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Creep and Plasticity of Hexagonal Polycrystals as Related to Single Crystal Slip

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The role of slip on basal, prismatic and pyramidal systems of hexagonal single crystals in determining inelastic polycrystalline behavior is studied using a uniform strain-rate upper bound and a self-consistent method. Steady power-law creep is considered. Included as a limiting case is rigid-perfectly plastic behavior, for which the upper bound to the yield stress of the polycrystal coincides with the Bishop-Hill bound for these materials. When the resolved shear stress needed to produce a given level of slip on the pyramidal systems is large compared to that on the other systems the upper bound lies well above the self-consistent estimate. Self-consistent theory indicates that overall inelastic deformation of a polycrystal is possible without pyramidal slip. Implications for hexagonal materials, including ice, are discussed.

INELASTIC behavior of hexagonal materials at the single crystal level is often highly anisotropic and a relatively large number of different slip and twinning systems have been reported.[1] In many of these materials a given level of basal and prismatic slip is produced by shear stresses which are much below the shear stress needed to cause pyramidal slip. Basal and prismatic systems together comprise only four linearly independent slip systems, allowing no inelastic straining along the hexagonal axis (c-axis) of the crystal. The additional mechanism which supplies this missing degree of freedom, whether pyramidal slip or twinning, has a strong influence on the overall inelastic behavior of the polycrystal.

In this paper combinations of basal, prismatic and pyramidal slip are considered; twinning is not specifically taken into account. Steady, power-law creep of polycrystalline aggregates is analyzed using two methods which have previously been reported in the literature:[2] i) a uniform strain-rate upper bound, and ii) a self-consistent method. The self-consistent method is more accurate than the upper bound and requires somewhat more effort to apply. As long as the inelastic anisotropy of the crystals is not too large, the bound and the self-consistent theory are in reasonably close agreement. This ceases to be true when anisotropy is large and shows up most dramatically when slip is suppressed completely on the pyramidal systems. Then, according to the uniform strain-rate bound calculation, the polycrystalline aggregate is rigid. In contradistinction, the self-consistent theory predicts that the polycrystal can still undergo overall inelastic deformation. This is possible because the strain-rate in each grain is not constrained to be the same as the overall strain-rate. Variations in strain-rate from grain to grain, depending on orientation, accommodate the inability of the crystals to strain along their c-axis.

POWER-LAW CREEP OF SINGLE CRYSTALS AND POLYCRYSTALS

Let $n_i^{(k)}$ be the unit normal to the slip plane of the k-th system and $m_i^{(k)}$ be the unit vector in the slip direction in the plane. Denote the slip tensor for the system by

$$\mu_{ij}^{(k)} = \frac{1}{2}(m_i^{(k)}n_j^{(k)} + m_j^{(k)}n_i^{(k)}). \qquad [1]$$

With σ_{ij} as the stress, the resolved shear stress on the system is

$$\tau^{(k)} = \sigma_{ij}\mu_{ij}^{(k)}. \qquad [2]$$

Let $\gamma^{(k)}$ denote the shear strain-rate (engineering definition) on the k-th system and let α be a reference strain-rate which will be used throughout the paper. Steady creep is considered and a power-law relation is assumed where

$$\gamma^{(k)} = \alpha|\tau^{(k)}/\tau_0^{(k)}|^n \cdot \mathrm{sign}(\tau^{(k)}). \qquad [3]$$

The quantity $\tau_0^{(k)}$ is taken to be positive and is called the reference shear stress for the k-th system. The strain-rate is the sum of contributions from each of the systems according to

$$\epsilon_{ij} = \sum_k \gamma^{(k)}\mu_{ij}^{(k)}. \qquad [4]$$

The polycrystal is assumed to be a large collection of randomly orientated single crystals bonded together with no sliding across their boundaries. Attention is restricted to a common value of n for all systems. Then the steady state behavior of the polycrystal is governed by an isotropic, pure power relation between the overall strain-rate and the overall stress as discussed in Ref. 2. In particular, the tensile behavior of the polycrystal, which will be emphasized here, can be expressed quite generally in terms of the overall uniaxial strain-rate $\bar{\epsilon}$ and stress $\bar{\sigma}$ by

$$\bar{\epsilon} = \alpha(\bar{\sigma}/\bar{\sigma}_0)^n. \qquad [5]$$

Thus, $\bar{\sigma}_0$ completely specifies the uniaxial behavior; it is called the uniaxial reference stress. It is a function of the single crystal reference shear stresses and n.

