and multiple system creep if strong interaction between systems occurs. Then, for present purposes, the τ_0's in (2.4) should be assigned values on the basis of data from multiple system creep tests, consistent with Kocks' idea.

The total strain-rate is the sum of the contributions from all systems and can be written as

$$\epsilon_{ij} = \sum_k \gamma^{(k)} \mu_{ij}^{(k)} = M_{ijpq}^c \sigma_{pq}, \tag{2.5}$$

where, from (2.4),

$$M_{ijpq}^c = \sum_k (\alpha/\tau_0^{(k)}) \left| \tau^{(k)}/\tau_0^{(k)} \right|^{n-1} \mu_{ij}^{(k)} \mu_{pq}^{(k)}. \tag{2.6}$$

We will call M^c the tensor of creep compliances, or briefly just the compliances, of the crystal. The compliances are homogeneous of degree $n-1$ in the stress so that

$$M^c(\lambda\sigma) = \lambda^{n-1} M^c(\sigma). \tag{2.7}$$

Let $F^c(\sigma)$ be the stress potential and $E^c(\varepsilon)$ the strain-rate potential of the crystal defined such that

$$\varepsilon = \partial F^c/\partial\sigma \quad \text{and} \quad \sigma = \partial E^c/\partial\varepsilon. \tag{2.8a, b}$$

For the present crystal law there is an unusually simple connection between F^c, E^c and the dissipation-rate, $\sigma\varepsilon$

$$\sigma\varepsilon = (n+1)F^c = [(n+1)/n]E^c = \sum_k \tau^{(k)}\gamma^{(k)}. \tag{2.9}$$

A further connection which can be verified directly is

$$M_{ijkl}^c = \frac{1}{n}\frac{\partial^2 F^c}{\partial\sigma_{ij}\,\partial\sigma_{kl}}. \tag{2.10}$$

It follows that the relation between a stress increment $d\sigma$ and the associated change $d\varepsilon$ in the steady creep-rate is

$$d\varepsilon = nM^c d\sigma. \tag{2.11}$$

Except for the factor n, M^c can be regarded as the stress-dependent 'incremental' compliances in the sense of (2.11); this additional property will be useful in the sequel.

The polycrystal is regarded as a large collection of perfectly bonded, randomly oriented single crystals of roughly the same size. Some exact relations for such a polycrystal in terms of single crystal behaviour are derived quickly below. More general treatments can be found in Hill (1967) for inelastic behaviour in general and in Rice (1970) for creep behaviour specifically. However, the structure of the steady creep constitutive relation of the polycrystal as it relates to the single crystal is so simple that it is revealing to start from first principles.

Consider a finite polycrystal with a definitive arrangement of single crystals. As a first possibility impose a uniform straining velocity $v_i = \bar{\epsilon}_{ij}x_j$ over the entire

outer surface of the polycrystal, where x_j is the Cartesian coordinate and the constant strain-rate quantity $\bar{\varepsilon}$ will be called the overall strain-rate. Define $\bar{\sigma}$ to be the average of the stress over the volume V of the polycrystal, i.e. $\bar{\sigma} = \{\sigma\}$ where

$$\{\} = V^{-1} \int_V (\,)\,\mathrm{d}V. \tag{2.12}$$

The single crystal potentials given by (2.9) are convex, as can readily be established, and this guarantees a unique solution to the boundary value problem posed for the polycrystal (Hill 1956). As a consequence of the pure power law relation (2.5) for the single crystals, the strain-rate ε and stress σ at every point are homogeneous functions of degree 1 and $1/n$, respectively, of $\bar{\varepsilon}$. The average stress is also homogeneous of degree $1/n$ in $\bar{\varepsilon}$ so that

$$\bar{\sigma}(\lambda\bar{\varepsilon}) = \lambda^{1/n}\bar{\sigma}(\bar{\varepsilon}); \quad \bar{\varepsilon}(\lambda\bar{\sigma}) = \lambda^n \bar{\varepsilon}(\bar{\sigma}). \tag{2.13}$$

Using the principle of virtual work one can show the following exact relations between the barred quantities and the local quantities

$$\bar{\sigma}\bar{\varepsilon} = \{\sigma\varepsilon\}, \quad \bar{\sigma}\,\mathrm{d}\bar{\varepsilon} = \{\sigma\,\mathrm{d}\varepsilon\}, \quad \bar{\varepsilon}\,\mathrm{d}\bar{\sigma} = \{\varepsilon\,\mathrm{d}\sigma\} \tag{2.14a, b, c}$$

where $\mathrm{d}v_i = \mathrm{d}\bar{\varepsilon}_{ij}x_j$ is an increment in the prescribed steady boundary velocity and $\mathrm{d}\bar{\sigma} = \{\mathrm{d}\sigma\}$ is the associated average stress change.

Define overall stress and strain-rate potentials in terms of the local potentials as

$$F(\bar{\sigma}) = \{F^c(\sigma)\}, \quad E(\bar{\varepsilon}) = \{E^c(\varepsilon)\}, \tag{2.15a, b}$$

or, from (2.14a) and (2.9), equivalently as

$$(n+1)F(\bar{\sigma}) = [(n+1)/n]\,E(\bar{\varepsilon}) = \bar{\sigma}\bar{\varepsilon}. \tag{2.16}$$

Next, using (2.8b) and (2.14b) together with (2.15b), one can show that

$$\bar{\sigma} = \partial E/\partial\bar{\varepsilon}. \tag{2.17}$$

Then, from the fact $\mathrm{d}(\bar{\sigma}\bar{\varepsilon}) = \mathrm{d}F + \mathrm{d}E$, it also follows that

$$\bar{\varepsilon} = \partial F/\partial\bar{\sigma}. \tag{2.18}$$

Rather than applying uniform straining boundary velocities we could instead apply uniform traction over the outer surface of the polycrystal according to $T_i = \bar{\sigma}_{ij}q_j$, where q is the outward unit normal to the surface and the constant stress quantity $\bar{\sigma}$ is called the overall stress. Now, $\bar{\varepsilon}$ is *defined* to be the average strain-rate, i.e. $\bar{\varepsilon} = \{\varepsilon\}$. All the relations, (2.13)–(2.18), also hold exactly for the uniform traction problem, although the precise functional dependence of $\bar{\varepsilon}$ on $\bar{\sigma}$, will be slightly different. However, if the polycrystal is macroscopically homogeneous with an overall size which is large compared to the characteristic grain size, then the distinction between uniform straining boundary conditions and uniform traction becomes negligible (Hill 1967). Henceforth we will assume this is the case. Accordingly, $\bar{\sigma}$ may be referred to interchangeably as the average, overall or macroscopic stress, with similar designations for the strain-rate $\bar{\varepsilon}$.

The overall stress potential $F(\overline{\sigma})$ defined in $(2.15a)$ is homogeneous of degree $n+1$ in $\overline{\sigma}$. A mathematical consequence of this homogeneity, which follows from Euler's theorem, is

$$\overline{\epsilon}_{ij} = \frac{\partial F}{\partial \overline{\sigma}_{ij}} = \frac{1}{n} \frac{\partial^2 F}{\partial \overline{\sigma}_{ij} \partial \overline{\sigma}_{kl}} \overline{\sigma}_{kl}. \tag{2.19}$$

In parallel to (2.5) or (2.10) for the single crystals, define the tensor of overall creep compliances as

$$M_{ijkl} = \frac{1}{n} \frac{\partial^2 F}{\partial \overline{\sigma}_{ij} \partial \overline{\sigma}_{kl}}, \tag{2.20}$$

and thus

$$\overline{\epsilon} = M\overline{\sigma}. \tag{2.21}$$

Note also that an increment in overall steady strain-rate $\mathrm{d}\overline{\epsilon}$ is related to $\mathrm{d}\overline{\sigma}$ by

$$\mathrm{d}\overline{\epsilon} = nM\mathrm{d}\overline{\sigma} \tag{2.22}$$

in analogue to (2.11).

Since the single crystal grains are randomly distributed the relation between $\overline{\sigma}$ and $\overline{\epsilon}$ is isotropic. In a uniaxial stressing of the polycrystal along any axis the tensile strain-rate $\overline{\epsilon}$ is, by (2.13), proportional to $(\overline{\sigma})^n$, where $\overline{\sigma}$ is the overall tensile stress. Throughout the paper it will be convenient to write, without loss in generality, the tensile relation as

$$\overline{\epsilon} = \alpha(\overline{\sigma}/\overline{\sigma}_0)^n, \tag{2.23}$$

where α is the same reference strain-rate introduced in (2.3). Thus, (2.23) is the defining equation for the overall tensile reference stress $\overline{\sigma}_0$; knowledge of $\overline{\sigma}_0$ completely specifies the tensile behaviour of the polycrystal. One of the aims of the paper will be to determine $\overline{\sigma}_0$ in terms of the characterizing parameters and structure of the single crystals.

3. UPPER BOUNDS FOR F.C.C. POLYCRYSTALS

A f.c.c. single crystal has twelve crystallographically similar slip systems. In the grain axes there are four slip planes of the $(1, 1, 1)$ type and three slip directions per plane of the $(1, 1, 0)$ type. The reference value of the resolved shear stress is the same for each system and we write $\tau_0^{(k)} = \tau_0, k = 1, 12$. This information completely specifies the crystal compliances in (2.6).

