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CXXVIII. A theoretical derivation of the plastic properties of a polycrystalline face-centred metal

J.F.W. Bishop [a] & R. Hill [a]

[a] H. H. Wills Physical Laboratory , University of Bristol
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CXXVIII. *A Theoretical Derivation of the Plastic Properties of a Polycrystalline Face-Centred Metal.*

By J. F. W. Bishop and R. Hill,
H. H. Wills Physical Laboratory, University of Bristol †.

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Summary

In continuation of a previous paper (Bishop and Hill 1951) it is conjectured that the work done in plastically deforming a polycrystal is approximately equal to that which would be done if the grains were free to deform equally. In conjunction with the principle of maximum plastic work, this enables the yield function of an aggregate to be calculated. This is done for an isotropic aggregate of face-centred cubic crystals, following a determination of the stresses needed to produce multi-slip. The theoretical yield criterion lies between those of Tresca and von Mises, in good agreement with observaton for copper and aluminum. It is shown further that the work-hardening of an aggregate would be a function only of the total plastic work if the grains hardened equally; the departure from this functional relation is expressed explicitly in terms of the non-uniform hardening.

§ 1. Résumé of Previous Work.

In a recent paper (Bishop and Hill 1951, henceforward referred to as BH) some general theorems were proved for an aggregate in which the crystals individually deform by slip according to the Schmid law. The theorems depend, in essence, on a principle of maximum plastic work for a homogeneously deformed single crystal (BH, equation (9)). This principle states that if a crystal is caused to deform plastically through an increment of strain $d\epsilon_{ij}$, the work done by the required stress σ_{ij} is not less than that done by any other stress σ^*_{ij} not violating the yield condition; thus

$$(\sigma_{ij}-\sigma^*_{ij})\, d\epsilon_{ij} \geqslant 0. \qquad (1)$$

The yield condition is that the component shear-stress in any of the possible slip-directions, and over the associated slip-planes, cannot exceed the corresponding critical shear-stress in the current state of hardening. The critical shear-stress may vary from one slip-direction to another, due to differential hardening, or may be different in the two opposite senses of the same slip-direction, due to a microscopic Bauschinger effect. In a statistically homogeneous aggregate, in which cohesion between crystals is maintained by multi-slip, the same principle was proved for the *macroscopic* stress S_{ij} and strain-increment dE_{ij}. (BH, equation (16)).

† Communicated by the Authors.

From this it was shown to follow immediately that, if the yield criterion for the aggregate is

$$f(\mathrm{S}_{ij})=0 \quad \ldots\ldots\ldots\ldots \quad (2)$$

in a certain state of hardening and anisotropy, then the relation between the ratios of the components of the stress and strain-increment tensors is

$$d\mathrm{E}_{ij}=h\,\frac{\partial f}{\partial \mathrm{S}_{ij}}\,df. \quad \ldots\ldots\ldots\ldots \quad (3)$$

The function f is, moreover, concave to the origin when regarded as a surface in stress hyperspace, and does not involve the hydrostatic component of S_{ij}. h is a function of the stress and strain-history, controlling the *magnitude* of the strain-increment produced by a further increment of stress.

The plastic behaviour of an aggregate is thus completely determined by the functions f and h. The present paper is concerned with their calculation for an aggregate of face-centred cubic crystals.

§ 2. The Basic Theorem.

Since the actual stress distribution σ_{ij} is in equilibrium, it follows by virtual work that

$$\int(\sigma_{ij}\,d\mathrm{E}_{ij})\,d\mathrm{V}=\mathrm{S}_{ij}\,d\mathrm{E}_{ij},$$

where the integral extends over a unit cube of aggregate (see BH. equation (14) and succeeding remarks). Let σ^*_{ij} be a stress which, at each point of the aggregate, would produce the strain $d\mathrm{E}_{ij}$ in a free crystal having the local orientation and hardening. The distribution σ^*_{ij} is, of course, not necessarily in equilibrium. Then, by (1),

$$(\sigma^*_{ij}-\sigma_{ij})\,d\mathrm{E}_{ij}\geqslant 0,$$

the equality holding in general only when the deviatoric parts of σ_{ij} and σ^*_{ij} are equal. Hence

$$\mathrm{S}_{ij}\,d\mathrm{E}_{ij}=\int(\sigma_{ij}\,d\mathrm{E}_{ij})\,d\mathrm{V}\leqslant d\mathrm{E}_{ij}\int\sigma^*_{ij}\,d\mathrm{V}. \quad \ldots\ldots \quad (4)$$