Details of the two methods for estimating $\bar{\sigma}_0$ are given in Ref. 2 and will not be repeated here. The uniform strain-rate calculation provides an upper bound to $\bar{\sigma}_0$. In the limit as $n \to \infty$ the crystals are rigid-ideally plastic and then the bound to $\bar{\sigma}_0$ is equal to the

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bound of Bishop and Hill.[3,2] For $n = 1$ the behavior is linear viscoelastic and the bound to $\bar{\sigma}_0$ is then just the Voigt bound. The version of the self-consistent theory used is adapted from Hill.[4] In this calculation the strain-rate and stress in each grain is determined by taking the grain to be spherical and by embedding it in an infinite matrix whose properties are those desired of the polycrystal. The overall stress and strain-rate are determined in terms of the corresponding single crystal quantities by self-consistent averaging over all grain orientations. In this approximate way grain interaction is taken into account without requiring the strain-rate to be the same in each grain. The self-consistent estimate of $\bar{\sigma}_0$ is not a bound, although for $n = 1$ it can be shown[5] that it falls between the tighter bounds of Hashin and Shtrikman,[6] as will be illustrated below.

For hexagonal crystals we specialize (Eq. [3]) further by denoting the reference shear stresses for the basal, prismatic and pyramidal systems as τ_A, τ_B and τ_C, respectively. Thus,

$$\left.\begin{array}{ll} \gamma = \alpha\,|\tau/\tau_A|^n \cdot \operatorname{sign}(\tau) & \text{for basal systems} \\ \gamma = \alpha\,|\tau/\tau_B|^n \cdot \operatorname{sign}(\tau) & \text{for prismatic systems} \\ \gamma = \alpha\,|\tau/\tau_C|^n \cdot \operatorname{sign}(\tau) & \text{for pyramidal systems} \end{array}\right\} \quad [6]$$

where the slip systems are depicted in Fig. 1. The two basal systems and three prismatic systems together supply four linearly independent systems, as already mentioned. The angle made by each of the six pyramidal planes to the c-axis is denoted by ϕ and, if ϕ is not 45 deg, this set provides five linearly independent systems by itself. In Fig. 1 the particular set of pyramidal systems illustrated is $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$. A discussion of the competition between the three types of slip systems for ideally plastic crystals is given by Chin and Mammel[7] and Thornburg and Piehler.[8]

UPPER BOUND TO $\bar{\sigma}_0$

For $n = 1$ the uniform strain-rate upper bound to $\bar{\sigma}_0$ is given by

$$\bar{\sigma}_0 = \frac{2}{5}\left[\frac{\tau_C}{3\sin^2 2\phi} + \frac{4\tau_B\tau_C}{2\tau_C + \tau_B\sin^2 2\phi} + \frac{2\tau_A\tau_C}{\tau_C + 2\tau_A\cos^2 2\phi}\right]. \quad [7]$$

This result holds for any set of six pyramidal planes each making an angle ϕ to the c-axis and arranged with 60 deg intervals between planes about this axis. Also, the slip direction is taken perpendicular to the intersection of the slip plane and the basal plane, such as shown in Fig. 1. The special role of the pyramidal systems can be seen by noting that $\bar{\sigma}_0 \to \infty$ as $\tau_C \to \infty$, whereas a finite limit is obtained if τ_A and/or τ_B become unbounded.