The limiting case $n = 1$ is special in that the compliances are stress-independent. The bounds and estimates calculated below can be carried out without recourse to numerical work only for this case. For $n = 1$, the compliance tensor necessarily has cubic symmetry with respect to the grain axes. In its axes of cubic symmetry, any diagonally symmetric fourth order tensor A is completely specified by the three quantities: $A_{1111} + 2A_{1122}$, $A_{1111} - A_{1122}$ and A_{1212}. By carrying out the summations indicated in (2.6), one finds

$$M^c_{1111} + 2M^c_{1122} = 0, \quad M^c_{1111} - M^c_{1122} = 2\alpha/\tau_0, \quad M^c_{1212} = \alpha/3\tau_0. \tag{3.1}$$

The first combination of terms in (3.1) is proportional to the volume change compliance which is identically zero in steady creep.

The upper bounds for the polycrystal can be based on the minimum principle for the strain-rates which has been given for power law materials by Hill (1965). Suppose 'uniform straining' is imposed on the outer surface of the polycrystal according to $v_i = \bar{\varepsilon}_{ij} x_j$. Among all velocity fields $\hat{\mathbf{v}}$ satisfying the prescribed velocity conditions on the outer surface, the actual field minimizes the functional†

$$\{E^c(\hat{\bar{\varepsilon}})\}, \tag{3.2}$$

where $\hat{\bar{\varepsilon}}$ is the strain-rate associated with $\hat{\mathbf{v}}$. The minimum value of (3.2) calculated from the actual fields is $E(\bar{\varepsilon})$ as defined by (2.15 b). The simplest upper bound is obtained by taking $\hat{\bar{\varepsilon}} = \bar{\varepsilon}$ everywhere in the polycrystal. Then the minimum principle gives

$$\{E^c(\bar{\varepsilon})\} \geqslant E(\bar{\varepsilon}). \tag{3.3}$$

Let σ^u denote the local stress associated with imposed uniform $\bar{\varepsilon}$. Multiply (3.3) by $(n+1)/n$, noting (2.9) and (2.16), to obtain the equivalent statement of the upper bound

$$\{\sigma^u\bar{\varepsilon}\} \geqslant \overline{\sigma\varepsilon}. \tag{3.4}$$

With $\bar{\varepsilon}$ imposed throughout, the stress in each crystalline grain is uniform and, from (2.6), must satisfy

$$\bar{\varepsilon}_{ij} = M^c_{ijkl}(\sigma^u)\,\sigma^u_{kl}. \tag{3.5}$$

In other words, to determine $E^c(\bar{\varepsilon})$ or $\sigma^u\bar{\varepsilon}$ for any grain it is first necessary to solve the nonlinear equation (3.5) for σ^u. The following extremum principle associated with this inverse problem can be shown to hold. Among all possible stresses $\hat{\sigma}, \sigma^u$ maximizes the function

$$\hat{\sigma}\bar{\varepsilon} - F^c(\hat{\sigma}) = \hat{\sigma}\bar{\varepsilon} - \frac{\alpha}{n+1}\tau_0 \sum_k |\hat{\tau}^{(k)}/\tau_0|^{n+1}, \tag{3.6}$$

where $\hat{\tau}^{(k)} = \hat{\sigma}\mu^{(k)}$. The importance of this principle is that it allows us to establish a connection with the maximum work principle of Bishop & Hill (1952) for the limiting case $n \to \infty$ corresponding to rigid/perfectly plastic behaviour. The Bishop–Hill principle states that, for all $\hat{\sigma}$ satisfying the constraints $|\hat{\tau}^{(k)}| \leqslant \tau_0$ for $k = 1, 12$, the actual stress maximizes $\hat{\sigma}\bar{\varepsilon}$. But (3.6) reduces to this principle as $n \to \infty$. This can be seen by noting: (i) $F^c(\sigma^u) \to 0$ as $n \to \infty$, from (2.9), with σ^u itself satisfying the constraints and (ii) for any $\hat{\sigma}$ satisfying the constraints, $F^c(\hat{\sigma}) \to 0$ as $n \to \infty$. The maximum principle associated with (3.6) then reduces to $\hat{\sigma}\bar{\varepsilon} \leqslant \sigma^u\bar{\varepsilon}$ which establishes the desired connection. Thus, in the limit $n \to \infty$, the stress σ^u corresponding to $\bar{\varepsilon}$ is the same as that calculated by the Taylor–Bishop–Hill scheme. Hence the limit for $n \to \infty$ of the present bound coincides with the Taylor–Bishop–Hill bound since (3.4) is the same as their overall bounding equation.

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† Intuitively, it may help to think in terms of strains rather than strain-rates and displacements rather than velocities, in which case the present formulation is a small strain theory for a class of nonlinear elastic crystals and polycrystals. With this interpretation (3.2) is just the strain energy functional of the polycrystal divided by its volume.

Let $|\bar{\varepsilon}| \equiv \sqrt{(2\overline{\varepsilon\varepsilon}/3)}$. Then one can show that σ^u can, without loss in generality, be written as

$$\sigma^u = (|\bar{\varepsilon}|/\alpha)^{1/n}\tau_0\,\omega, \tag{3.7}$$

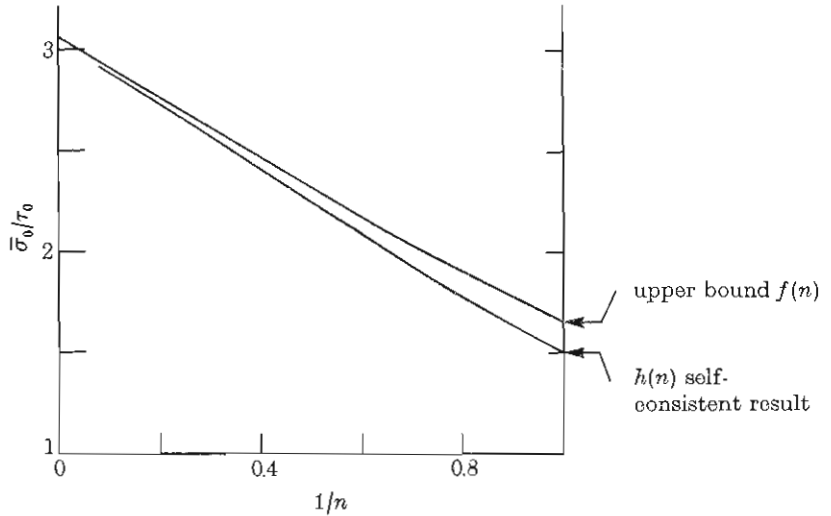where ω depends only on n, the orientation of the grain and $\bar{\varepsilon}/|\bar{\varepsilon}|$.

FIGURE 1. Upper bound and self-consistent result for the tensile reference stress of an f.c.c. polycrystal.

(a) Upper bound to the tensile reference stress

In simple tension along the 3-axis, the nonzero components of the overall stress and strain-rate are

$$\bar{\sigma}_{33} = \bar{\sigma} \quad \text{and} \quad \bar{\varepsilon}_{33} = -2\bar{\varepsilon}_{11} = -2\bar{\varepsilon}_{22} \equiv \bar{\varepsilon} = |\bar{\varepsilon}|. \tag{3.8}$$

The upper bound statement (3.4) can be written as

$$\{\sigma^u\bar{\varepsilon}\} \geqslant \bar{\sigma}\bar{\varepsilon}. \tag{3.9}$$

But, by (2.23), $\bar{\sigma} = (\bar{\varepsilon}/\alpha)^{1/n}\bar{\sigma}_0$ and, from (3.7) and (3.8), the upper bound can be restated as

$$\bar{\sigma}_0/\tau_0 \leqslant f(n) \quad \text{where} \quad f(n) = \{\omega\bar{\varepsilon}\}/\bar{\varepsilon}. \tag{3.10}$$

The upper bound calculation specified by (3.10) is discussed further in the appendix. The numerical method uses a highly efficient procedure for solving for σ^u (or ω) from (3.5). The volume integration defined in (2.12) is replaced by a uniformly weighted integration over all orientations of the grain axes with respect to the specimen axes. This integration is in turn replaced by a sum over discrete orientations. Sufficiently many discrete orientations are taken to ensure an accuracy in $f(n)$ to within 0.5 %. The results of this calculation are shown as the upper curve in figure 1, where $f(n)$ is plotted against $1/n$, and in table 1.

As already mentioned, the calculation of (3.10) can be carried out analytically when $n = 1$. The result is the Voigt-type bound.

$$f(1) = \tfrac{33}{20}. \tag{3.11}$$

The largest value of n for which $f(n)$ was calculated was $n = 10$; but, in accord with our previous discussion, the curve in figure 1 is extrapolated to the well known Taylor value

$$f(\infty) = 3.06. \tag{3.12}$$

(b) Upper bound in shear and bounding potentials

Consider a pure shearing of the polycrystal $(\overline{\sigma}_{12}, \overline{\varepsilon}_{12})$ with the overall reference stress in shear $\overline{\tau}_0$ defined by the equation

$$\overline{\varepsilon}_{12} = \alpha(\overline{\sigma}_{12}/\overline{\tau}_0)^n. \tag{3.13}$$

Now, $|\overline{\varepsilon}| = 2\overline{\varepsilon}_{12}/\sqrt{3}$, and (3.4) can be reduced to

$$\overline{\tau}_0/\tau_0 \leqslant g(n) \quad \text{where} \quad g(n) = (2/\sqrt{3})^{1/n}\{\omega_{12}\}. \tag{3.14}$$

The result of this calculation is given in table 1 and is shown as a solid line curve in figure 2. For $n = 1, g(1) = \tfrac{11}{10}$; and for $n \to \infty$, the curve is extrapolated to the Bishop–Hill value $g(\infty) = 1.656$.