On the other hand, by integrating (1) through a unit cube of aggregate, we obtain

$$\mathrm{S}_{ij}\,d\mathrm{E}_{ij}\geqslant\int(\sigma^*_{ij}\,d\epsilon_{ij})\,d\mathrm{V}.$$

Assuming that there can be no statistical correlation between any components of σ^*_{ij} and $d\epsilon_{ij}$,

$$\int(\sigma^*_{ij}\,d\epsilon_{ij})\,d\mathrm{V}=\int\sigma^*_{ij}\,d\mathrm{V}\times\int(d\epsilon_{ij})\,d\mathrm{V}=d\mathrm{E}_{ij}\int\sigma^*_{ij}\,d\mathrm{V},$$

provided there is no rupture or relative sliding of the grains. Hence

$$\mathrm{S}_{ij}\,d\mathrm{E}_{ij}\geqslant d\mathrm{E}_{ij}\int\sigma^*_{ij}\,d\mathrm{V}. \quad \ldots\ldots\ldots \quad (5)$$

On combining (4) and (5) we obtain the theorem on which the possibility of a calculation of the function f depends :

$$\mathrm{S}_{ij}\,d\mathrm{E}_{ij}=d\mathrm{E}_{ij}\int\sigma^*_{ij}\,d\mathrm{V}. \quad \ldots\ldots\ldots \quad (6)$$

In words: the actual work done is equal to the work that would be done if the grains all underwent the same (macroscopic) strain.

In particular, when the slip-directions in any one grain all have the same critical shear-stress τ (in both senses), we may define an average value $\bar{\tau}$ for the aggregate, such that

$$\bar{\tau}=\int\tau\, dV.$$

Then, if σ^*_{ij} would produce a strain dE_{ij} in a grain with critical shear stress τ, $\bar{\sigma}^*_{ij}=\bar{\tau}\sigma^*_{ij}/\tau$ would produce the same strain in a grain of the same orientation but with critical shear stress $\bar{\tau}$. Hence

$$\bar{\tau}\int\sigma^*_{ij}\, dV=\int\tau\bar{\sigma}^*_{ij}\, dV=\bar{\tau}\int\bar{\sigma}^*_{ij}\, dV,$$

assuming that there is no correlation between $\bar{\sigma}^*_{ij}$ and τ. Therefore:

$$\int\sigma^*_{ij}\, dV=\int\bar{\sigma}^*_{ij}\, dV,$$

and so, from (6),

$$S_{ij}\, dE_{ij}=dE_{ij}\int\bar{\sigma}^*_{ij}\, dV. \quad \ldots \ldots \quad (7)$$

We can thus evaluate the work using the average value of the critical shear stress in the aggregate.

But equations (5) and (6) cannot be strictly true since (6) implies that the deviatoric part of σ_{ij} is equal to that of σ^*_{ij}, all components of which are generally discontinuous across grain boundaries or wherever else the lattice orientation changes. (It is shown later that a general strain can only be produced by some one of a *finite* set of stresses.) However, we are inclined to think (though we have not found a rigorous proof) that equation (6) is not much in error, and we assume it as an approximation.

§ 3. Method of Calculation of the Yield Function.