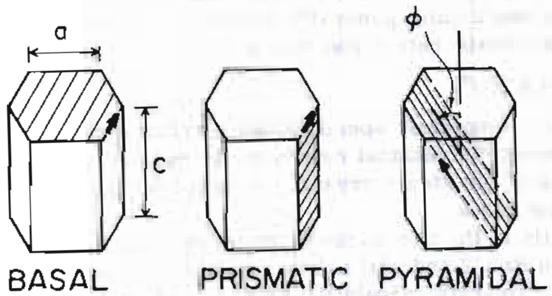

Fig. 1—Slip systems. Pyramidal system illustrated is $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$.

The problem for the limit of rigid-ideally plastic single crystals ($n \to \infty$) can be formulated in the manner of Bishop and Hill[3] with numerical results obtained by a linear programming algorithm.[9] This procedure was used to generate the results for this limit in the figures which follow. Thornburg and Piehler[8] have produced an extensive list of stress states capable of activating different combinations of slip and twinning systems for hexagonal crystals. For the present purposes it proved easiest to include the linear programming procedure directly as part of the complete calculation program. For values of n in the range $1 < n < \infty$ calculations were performed using the method described in Ref. 2.

The examples discussed below were chosen with the primary purpose of bringing out the role of the pyramidal systems. Figure 2 displays the upper bound and the self-consistent estimate (to be introduced below) as a function of $1/n$ for two levels of τ_C relative to τ_A and τ_B. In these examples $\phi = 31.5$ deg corresponding to $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$ systems for the ideal ratio $c/a = 2\sqrt{(2/3)}$. When $\tau_C = 5\tau_A = 5\tau_B$, as in the lower curves in Fig. 2, the two methods are still in reasonable agreement. For larger single crystal anisotropy the methods begin to diverge, as will be discussed in the next section.

If the resistance to creep on the basal and prismatic systems is small compared to that on the pyramidal

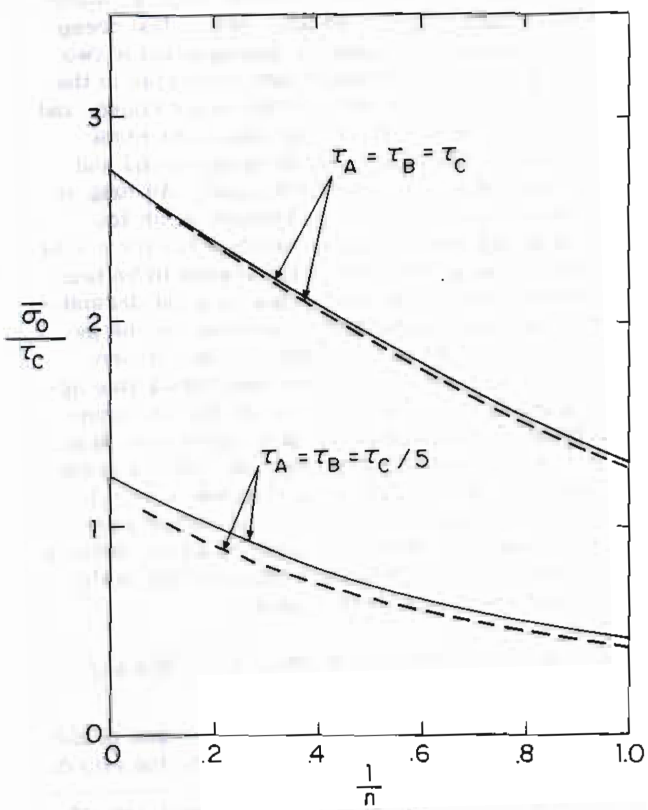

Fig. 2—Comparison of upper bound (solid line curve) and self-consistent result (dashed line curve).