TABLE 1

$1/n$	$f(n)$	$g(n)$	$h(n)$	$A(n)$	$B(n)$	$C(n)$	$D(n)$
1.0	33/20	11/10	3/2	2/5	9/10	4/15	3/5
0.8	1.90	1.24	1.78	0.460	1.03	0.320	0.669
0.6	2.18	1.37	2.08	0.573	1.16	0.385	0.739
0.4	2.48	1.50	2.41	0.733	1.31	0.459	0.807
0.3	2.62	1.55	2.57	0.828	1.39	0.497	0.836
0.2	2.77	1.58	2.73	0.925	1.46	0.535	0.860
0.1	2.92	1.63	2.89	1.030	1.54	0.575	0.883
0	3.06†	1.656†	3.04‡	1.154†	1.633†	0.62‡	0.90‡

† Calculated as discussed in text.   ‡ Extrapolated value.

For general overall strain-rates $\overline{\varepsilon}$ define an upper bound strain-rate potential as

$$E_u(\overline{\varepsilon}) = \{E^{\mathrm{c}}(\overline{\varepsilon})\}, \tag{3.15}$$

where, from (3.3), $E_u(\overline{\varepsilon}) \geqslant E(\overline{\varepsilon})$. The associated upper bound stress potential is

$$F_u(\overline{\sigma}) = n^{-1}E_u(\overline{\varepsilon}) \quad \text{where} \quad \overline{\sigma} = \partial E_u/\partial\overline{\varepsilon}. \tag{3.16}$$

The definition of $\overline{\sigma}$ in (3.16) is equivalent to $\overline{\sigma} = \{\sigma^u\}$ where σ^u is given in terms of $\overline{\varepsilon}$ by (3.5). Since the overall behaviour is isotropic and independent of $\overline{\sigma}_{kk}$, F_u must be a function of the two invariants

$$\overline{\sigma}_e = \sqrt{(3\overline{s}_{ij}\overline{s}_{ij}/2)}, \quad \overline{s}_{ij}\overline{s}_{ik}\overline{s}_{jk}, \tag{3.17}$$

where $\overline{s}$ is the deviator stress.

Consider the simplest approximation in which F_u is taken to depend on $\bar{\sigma}_e$ alone. With $\bar{\sigma}_0 = f(n)\tau_0$, the choice

$$F_u = [\alpha\bar{\sigma}_0/(n+1)](\bar{\sigma}_e/\bar{\sigma}_0)^{n+1} \tag{3.18}$$

brings the potential into coincidence with the upper bound results for tension. In simple shear (3.18) gives

$$\bar{\epsilon}_{12} = \partial F_u/\partial \bar{\sigma}_{12} \Rightarrow \bar{\epsilon}_{12} = (\alpha\sqrt{3}/2)(\sqrt{3}\bar{\sigma}_{12}/\bar{\sigma}_0)^n. \tag{3.19}$$

By comparing (3.19) and (3.13), one obtains the approximate upper bound to $\bar{\tau}_0/\tau_0$ as

$$\bar{\tau}_0/\tau_0 = (2/\sqrt{3})^{1/n}f(n)/\sqrt{3}. \tag{3.20}$$

This is shown as the upper dashed curve in figure 2.
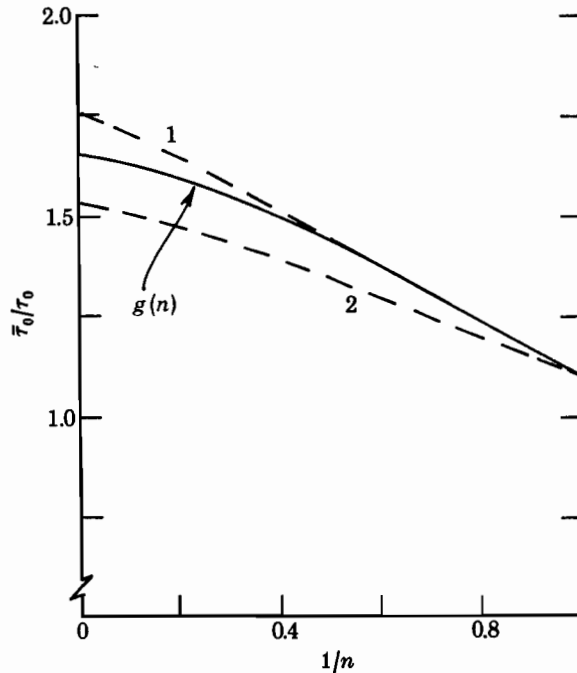
FIGURE 2. Upper bound to the reference stress in shear for f.c.c. polycrystals and comparison with estimates obtained from the uniaxial bound using two phenomenological theories: 1, Based on the effective stress from (3.20) and 2, based on the maximum shear stress from (3.22).

The assumption of a universal relation between the maximum shear strain-rate and maximum shear stress is another criterion which is commonly used to convert back and forth from uniaxial data to shear data in an isotropic material. Applying this criterion to convert the uniaxial relation (2.23) to pure shear gives

$$\bar{\epsilon}_{12} = (3\alpha/4)(2\bar{\sigma}_{12}/\bar{\sigma}_0)^n. \tag{3.21}$$

Comparing (3.21) and (3.13), again with $\bar{\sigma}_0 = f(n)\,\tau_0$, gives

$$\bar{\tau}_0/\tau_0 = (4/3)^{1/n} f(n)/2 \tag{3.22}$$

which is shown as the lower dashed curve in figure 2.

At $n = 1$ the two estimates (3.20) and (3.22) necessarily coincide with the actual bound. At the other limit, $n = \infty$, the actual bound falls roughly half way between the two estimates. However, over the range $1 < n < 5$ the estimates based on the approximate potential (3.18) appear to be inherently better than those based on the maximum shear stress criterion. In fact, for $n \leqslant 3$ the results of figure 2 suggest that the simple potential (3.18) supplies a rather accurate approximation to the actual uniform strain-rate upper bound. A potential such as (3.18) which is based on the single invariant $\bar{\sigma}_e$ is frequently taken as a phenomenological characterization of steady creep behaviour (Odqvist 1960; Rabotnov 1969).

4. Self-consistent theory for steady creep of polycrystalline materials

For macroscopically homogeneous deformations of a polycrystal the overall stress and strain-rates are just the averages of their local values, as discussed in §2, i.e.

$$\bar{\sigma} = \{\sigma\}, \quad \bar{\varepsilon} = \{\varepsilon\}. \tag{4.1\,a, b}$$

The self-consistent model provides an approximate procedure for calculating the stress and strain-rate in each individual crystalline grain and, through (4.1), provides an estimate of the overall behaviour. As it applies to linearly elastic polycrystals and composites, self-consistent theory has been developed by Hershey (1954), Kröner (1958), Budiansky (1965) and Hill (1965). Two different models have been proposed to extend the theory to include time-independent plasticity: (i) the K.B.W. model of Kröner (1961) and Budiansky & Wu (1962) and (ii) Hill's (1965) model. Both models are formulated to deal with incremental behaviour. That is, these models relate increments in overall stress and strain to the single crystal incremental behaviour at each stage of the deformation history. A comparative study of the models as they apply to the plastic deformation of polycrystals was given by Hutchinson (1970). While the K.B.W. is computationally the simpler of the two, the Hill model is more realistic, particularly in the way that it deals with overall anisotropy. Hill's scheme will be applied here to the steady problem. First, we will formulate the steady creep problem in incremental form and apply the self-consistent theory to calculate the overall behaviour for an incremental step. Then we will show that the incremental self-consistent equations can be 'integrated-up' to a convenient form. Finally, it will be shown that the resulting self-consistent equations can be arrived at directly via a short cut interpretation.

A related study of non-steady creep of f.c.c. polycrystals was conducted by Brown (1970) using the K.B.W. model. He assumed the same single crystal law (2.3)

used here. Under a step application of overall stress the crystals are stressed elastically at the start. Initially the crystals respond in a non-steady manner, but with increasing time the stresses in the grains relax to their steady-state values, which, for the K.B.W. model, are identical to those predicted by the uniform strain-rate upper bound. Thus, the limiting steady-state relation between the overall stress and strain-rate according to Brown's formulation of the K.B.W. model is precisely that given by the procedures of the previous section.