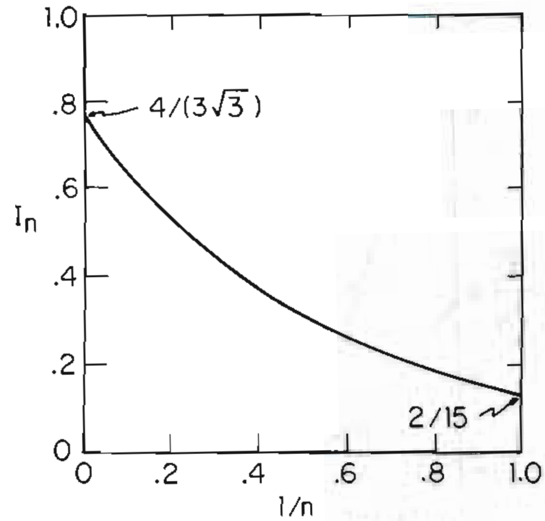

Fig. 3—Values of I_n from Eq. [9].

systems, then the pyramidal systems essentially control the upper bound. In the limiting case where there is no resistance to glide on the basal and prismatic systems, *i.e.*, $\tau_A = \tau_B = 0$, the upper bound to $\bar{\sigma}_0$ can be obtained in closed form. Then each crystal can support only a uniaxial stress aligned with the c-axis plus a hydrostatic component. The result for the uniform strain-rate bound to $\bar{\sigma}_0$ for this case is found to be

$$\bar{\sigma}_0 = \tau_C I_n [\sin 2\phi]^{-(n+1)/n} \qquad [8]$$

where

$$I_n = \int_0^{\pi/2} \sin\theta \, |2 - 3\sin^2\theta|^{(n+1)/n} d\theta. \qquad [9]$$

Values of I_n are plotted in Fig. 3; $I_1 = 2/15$ in agreement with Eq. [7] for $n = 1$ and, for $n \to \infty$, $I_n \to 4/(3\sqrt{3})$. Eq. [8] applies to any six pyramidal planes as specified in connection with Eq. [7].

The approach to Eq. [8] is shown in Fig. 4 where the upper bound to $\bar{\sigma}_0/\tau_C$ is plotted against τ_B/τ_C for the case $\tau_A = \tau_B/10$ and for the same pyramidal systems chosen in the calculations for Fig. 2.

SELF-CONSISTENT ESTIMATE OF $\bar{\sigma}_0$

If $n = 1$ the self-consistent equation can be obtained in closed form. It is also of interest to make comparisons with the tighter upper and lower bounds of Hashin and Shtrikman[6] (abbreviated as H.-S.) and Walpole[5] when $n = 1$. All three equations can be summarized compactly as follows:

$$\bar{\sigma}_0 = 9\eta/(3 - 8\eta\zeta) \qquad [10]$$

$$\eta = \frac{3}{10}\left[\frac{1}{2(2\zeta + 3d)} + \frac{1}{2\zeta + 3e} + \frac{1}{2\zeta + 3f}\right]$$

$$d = (9/8)\tau_C^{-1}\sin^2 2\phi$$

$$e = (3/8)\tau_B^{-1} + (3/16)\tau_C^{-1}\sin^2 2\phi$$

$$f = (3/8)\tau_A^{-1} + (3/4)\tau_C^{-1}\cos^2 2\phi$$

where

$$\zeta = \begin{cases} \text{smallest of } (d, e, f) \text{ for upper bound} \\ \text{largest of } (d, e, f) \text{ for lower bound} \\ 3/(4\bar{\sigma}_0) \text{ for self-consistent result.} \end{cases}$$

For the H.-S. bounds Eq. [10] is explicit; for the self-consistent result it is necessary to solve Eq. [10] using some simple iteration or root-finding scheme.

A numerical comparison of the uniform strain-rate bound Eq. [7], the uniform stress lower bound (details omitted), the two H.-S. bounds, and the self-consistent estimate are shown in Fig. 5. In this example basal creep occurs easily compared to prismatic creep ($\tau_A = \tau_B/10$) and the effect of the pyramidal systems is seen through the ratio τ_B/τ_C. As $\tau_C \to \infty$ (*i.e.*, $\tau_B/\tau_C \to 0$) the self-consistent estimate of $\bar{\sigma}_0/\tau_B$ remains finite, as do the two lower bounds, but the two upper bounds are unbounded. Thus according to the self-consistent theory, it is not always necessary to have five linearly independent slip systems for overall deformation to occur. With glide on the pyramidal systems suppressed ($\tau_C \to \infty$) there are only four linearly independent systems available, as previously mentioned, and [10] continues to hold with $d = 0$, $e = 3/(8\tau_B)$, and $f = 3/(8\tau_A)$.

The self-consistent results of Fig. 2 plotted against $1/n$ were calculated using the method in Ref. 2. The self-consistent problem for the limiting case of rigid-perfectly plastic crystals ($n \to \infty$) can be formulated separately involving quadratic programming. A computer program for this limit was not written; $n = 10$ was the largest value used in the calculations. The property discussed above for $n = 1$ holds for all n. That is, according to the self-consistent model, overall inelastic deformation occurs even when slip cannot take place on the pyramidal systems.

The example in Fig. 6 also illustrates the point made in connection with Fig. 5 but now with $n = 3$ and for other parameters chosen to represent ice discussed in the next section. As in the previous example, the deviation between the two predictions becomes large when $\tau_C > 3\tau_B$. With glide entirely sup-

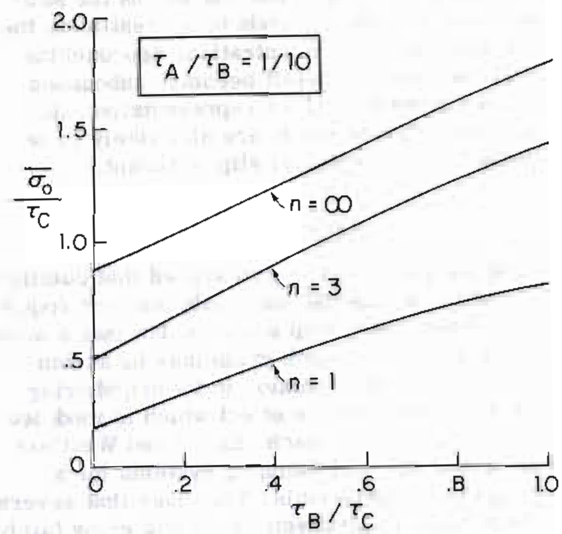

Fig. 4—Approach of upper bound to limiting case (Eq. [8]) where resistance to creep on basal and prismatic systems vanishes.

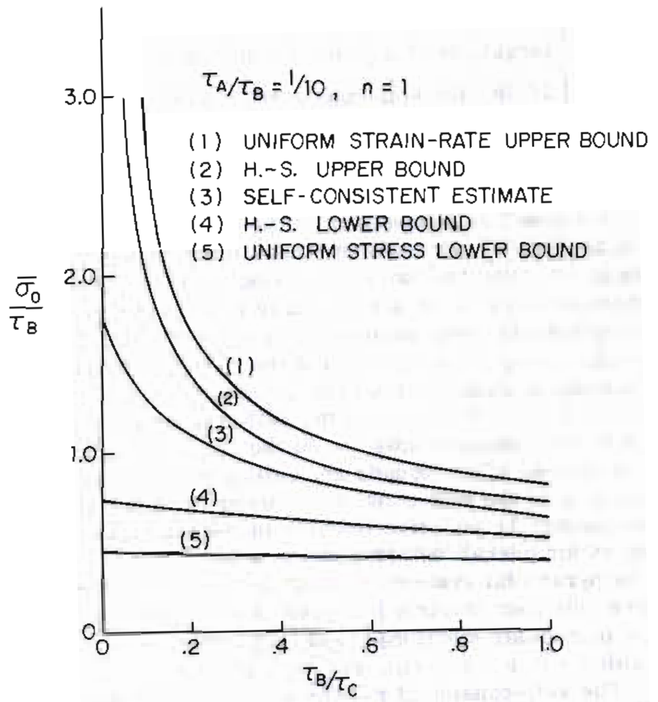

Fig. 5—Self-consistent results and various bounds for $n = 1$. ($\phi = 31.5$ deg).