(a) Formulation as an incremental problem relating $d\varepsilon$ and $d\overline{\sigma}$

Let $\overline{\sigma}$ be applied to the polycrystal and suppose (for the moment) that the stress σ in each grain is known and is uniform within each grain. From (2.6) and (2.11) the instantaneous incremental compliances are then also known in each grain; within a grain a stress increment is related to an increment in steady strain-rate by $d\varepsilon = nM^c d\sigma$. Apply an increment of overall stress $d\overline{\sigma}$ to the polycrystal. We wish to calculate the increment in overall steady strain-rate $d\overline{\varepsilon}$. Equivalently, from (2.22), we will calculate the instantaneous overall incremental compliances nM in terms of the single crystal compliances nM^c. To do this we will follow the prescription for the application of the self-consistent method to incrementally linear problems as laid out by Hill (1965). The typical grain with uniform instantaneous compliances nM^c is taken to have a spherical shape (or, more generally, an ellipsoidal shape) with its crystal axes orientated in a definite way with respect to the specimen axes. The grain is embedded in an infinite matrix with instantaneous compliances nM which are the unknown overall incremental compliances. The overall stress increment $d\overline{\sigma}$ is applied to the matrix at infinity. Self-consistency requires that

$$d\overline{\sigma} = \{d\sigma\}, \tag{4.2}$$

where $\{\ \}$ denotes the properly weighted average over all shapes and orientations. In the present study we restrict attention to spherical shapes and a random distribution of grain orientations so that $\{\ \}$ denotes an equally weighted average over all orientations.

Eshelby's (1957) well known general solution to the isotropic elastic inclusion problem can be used to solve for $d\sigma$ in the grain in terms of $d\overline{\sigma}$. An important property of this solution is that, for spherical or ellipsoidal grains with uniform compliances, $d\sigma$ is uniform within the grain. Denote the fourth order concentration tensor relating $d\sigma$ and $d\overline{\sigma}$ by B^c so that

$$d\sigma = B^c d\overline{\sigma}. \tag{4.3}$$

The most convenient general expression for B^c is obtained using the fourth order constraint tensor M^* introduced by Hill in the following way. Remove the spherical grain and $d\overline{\sigma}$ at infinity; apply a traction $d\sigma_{ij}^* n_j$ over the surface of the spherical void, where n is the inward unit normal to the void surface and $d\sigma^*$ is constant. The instantaneous incremental compliances of the infinite matrix are still nM. The resulting deformation of the void surface corresponds to a uniform straining

$d\varepsilon^*$ in the sense that the velocity-increment at any point on the surface is given by $dv_i = d\varepsilon_{ij}^* x_j$ (plus a possible rigid body contribution). The constraint tensor is defined by

$$d\varepsilon^* = -nM^* d\sigma^*, \tag{4.4}$$

where we carry along in the definition the multiplicative factor n present in the overall incremental compliances. Since M has diagonal symmetry, it can be shown that M^* does. For spherical shapes, M^* depends only on M. Calculations carried out here will be restricted to overall uniaxial tension for which M and M^* have transverse isotropy with respect to the tensile axis. General formulas for M^* are available for this case as discussed in the appendix.

The constraint tensor can be used to relate the discrepancy between the strain-rate increment at infinity and that in the grain to the corresponding discrepancy in stress increments

$$d\bar{\varepsilon} - d\varepsilon = -nM^*(d\bar{\sigma} - d\sigma). \tag{4.5}$$

Using (2.11) and (2.22), one can rewrite (4.5) as

$$(M^* + M^c) d\sigma = (M^* + M) d\bar{\sigma}. \tag{4.6}$$

Hence, by (4.3),

$$B^c = (M^* + M^c)^{-1} (M^* + M). \tag{4.7}$$

From (4.2) and (4.3), the self-consistent condition is

$$\{B^c\} = I, \tag{4.8}$$

where I is the fourth order identity tensor in (1.1). Alternatively, since

$$d\varepsilon = nM^c B^c d\bar{\sigma}, \quad d\bar{\varepsilon} = \{d\varepsilon\} \quad \text{and} \quad d\bar{\varepsilon} = nM d\bar{\sigma},$$

another self-consistent equation is

$$M = \{M^c B^c\}. \tag{4.9}$$

A variation which combines (4.8) and (4.9) is

$$\{(M - M^c) B^c\} = 0. \tag{4.10}$$

As Hill (1965) has shown, the self-consistent equations (4.8)–(4.10), as well as other variants, are completely equivalent for spherical grains. Equation (4.10) has a slight advantage over the other two, for numerical work, in that $(M - M^c) B^c$ has diagonal symmetry, while the same is not true in general for B^c and $M^c B^c$.†

In deriving (4.8)–(4.10) it was assumed that the stress σ in each grain, and consequently M^c, was known at the overall stress $\bar{\sigma}$. It remains to close the system of equations by integrating the incremental equations from the state of zero stress to the overall stress $\bar{\sigma}$. We are free to choose any overall history to reach $\bar{\sigma}$ since the end state is independent of history. The simplest is to take the proportional history

$$\lambda\bar{\sigma}, \quad 0 \leqslant \lambda \leqslant 1, \tag{4.11}$$

† It can be shown that $(M - M^c) B^c = (M^* + M)(M^* + M^c)^{-1}(M^* + M) - (M^* + M)$ from which diagonal symmetry of this combination is obvious.

so that corresponding to $d\lambda$ is the increment $d\overline{\sigma} = \overline{\sigma}\,d\lambda$ in the overall stress. Because of the pure power relation between the strain-rate quantities and the stress quantities, the stress in each grain increases in direct proportion to λ (in the actual boundary value problem as well as the self-consistent model) and therefore in a typical grain the stress is $\lambda\sigma$ where σ, as previously introduced, is the stress associated with $\overline{\sigma}$. Now we exploit the homogeneous stress dependence of the compliances and the constraint tensor according to

$$M^c(\lambda\sigma) = \lambda^{n-1}M^c(\sigma), \quad M(\lambda\overline{\sigma}) = \lambda^{n-1}M(\overline{\sigma}), \quad M^*(\lambda\overline{\sigma}) = \lambda^{n-1}M^*(\overline{\sigma}). \quad (4.12)$$

An immediate consequence of (4.12) is that B^c in (4.7) for each grain is independent of λ and depends only on the end state. Thus, integration of (4.3) gives

$$\sigma = B^c\overline{\sigma}. \quad (4.13)$$

Also, from (2.11) and (4.12), $d\varepsilon = n\lambda^{n-1}M^c(\sigma)\,\sigma\,d\lambda$; integration from $\lambda = 0$ to $\lambda = 1$ gives

$$\varepsilon = M^c(\sigma)\,\sigma. \quad (4.14)$$

Similarly, (2.22) can be integrated to give

$$\overline{\varepsilon} = M(\overline{\sigma})\,\overline{\sigma}. \quad (4.15)$$

The system of equations has thus been integrated to a total form. The complete system of equations used here in the numerical calculation of the overall compliances M in terms of a given $\overline{\sigma}$ can be summarized as

$$\sigma = B^c\overline{\sigma}, \quad B^c = (M^* + M^c)^{-1}(M^* + M), \quad \{(M - M^c)\,B^c\} = 0, \quad (4.16a, b, c)$$

where M^c depends on σ according to (2.6) and M^* depends on M as described further in the appendix.

(b) Interpretation as a total problem relating $\overline{\varepsilon}$ and $\overline{\sigma}$

Having arrived at (4.16) via an incremental formulation, we can now give an interpretation in terms of a total formulation. Equations (4.16), together with (4.13)–(4.15), are precisely those one would obtain from the model as depicted in figure 3. Now the typical spherical grain has compliances $M^c(\sigma)$, in the sense of (4.14); and the infinite matrix has the unknown *uniform* compliances $M(\overline{\sigma})$, as in (4.15), where $\overline{\sigma}$ is applied at infinity. In applying the self-consistent scheme, regard M as fixed in the sense that (4.15) provides a linear relation between $\overline{\varepsilon}$ and $\overline{\sigma}$. The resulting equations are then (4.13)–(4.16) so that this total formulation is completely equivalent to the integrated incremental equations. The equivalence depends crucially on the pure power character of the constitutive law which permits the two interpretations for the compliances, (2.21) and (2.22).

The total formulation brings out one feature of the self-consistent scheme, as it is applied here, which is somewhat obscured by the incremental derivation. The

infinite matrix is assigned the unknown overall compliances (as in an application to a linear material) but, in addition, these compliances are taken to depend on the average stress $\bar{\sigma}$ in the matrix and not on the local stress in the matrix. (Of course, for a linear material this distinction does not arise.) Thus, grain interaction is approximated by 'smearing out' all grains surrounding the typical spherical grain, as usual, but, in addition, stress induced variations of the compliances in the surrounding grains are smeared out as well.

An alternative self-consistent scheme suggested by the above discussion would allow the unknown overall compliances to depend on the local stress in the matrix according to $M(\sigma)$. Although this modification is likely to give somewhat improved estimates of overall material behaviour, the computational aspects become almost prohibitive. However, Huang (1971) has carried out the necessary calculations for the plane deformation of a nonlinear material with rigid circular fibers. To do so he was forced to assume an approximate functional form for $M(\sigma)$.
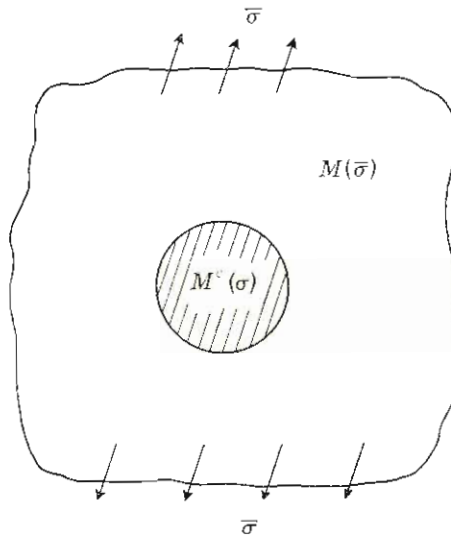
FIGURE 3. Self-consistent model.

(c) *Self-consistent results for f.c.c. polycrystals in tension*

With the tensile reference stress $\bar{\sigma}_0$ defined in (2.23), the self-consistent result can be presented as

$$\bar{\sigma}_0/\tau_0 = h(n). \tag{4.17}$$

In the limit $n = 1$ the compliances (3.1) are stress-independent with cubic symmetry. The overall compliances are isotropic since a random distribution of grain orientation is assumed. The overall moduli can be calculated in closed form (details are omitted); when translated into the form (4.17), the result is

$$h(1) = \tfrac{3}{2}. \tag{4.18}$$

Some feeling for the accuracy of the self-consistent result for $n = 1$ can be had by comparing it with the following rigorous upper and lower bounds:

$$\frac{5}{6}\frac{3}{2} < \frac{63}{66}\frac{3}{2} \leqslant \frac{\bar{\sigma}_0}{\tau_0} \leqslant \frac{129}{126}\frac{3}{2} < \frac{11}{10}\frac{3}{2}. \tag{4.19}$$

(Reuss)   (H.-S.)   (H.-S.)   (Voigt)

The outermost bounds are the simple Reuss and Voigt (3.11) values. The inner bounds, denoted by H.–S. are obtained by using the procedures of Hashin & Shtrikman (1962) and Walpole (1966). (Again, details of these calculations need not be included here.) From (4.19), the self-consistent estimate can be in error by at most 4 % when $n = 1$.

In the nonlinear range, $n > 1$, the solution to the self-consistent equations depends on the overall stress $\bar{\sigma}$ in a highly implicit way and use of a numerical iteration procedure becomes essential. In principle, the scheme adopted here is as follows. Take $\bar{\sigma}$ to be prescribed and assume that at any stage of the iterative process an estimate of M (and therefore M^*) is available. The compliances of any grain M^c are the function of the stress σ in the grain given by (2.6), and σ is in turn a function of $\bar{\sigma}$ through (4.16a). Thus, even with $\bar{\sigma}$, M and M^* specified, the calculation of σ, M^c and B^c is not explicit but must be calculated in an iterative fashion. This sub-step is performed for each grain orientation by using a highly efficient Newton method described in the appendix. Once calculated, the values of M^c and B^c are used to obtain an improved estimate of M from (4.16c). This higher level iteration is also based on Newton's method with its associated rapid convergence. The numerical method takes advantage of the fact that results over the entire range of n are desired. Results for the linear case, $n = 1$, are used as the starting point in the iterations for $1/n = 0.8$, for example, and, when convergence has been obtained in this case, that solution is in turn used to start off iterations for a smaller value of $1/n$. Sufficiently many grain orientations were taken to ensure that the calculated values of $h(n)$ given in table 1 are in error by less than 1 %. Further details of the numerical procedure are given in the appendix.

A plot of $h(n)$ is included with the upper bound in figure 1. Perhaps the most significant aspect of this comparison is the decreasing discrepancy between the two sets of results with increasing n.[†] The largest value of n used in the self-consistent calculation was $n = 10$; extrapolation of $h(n)$ from $1/n = \frac{1}{10}$ to $1/n = 0$ in figure 1 suggests that the limit value $h(\infty)$ is very close to the Taylor upper bound value 3.06. A straight line approximation passing through the values $\frac{3}{2}$ at $n = 1$ and 3.06 at $n = \infty$ provides an excellent approximation to the self-consistent results, namely,

$$\bar{\sigma}_0/\tau_0 = 3.06 - 1.56/n. \tag{4.20}$$

The limit value $\bar{\sigma}_0/\tau_0 = 3.06$ is sometimes used in the metallurgical literature to convert steady creep shear data for single crystals to equivalent tensile data for

[†] We have not calculated the analogue of the Reuss lower bound for $n > 1$ since it is unrealistically low.

polycrystals or vice versa. Aside from the difficulty of properly accounting for the dependence of τ_0 on grain size, the use of 3.06 rather than (4.20) leads to an error in the strain-rate in this conversion which is roughly a factor of 2 for all values of n.

5. UPPER BOUNDS FOR IONIC POLYCRYSTALS

We consider ionic crystals which can slip on the two systems shown in figure 4: the A-systems, $\{110\}\langle110\rangle$, and the B-systems, $\{100\}\langle100\rangle$. The A-systems include only two linearly independent μ's; the B-systems include three linearly independent μ's. Together they comprise five linearly independent systems. An additional property, which is easily established and which will be significant in the analysis below, is that the μ's of the A-systems are orthogonal to those of the B-systems, i.e.

$$\mu^{(k)}\mu^{(m)} = 0, \quad \text{for } k \text{ in A and } m \text{ in B.} \tag{5.1}$$

Gilman (1961) has given an extensive background discussion of the inelastic properties of a large number of ionic materials. Many polycrystalline ionic materials, ceramics being examples, are extremely brittle at low or even room temperatures due to the fact that slip on a B-system requires inordinately high stress for its activation. As a result each crystal has effectively only two linearly independent slip systems and a general inelastic accommodation of the crystals is not possible. At higher temperatures the stress required to cause slip on the B-systems may become sufficiently low to provide a full complement of five linearly independent systems and then an overall inelastic deformation of the polycrystal becomes possible.

For such ionic crystals (2.3) specializes to

$$\begin{aligned}
\gamma^{(k)} &= \alpha(\tau^{(k)}/\tau_A)^n \quad \text{for} \quad \text{A-systems,} \\
\gamma^{(k)} &= \alpha(\tau^{(k)}/\tau_B)^n \quad \text{for} \quad \text{B-systems,}
\end{aligned} \tag{5.2}$$

where τ_A and τ_B will be called the reference stresses for the A and B systems and n is restricted to be the same for both systems. Some data of Gilman (1959) for lithium fluoride crystals is included in figure 4 to show the strong temperature dependence of the critical resolved shear stress for this material. Gilman's tests were run at a strain-rate on the order of 10^{-5} s^{-1}. His data was not taken under steady conditions, so the plots of the shear stresses in figure 4 can only be regarded as qualitative estimates of τ_A and τ_B for present purposes.

For $n = 1$ the tensor of compliances of the crystal can be calculated simply. In the cubic axes of the crystal the compliances are completely specified by

$$M^c_{1111} + 2M_{1122} = 0, \quad M^c_{1111} - M^c_{1122} = 3\alpha/2\tau_A, \quad M^c_{1212} = \alpha/2\tau_B. \tag{5.3}$$

The compliances are isotropic if $\tau_A = 3\tau_B/2$.

We now investigate the uniform strain-rate upper bound which was discussed in §3 for a polycrystal with randomly orientated ionic crystals. It is convenient to exploit the property (5.1) for orthogonality between the two sets of slip systems.

For any trial stress in (3.6) we can always write $\hat{\sigma} = \hat{\sigma}_A + \hat{\sigma}_B$ where $\hat{\sigma}_A \mu^{(k)} = 0$ for k in B and $\hat{\sigma}_B \mu^{(k)} = 0$ for k in A. Then (3.6) becomes

$$\hat{\sigma}\bar{\varepsilon} - F^c(\hat{\sigma}) = \left[\hat{\sigma}_A\bar{\varepsilon} - \frac{\alpha\tau_A}{n+1}\sum_A |\mathcal{T}^{(k)}/\tau_A|^{n+1}\right] + \left[\hat{\sigma}_B\bar{\varepsilon} - \frac{\alpha\tau_B}{n+1}\sum_B |\mathcal{T}^{(k)}/\tau_B|^{n+1}\right], \quad (5.4)$$

where $\mathcal{T}^{(k)} = \hat{\sigma}_A \mu^{(k)}$ for k in A and $\mathcal{T}^{(k)} = \hat{\sigma}_B \mu^{(k)}$ for k in B. The decomposition in (5.4) shows that to maximize $\hat{\sigma}\bar{\varepsilon} - F^c(\hat{\sigma})$ each of the two parts may be maximized
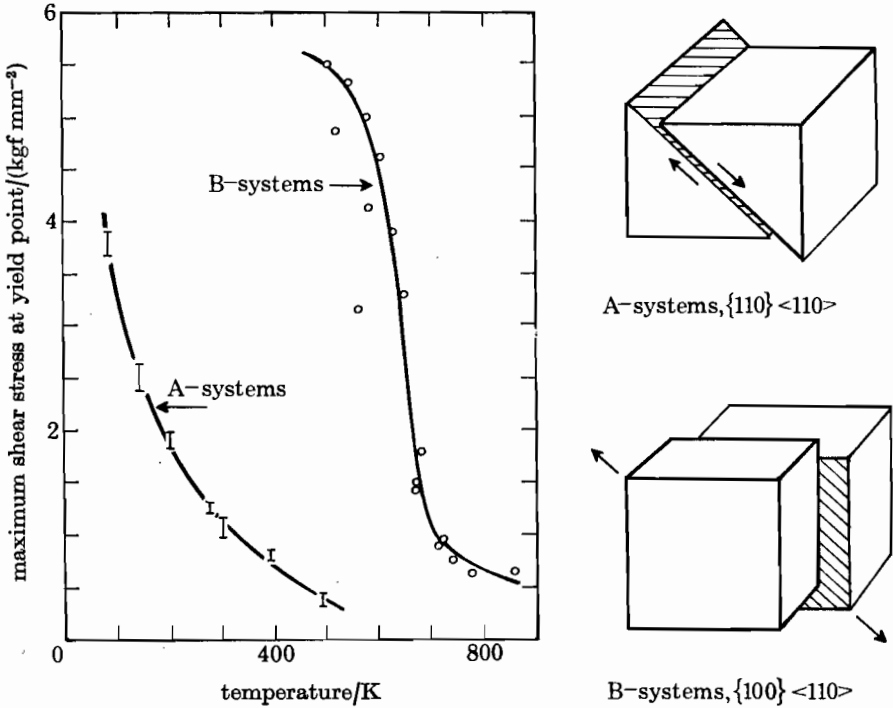
FIGURE 4. Gilman's (1959) data for the yield stresses on the two systems of lithium fluoride single crystals.