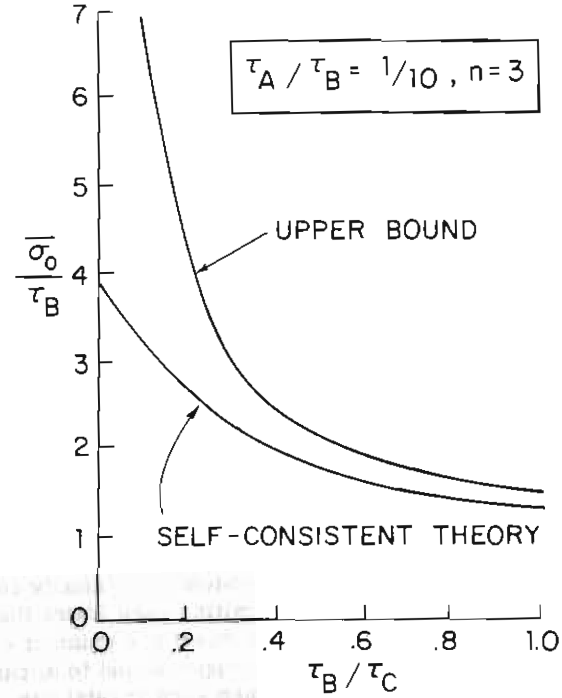

Fig. 6—Self consistent results and upper bound for $n = 3$. Pyramidal systems are $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$ with $\phi = 31.5$ deg.

pressed on the pyramidal systems, $\bar{\sigma}_0 \cong 3.9\tau_B$ (with $\tau_A = \tau_B/10$). By comparison the result for a fcc polycrystal at $n = 3$ is $\bar{\sigma}_0 \cong 2.5\tau_0$, where τ_0 is the reference shear stress for each of the $\{111\}\langle110\rangle$ systems of the single crystal.[2]

Any rigidity on the microscopic level renders the uniform strain-rate upper bound infinite. Perhaps the simplest system where this is seen is in connection with the elastic properties of an isotropic elastic matrix with embedded rigid particles. Both the uniform strain bound and the Hashin-Shtrikman upper bound to the shear modulus are infinite. The self-consistent result for this modulus[10,11] is finite and is known to be accurate at low volume concentrations of particles. At higher volume concentrations the self-consistent method probably tends to overestimate the modulus, and at volume concentrations approaching about 50 pct the estimate itself becomes unbounded. If this simpler system is at all representative, the self-consistent estimates of $\bar{\sigma}_0$ are also likely to be overestimates when pyramidal slip is absent.

DISCUSSION

Kocks and Westlake[12] have also argued that ductility of polycrystalline hexagonal materials may not require five linearly independent slip systems, but that a missing degree of freedom in each grain may be accommodated by inelastic deformation in its neighboring grains. This is precisely the effect which is modeled by the self-consistent approach. Kocks and Westlake tabulate observed slip and twinning systems for a number of hexagonal materials. They note that several of these materials in polycrystalline form enjoy fairly extensive ductility yet do not appear to display either pyramidal slip or twinning. They suggest that the lack of the fifth degree of freedom primarily influences the amount of ductility by increasing the stress concentration in each grain and thereby hastening fracture.

Twinning is observed in many hexagonal close packed metals and can make an important contribution to the inelastic accommodation of abutting grains as discussed by Chin.[13] At higher temperatures and lower overall stress levels characteristic of the creep regime, twinning becomes increasingly difficult compared to slip in many materials, and the role of the pyramidal slip becomes more important. Even a relatively "hard" pyramidal system has a considerable influence on the overall creep-rate as long as it permits some creep. For example, in Fig. 6 $\bar{\sigma}_0$ increases from roughly $2\tau_B$ to $3.9\tau_B$ as τ_C increases from $3\tau_B$ to ∞, according to the self-consistent theory.