independently, since the terms in one of the square brackets are completely independent of those in the other. As a consequence, the maximizing stress σ^u must be of the form

$$\sigma^u = (|\bar{\varepsilon}|/\alpha)^{1/n}[\tau_A\,\omega_A + \tau_B\,\omega_B] \quad (5.5)$$

for all combinations of τ_A and τ_B. Here ω_A and ω_B depend on n, grain orientation and $\bar{\varepsilon}/|\bar{\varepsilon}|$ but *not* on τ_A or τ_B. The upper bound (3.4) for prescribed $\bar{\varepsilon}$ can be written as

$$\bar{\sigma}\bar{\varepsilon} \leqslant (|\bar{\varepsilon}|/\alpha)^{1/n}[\tau_A\{\omega_A\,\bar{\varepsilon}\} + \tau_B\{\omega_B\,\bar{\varepsilon}\}]. \quad (5.6)$$

In words, the upper bound to the dissipation-rate, for a prescribed $\bar{\varepsilon}$, is a linear combination of τ_A and τ_B. This property cannot be expected to hold when the two sets of slip systems are not mutually orthogonal.

(a) *Upper bound to the tensile reference stress*

In simple tension, as in (3.8) with $\bar{\sigma}_0$ defined in (2.23), the upper bound (5.6) can be reduced to

$$\bar{\sigma}_0 \leqslant A(n)\tau_A + B(n)\tau_B, \tag{5.7}$$

where $A(n) = \{\omega_A\bar{\varepsilon}\}/\bar{\varepsilon}$ and $B(n) = \{\omega_B\bar{\varepsilon}\}/\bar{\varepsilon}$. For $n = 1$ the calculations can be carried out analytically leading to

$$A(1) = \tfrac{2}{3}, \quad B(1) = \tfrac{9}{10}. \tag{5.8}$$

For $n > 1$ numerical calculations are required but these are not different in principle from these carried out for the f.c.c. structure. Plots of $A(n)$ and $B(n)$ are shown in
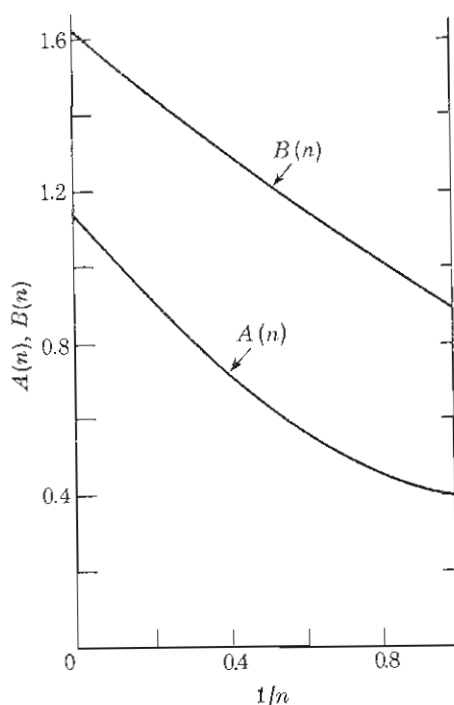
FIGURE 5. Upper bound to the tensile reference stress for ionic polycrystals:
$$\bar{\sigma}_0 \leqslant A(n)\,\tau_A + B(n)\,\tau_B.$$

figure 5 and numerical values are given in table 1. Limiting values corresponding to rigid/perfectly plastic single crystals ($n \to \infty$) are

$$A(\infty) = 1.154, \quad B(\infty) = 1.633 \tag{5.9}$$

and are accurate to four significant figures. To determine these values we have used the analytic expressions for ω_{A33} and ω_{B33}, in our notation, which were obtained by Chin (1973) in his study of the deformation of perfectly plastic ionic crystals. We evaluated $\{\omega_{A33}\}$ and $\{\omega_{B33}\}$ using numerical integration. From figure 5 it is seen

that the results for large, but finite, n extrapolate smoothly into the limiting values (5.9), even though the results for finite n were obtained using an entirely different numerical procedure. This must be the case since the limit as $n \to \infty$ of the maximum principle associated with (5.4) is the Bishop–Hill maximum work principle.

Thus the analogue for the ionic structure of the Taylor result for the tensile limit load of an f.c.c. polycrystal of rigid-perfectly plastic single crystals (i.e. $\bar{\sigma}_0 \leqslant 3.06 \, \tau_0$) is

$$\bar{\sigma}_0 \leqslant 1.154 \, \tau_A + 1.633 \, \tau_B. \tag{5.10}$$

If τ_A and τ_B differ widely, texturing effects, such as those discussed by Chiu & Mammel (1973), may be important. Then the assumption of a random distribution of grain orientations used in calculating (5.10) must be replaced by distributions with preferred orientations.

(b) Upper bound in pure shear and approximate bounding potentials

In a macroscopic pure shearing with the overall reference stress in shear $\bar{\tau}_0$ defined by (3.13), the upper bound (5.6) reduces to

$$\bar{\tau}_0 \leqslant C(n) \, \tau_A + D(n) \, \tau_B, \tag{5.11}$$

where $C(n) = (2/\sqrt{3})^{1/n} \{\omega_{A12}\}$ and $D(n) = (2/\sqrt{3})^{1/n} \{\omega_{B12}\}$. For $n = 1$,

$$C(1) = \tfrac{4}{15}, \quad D(1) = \tfrac{3}{5}. \tag{5.12}$$

Numerical values of C and D are given in table 1 and plots are shown in figure 6. By extrapolating to the limit $1/n \to 0$, we find

$$\bar{\tau}_0 \leqslant 0.62 \, \tau_A + 0.90 \, \tau_B. \tag{5.13}$$

Proceeding as was done for f.c.c. polycrystals, we compare (5.11) with the estimates of $\bar{\tau}_0$ obtained from $\bar{\sigma}_0$ by using the two most common phenomenological theories. Using (3.18) with $\bar{\sigma}_0 = A\tau_A + B\tau_B$, we find after manipulations similar to those used in the f.c.c. comparison

$$\bar{\tau}_0 = (1/\sqrt{3})\,(2/\sqrt{3})^{1/n} [A(n) \, \tau_A + B(n) \, \tau_B]. \tag{5.14}$$

Similarly, using the conversion based on maximum shear stress and maximum shear strain-rate, we find

$$\bar{\tau}_0 = (\tfrac{1}{2})\,(\tfrac{4}{3})^{1/n} [A(n) \, \tau_A + B(n) \, \tau_B]. \tag{5.15}$$

The multiplicative factors of τ_A and τ_B in (5.14) and (5.15) are compared with $C(n)$ and $D(n)$ in figure 6. The conclusion for ionic polycrystals is similar to that drawn for f.c.c. polycrystals. Use of the single invariant $\bar{\sigma}_e$ to represent multi-axial states appears to involve little error in the bounding potential.
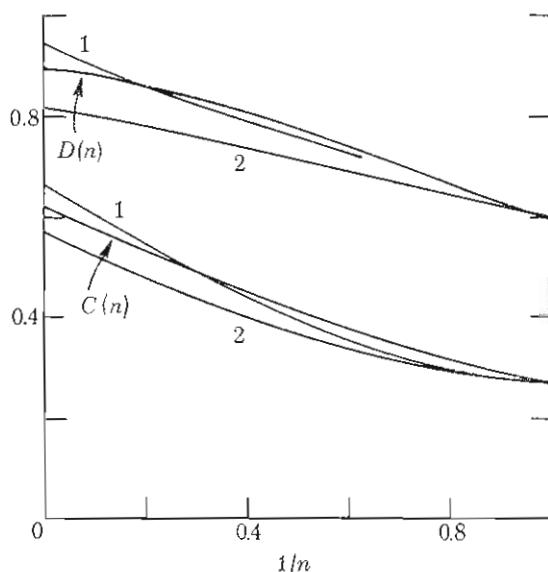
FIGURE 6. Upper bound to the reference stress in shear for ionic polycrystals,
$$\bar{\tau}_0 \leqslant C(n)\,\tau_A + D(n)\,\tau_B,$$
and comparison with estimates obtained from the uniaxial bound using two phenomeno-
logical theories: (1) based on the effective stress from (5.14) and (2) based on the maximum
shear stress from (5.15).