The present results can be used to infer information about the pyramidal systems of ice. A number of direct measurements of steady creep on basal and prismatic systems have been made for single crystal ice. Weertman[14] has compared some of this data with uniaxial steady creep data for polycrystalline specimens, all data being normalized to $-10°$C. Figure 7 is abstracted from Weertman's Fig. 4 and includes, in addition, two theoretical curves (shown dashed) for the polycrystal from the present analysis. (See Fig. 4 of Ref. 14 for more detail on the experimental data.) The single crystal data has been converted to equivalent uniaxial form in Fig. 7 using $\sigma = \sqrt{3}\tau$ and $\epsilon = \gamma/\sqrt{3}$, following Weertman, and the polycrystal data falls within the shaded band. The theoretical curves for the polycrystal were derived from the data for the prismatic systems using the self-consistent results of Fig. 6 and picking two values of τ_B/τ_C to bracket the polycrystalline data. For the prismatic systems $n = 3$. This value was used in the theoretical calculations; n is slightly less for the

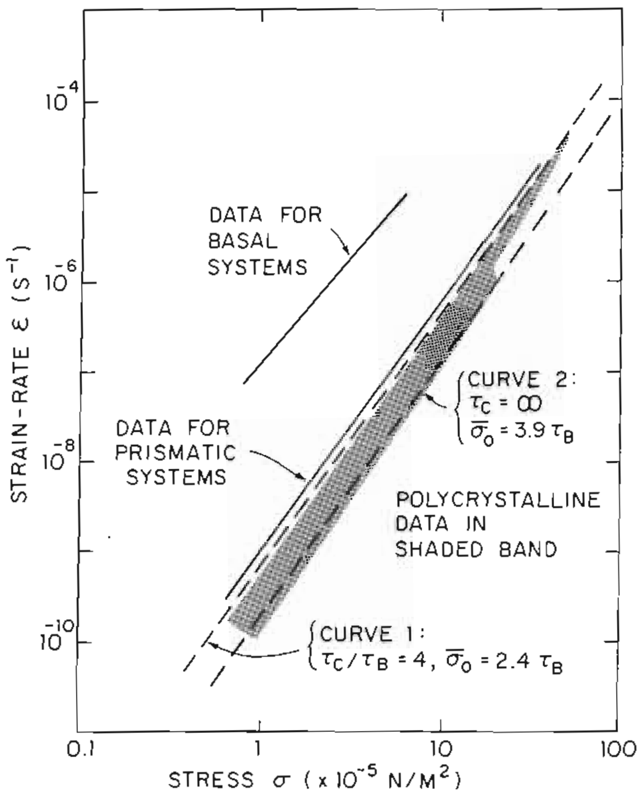

Fig. 7—Collected experimental data for ice at −10°C from Weertman, and comparison with theoretical curves (1 and 2) for polycrystal derived from data for prismatic systems.

basal systems but, since τ_A/τ_B is so small ($\simeq 0.1$), the resistance to creep on the basal systems could be neglected altogether with little change in the results. Curve 1 in Fig. 7 corresponds to the choice $\tau_B/\tau_C = 1/4$ so that (from Fig. 6) $\overline{\sigma}_0 = 2.4\tau_B$, which then permits one to determine Curve 1 from the prismatic data. Curve 2 corresponds to $\tau_B/\tau_C = 0$ with $\overline{\sigma}_0 = 3.9\tau_B$. In conclusion, the self-consistent model indicates that the experimental data for ice is compatible with very "hard" pyramidal systems. Direct measurement of pyramidal glide in ice has not yet been reported; nor has any other mechanism been reported which will supply c-axis straining, except possibly void growth at low pressures. However, there is some evidence, based on observations of etch channels, that glide on the pyramidal systems $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$ may occur.[15]

The present study has been limited to isotropic distributions of single crystals. Texture development associated with large straining has not been addressed but is clearly an important aspect of hexagonal material behavior because of large anisotropy at the single crystal level. The present study does, however, serve to emphasize that, in the study of texture effects based on the widely used Bishop-Hill bound, one must not lose sight of the fact that the upper bound may in fact substantially overestimate the yield strength of the material.

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