6. SELF-CONSISTENT RESULTS FOR IONIC POLYCRYSTALS

The self-consistent theory described in §4 was also applied to the tensile be-
haviour of ionic polycrystals with randomly orientated single crystals. For $n = 1$,
the overall moduli are isotropic and can be calculated in terms of M^c specified by
(5.3). The self-consistent calculation gives

$$\bar{\sigma}_0 = \tfrac{1}{4}\tau_B[1 + (1 + 16\tau_A/\tau_B)^{\frac{1}{2}}].\tag{6.1}$$

This prediction is compared with various bounds in figure 7 where, to cover the
entire range of τ_A and τ_B, $\bar{\sigma}_0$ has been normalized by τ_A for $\tau_B < \tau_A$ and by τ_B for
$\tau_A < \tau_B$. With $n = 1$, (5.7) is the Voigt upper bound; the Reuss lower bound is

$$\bar{\sigma}_0 \geqslant (\tfrac{5}{2})\,(1/\tau_A + 1/\tau_B)^{-1}.\tag{6.2}$$

The bounds obtained by the methods of Hashin & Shtrikman (1962) and Walpole
(1966) can be expressed as

$$\bar{\sigma}_0 \leqslant (\tfrac{5}{2})\,(1/\tau_A + 1/\tau_B)^{-1} \times \text{the greater of } (\psi_1, \psi_2),\tag{6.3}$$

$$\bar{\sigma}_0 \geqslant (\tfrac{5}{2})\,(1/\tau_A + 1/\tau_B)^{-1} \times \text{the smaller of } (\psi_1, \psi_2),\tag{6.4}$$

where
$$\psi_1 = [19 + 4\tau_A/\tau_B]/[10 + 25(1 + \tau_B/\tau_A)^{-1}],$$
$$\psi_2 = [32 + 27\tau_B/\tau_A]/[20 + 75(1 + \tau_A/\tau_B)^{-1}].$$

All bounds coincide when $\tau_B/\tau_A = \frac{2}{3}$ since the crystal compliances are isotropic. Otherwise, the self-consistent results fall roughly halfway between the inner bounds, and these are relatively close as long as τ_A and τ_B do not differ by more than a factor of about five.

The simple property of the upper bound (5.7), whereby the bound was a linear combination of τ_A and τ_B, obviously does not carry over to the self-consistent results. Thus $\bar{\sigma}_0$ must be calculated independently for each value of τ_A/τ_B. We have calculated $\bar{\sigma}_0$ as a function of n for three values of τ_A/τ_B chosen to typify the range of
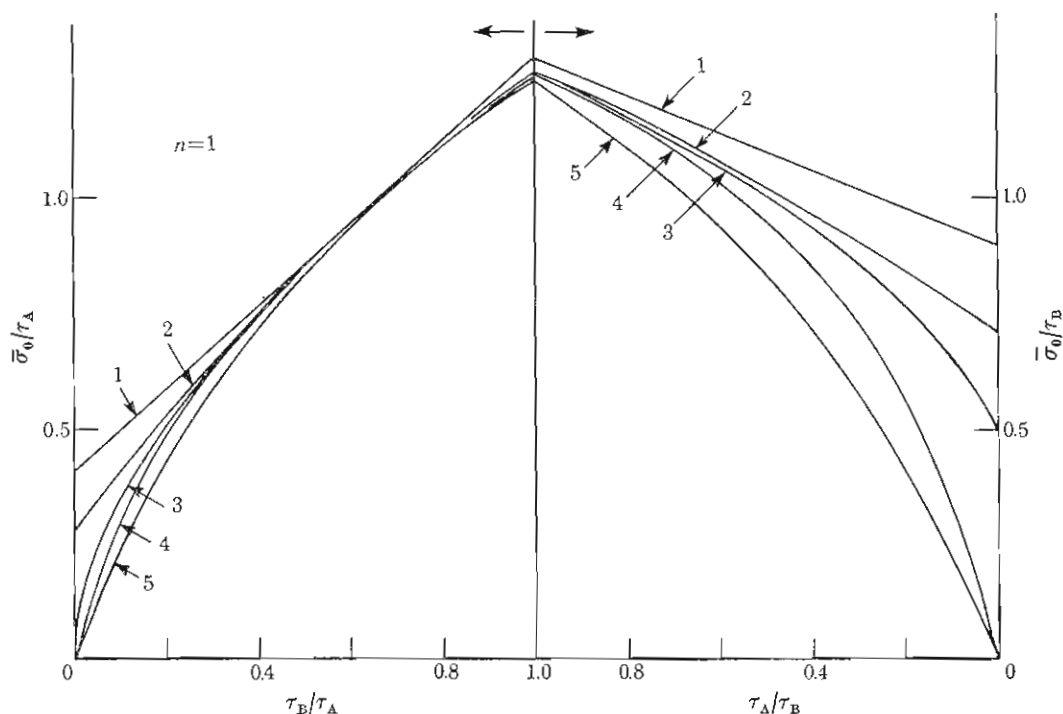
FIGURE 7. Comparison of self-consistent results and various bounds for linear viscoelastic behaviour ($n = 1$) of ionic polycrystals. 1, Voigt upper bound; 2, H.–S. upper bound; 3, Self-consistent result; 4, H.–S. lower bound; 5, Reuss lower bound.

possibilities, i.e. $\tau_A/\tau_B = 10$, 1, $\frac{1}{5}$. For $\tau_A/\tau_B = 1$, the self-consistent result falls below the upper bound (5.7) by only 3 % when $n = 1$ and this difference diminishes as n increases. For $\tau_A/\tau_B = 10$ and $\frac{1}{5}$ the discrepancy between the self-consistent results and the upper bound (5.7) is considerable when $n = 1$. However, for larger n the discrepancy diminishes significantly as can be seen in the two plots of figure 8. We are again led to conclude that in the highly nonlinear range characteristic of the creep of most materials ($n \geqslant 3$) the uniform strain-rate upper bound is reasonably accurate, assuming one is willing to use the self-consistent predictions as a standard of comparison.
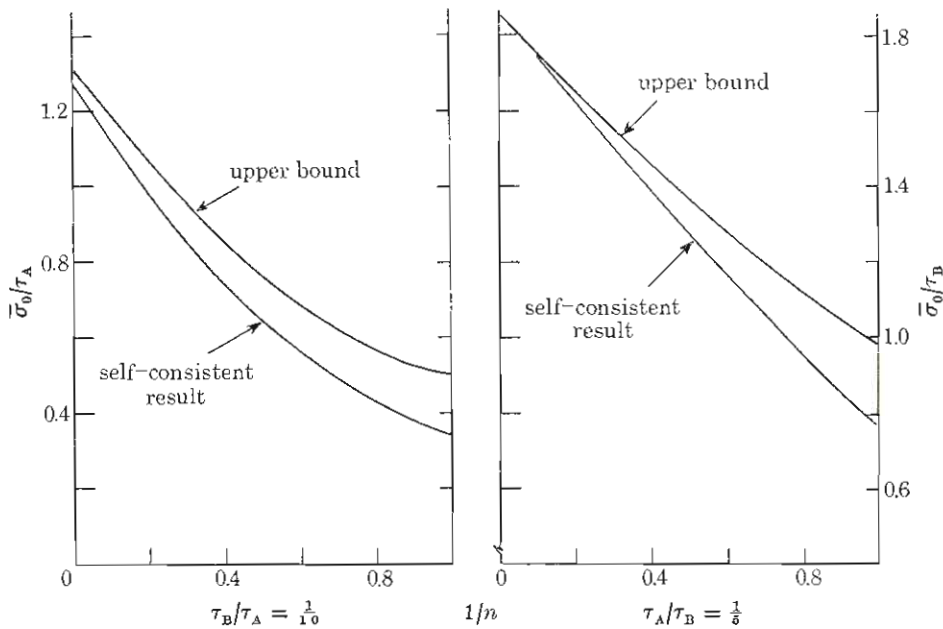
FIGURE 8. Upper bounds and self-consistent results for the tensile reference stress of ionic polycrystals.

7. CONCLUSIONS AND DISCUSSION

Self-consistent theory and the uniform strain-rate upper bound have been employed to estimate the properties of a class of nonlinear materials with a pure power stress dependence. Numerical work associated with the self-consistent method is more complicated than for the upper bound but is still far from being prohibitive. Significantly, the discrepancy between the upper bound and the self-consistent results is relatively small for $n \geqslant 3$ in each example considered here.

The results contained within provide a basis for converting single crystal steady creep data to polycrystal data and vice versa, although the usual difficulties involved in such conversions still remain. In particular, the single crystal data must be representative of the size of grain in the polycrystal. The creep law taken to describe single crystal behaviour neglects interaction effects between actively creeping systems. This is likely to be an over-simplification. A careful correlation of single crystal data and polycrystalline data brought into correspondence through the formulas presented here should shed some light on this question. Grain boundary sliding has been neglected which may render the present results invalid in certain ranges of temperature and stress, as has already been discussed.

Exploration of steady creep potentials has been limited to comparing bounds in tension and shear. The most commonly used steady creep law, based on the single effective stress invariant $\bar{\sigma}_e$ in (3.17), appears to account for multi-axial stress

dependence reasonably accurately, even more so in creep applications in the range $n \leqslant 5$ than for time-independent plasticity. This finding is generally in accord with Rabotnov's (1969, ch. V, §§ 77 and 78) conclusion based on his extensive examination of experimental data for a number of different metals in tension and shear.

The self-consistent model can be extended without essential additional difficulty to analyse effects such as texturing where a non-random distribution of crystal orientations is present. In incremental form, it can also be applied to the calculation of non-steady creep behaviour. As mentioned earlier, Brown (1970) examined non-steady behaviour using the K.B.W. model and the same steady single crystal constitutive relation used here. In his study non-steady effects were due entirely to grain interaction. Non-steady single crystal mechanisms are also likely to make a major contribution to non-steady polycrystalline behaviour. Mitra & McLean (1966) have performed some critical tests related to work hardening and recovery mechanisms in non-steady creep, and Ponter & Leckie (1975) have incorporated the features of their experimental findings into a phenomenological creep law for multi-axial stress states. Further work along the lines carried out here should provide some guidelines for the formulation of such phenomenological theories.

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Appendix

(a) *Numerical method for upper bound calculations*

With prescribed $\bar{\varepsilon}$, (3.5) must be solved for σ^u for each grain orientation. This requires an iterative procedure. Let σ denote the estimate of σ^u at any stage in the iteration process and let $\sigma + \Delta\sigma$ be the next estimate. Solving for $\Delta\sigma$ from (3.5), one finds that to order $|\Delta\sigma|^2$

$$\Delta\sigma = [(\partial M^c/\partial\sigma_{pq})\,\sigma_{pq} + M^c]^{-1}\,[\bar{\varepsilon} - M^c\sigma], \tag{A 1}$$

where M^c and its partial derivatives are evaluated at σ. One can show directly from the definition of M^c in (2.6), or simply as a consequence of the homogeneous dependence on stress, that

$$(\partial M^c/\partial\sigma_{pq})\,\sigma_{pq} = (n-1)\,M^c. \tag{A 2}$$

Thus, (A. 1) reduces to the attractive form

$$\Delta\sigma = (1/n)\,(M^{c-1}\bar{\varepsilon} - \sigma). \tag{A 3}$$

Since the material is inherently incompressible, M^c is singular. For numerical work this is easily overcome by converting σ and $\bar{\varepsilon}$ to 5-component vectors with an appropriate conversion of M^c. In this way, M^c becomes non-singular; the inverse of M^c in (A 3) is to be taken in this sense.

An iterative procedure based on repeated use of (A 3) leads to the rapid convergence associated with Newton's method. To start off each iteration we used the value of σ^u for the same grain orientation at a slightly smaller value of n. This proved to be a highly efficient way to cover the range $0 < 1/n \leqslant 1$. At $n = 1$ no iteration is needed. Typically, steps of $1/n = \frac{1}{10}$ were used. Calculations were made for values of n as large as 20; but for $n > 10$ rather small steps in $1/n$ were necessary to avoid poor starting values.

The integrations over all orientations were replaced by summations over a discrete number of orientations using a standard numerical integration technique. In overall tension, symmetry permits integration over only one of the spherical triangles associated with the Euler angles which relate the crystal axes to the specimen axes. In this case 36 orientations were chosen. In pure shear it is necessary

to integrate over the spherical triangle plus the third Euler angle; but, again, symmetry permits a considerable reduction of the number of integration stations, so that 105 stations gave accuracy to within 1 % when $n = 1$.

(b) Numerical method for self-consistent calculations

First, the method for solving for σ, M^c and B^c for each grain will be discussed given that M and $\overline{\sigma}$ are specified. Then a method for obtaining M from the self-consistent equations will be given.

In simple tension specified by (3.8), M must have transverse isotropy with respect to the 3-axis. In this case M^* also has transverse isotropy and a definite recipe for M^* is available (Hutchinson 1970).† One minor difficulty with this recipe is that it does not apply for a strictly incompressible solid, even though M^* itself is non-singular and well defined.‡ Since in the present application M is incompressible, it was necessary to include a very small compressibility compliance in M, but only for the purpose of calculating M^*. Using the isotropic case as a gauge, we chose the compressibility sufficiently small to ensure that M^* was accurate to four significant figures. In the presence of significant anisotropy, numerical experimentation indicated the same degree of accuracy.

Given $\overline{\sigma}$, M and M^* the problem for σ, M^c and B^c in (4.16a, b) and (2.6) is still nonlinear since M^c depends on σ. Let σ denote the estimate at any iterative step and let $\sigma + \Delta\sigma$ denote the estimate at the next step. Application of Newton's method to (4.16a, b) and (2.6) can be shown to give

$$\Delta\sigma = [(M^* + nM^c)^{-1}(M^* + M^c)](B^c\overline{\sigma} - \sigma), \tag{A 4}$$

where M^c and B^c are evaluated by using σ. With a good starting value σ, repeated application of (A 4) gives quadratic convergence associated with Newton's method. As in the upper bound calculation, a value of σ associated with the solution at a slightly larger value of $1/n$ was used to start each iteration.

The overall compliances M are also obtained by a rapidly convergent iterative process. Since the material is incompressible and transversely isotropic, only three independent constants are needed to specify M. For components in the specimen axes, let $2c_1 = M_{1111} + M_{1122}$, $2c_2 = M_{1111} - M_{1122}$ and $c_3 = M_{1313}$. Then,

$$\left.\begin{array}{ll} M_{1111} = c_1 + c_2, \quad M_{3333} = 4c_1, \quad M_{1122} = c_1 - c_2, \\ \qquad M_{1133} = -2c_1, \quad M_{1212} = c_2. \end{array}\right\} \tag{A 5}$$

† The recipe for M^* is based on a solution by Kneer (1965). As pointed out by Hutchinson (1970), and by Lin & Mura (1973) and Gubernatis & Krumhansl (1975), there are several minor errors in Kneer's results. There are also two misprints in table 1 given by Hutchinson (1970): The last term in a_3 should be $-2L_{13}L_{44}L_{66}$ instead of $-2L_{13}L_{11}L_{66}$ and the first term in $A^{(2)}_{1313}$ should be $L_{11}L_{33}$ instead of $L_{11}L_{13}$.

‡ The difficulty lies in the fact that the formula for M^* involves components of the moduli $L = M^{-1}$ and not the compliances. It should be possible to obtain M^* explicitly in terms of M for the incompressible case, but neither a direct calculation nor a limiting process appeared very tractable from our exploratory efforts.

With $\bar{\sigma}$ specified and given any M in the form (A 5), let

$$H = \{(M - M^c)\, B^c\}, \tag{A 6}$$

where M^c and B^c (at any stage in the iteration of the overall compliances) are functions of orientation and the current value of M which can be calculated as discussed in the previous paragraph. Since $(M - M^c)\, B^c$ has diagonal symmetry, H does. In addition,

$$H_{kkij} = H_{ijkk} = 0. \tag{A 7}$$

Since M and M^* have transverse isotropy with respect to the 3-axis and since (A 6) is an equally weighted integration over all orientations, H must also have transverse isotropy with respect to the 3-axis. This property, combined with (A 7), implies that H, like M, is completely specified by three independent constants. A convenient choice for these constants, as will be discussed later, is

$$H_1 = H_{ijij}, \quad H_2 = H_{\alpha\beta\alpha\beta}, \quad H_3 = H_{\alpha\alpha\beta\beta}, \tag{A 8}$$

where i and j sum from 1 to 3 as usual. In (A 8), H_2 and H_3 are defined in the specimen axes with α and β summed only over 1 and 2.

With $\bar{\sigma}$ specified, H is a function of M and by (A 5) and (A 8) we can indicate this functional dependence as $H_i(c_j)$ with $i = 1, 3$ and $j = 1, 3$. By (4.16 c), the self-consistent equation for M is $H = 0$ which will be satisfied if and only if

$$H_1 = H_2 = H_3 = 0.$$

Let c_j be the current estimate of the compliances in the iterative process and let $c_i + \Delta c_i$ be the values sought, i.e. $H_i(c_j + \Delta c_j) = 0$. The equations for Δc_j associated with Newton's method are

$$\sum_{j=1}^{3} (\partial H_i / \partial c_j)\, \Delta c_j = -H_i \quad (i = 1, 3), \tag{A 9}$$

where H_i and its derivatives in (A 9) are evaluated at c_j. An explicit expression for the derivatives of H_i in (A 9) can be obtained from the governing equations (4.16), but the expressions are extremely involved and too complicated to be useful for numerical work. Instead, the derivatives were evaluated numerically by an easily implemented procedure according to formulas such as

$$\partial H_i / \partial c_1 \cong [H_i(c_1 + \delta, c_2, c_3) - H_i(c_1, c_2, c_3)]/\delta, \tag{A 10}$$

where δ is taken as a very small fraction of c_1.

The advantage of the choice of constants H_i in (A 8) is that each contribution, $(M - M^c)\, B^c$, in (A 6) to these constants is invariant with respect to rotations of the grain axes about the overall tensile axis (the 3-axis of the specimen axes). Thus, symmetry permits the integration in (A 6) to be reduced to an integration over just one standard spherical triangle. As in the upper bound calculation, this is done numerically using 36 discrete orientations. For $n = 1$, the numerical results were always within 0.5 % of the exact values from (4.18) or (6.1).

Computation of $h(n)$ for the f.c.c. polycrystal took 2 min of c.p.u. time on an IBM 370/168 computer. Calculation of $f(n)$ for the upper bound took about 0.5 min.