The way in which f can be calculated is conveniently visualized geometrically. A strain increment dE_{ij} can be considered as a free vector in stress hyperspace. According to (6) the scalar product $S_{ij}\, dE_{ij}$ is calculable in terms of the slip properties of a single crystal. The extremity of the stress vector S_{ij}, corresponding to a strain-increment dE_{ij}, is thus known to lie on a plane which is perpendicular to dE_{ij} and whose distance from the origin is

$$\frac{dE_{ij}\int\sigma^*_{ij}\, dV}{(dE_{ij}dE_{ij})^{1/2}}. \quad \ldots \ldots \quad (8)$$

(Although the point $\int\sigma^*_{ij}\, dV$ lies on the plane, it does not, of course, necessarily coincide with S_{ij}.) Now according to (3), the normal to the yield surface at the point S_{ij} is parallel to dE_{ij}, and so perpendicular to the plane. The plane is therefore tangential to the yield surface at S_{ij}. The surface is thereby found as the envelope of planes whose distances from the origin are given by (8). Since possible strains have zero hydrostatic part (being the result of simultaneous simple shears), the surface is cylindrical with generators parallel to the direction δ_{ij}.

When the aggregate as a whole is isotropic the principal axes of the stress and strain-increment tensors are coincident, and we only need to consider the relation between their principal values represented in three dimensional space. The aggregate will be statistically isotropic when the orientations of grains in the same state of hardening are randomly distributed ; this condition must be satisfied for each of the various states of hardening at any moment in the differentially-hardened aggregate (if not, the aggregate might be anisotropic despite the absence of a preferred orientation).

The numerical calculations in the present paper are restricted to such an isotropic aggregate in which, moreover, the slip-directions in any grain are equally hardened (so that equation (7) is applicable). The development of deformation textures and their effect on the yield surface is left to a later paper.

§ 4. Multi-Slip in a Face-Centred Cubic Crystal.

At ordinary temperatures and rates of strain, glide occurs in a face-centred cubic crystal on the octahedral planes in the directions of the octahedron edges. Each of the four distinct glide-planes contains three possible slip-directions, making twelve in all, each of which has two opposite senses. The positive senses of the slip-directions are arbitrarily chosen here according to the following Table ; letters a, b, c, d refer to the four glide-planes, and with suffixes 1, 2, or 3, denote incremental shears in the respective positive senses. The components, referred to the

Plane	(111)			$(\bar{1}\bar{1}1)$			$(\bar{1}11)$			$(1\bar{1}1)$		
Shear	a_1	a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3	d_1	d_2	d_3
Direction	$01\bar{1}$	$\bar{1}01$	$1\bar{1}0$	$0\bar{1}\bar{1}$	101	$\bar{1}10$	$01\bar{1}$	101	$\bar{1}\bar{1}0$	$0\bar{1}\bar{1}$	$\bar{1}01$	110

cubic axes, of the strain tensor $d\epsilon_{ij}$ due to simultaneous shears in the twelve directions are given by the equations (Taylor 1938 a)

$$\left.\begin{aligned}
\sqrt{6}\, d\epsilon_{11} &= -a_2+a_3-b_2+b_3-c_2+c_3-d_2+d_3, \\
\sqrt{6}\, d\epsilon_{22} &= a_1-a_3+b_1-b_3+c_1-c_3+d_1-d_3, \\
\sqrt{6}\, d\epsilon_{33} &= -a_1+a_2-b_1+b_2-c_1+c_2-d_1+d_2, \\
2\sqrt{6}\, d\epsilon_{23} &= a_2-a_3-b_2+b_3+c_2-c_3-d_2+d_3, \\
2\sqrt{6}\, d\epsilon_{31} &= -a_1+a_3+b_1-b_3+c_1-c_3-d_1+d_3, \\
2\sqrt{6}\, d\epsilon_{12} &= a_1-a_2+b_1-b_2-c_1+c_2-d_1+d_2.
\end{aligned}\right\} \quad . \quad . \quad . \quad (9)$$

Any possible strain has five independent components (the hydrostatic part being zero), and therefore in general can only be produced by multi-slip over a group of directions containing an independent set of five.

Of the ${}^{12}C_5=792$ sets of five shears, only 384 are independent. The remaining 408 include dependent combinations of type

$$a_1+a_2+a_3=0 \qquad (144),$$
$$a_1+b_2+d_3=0 \qquad (228),$$
$$a_1-b_1+c_1-d_1=0 \qquad (36),$$

or their equivalents ; these equations are to be interpreted as meaning that such combinations of *unit* shears produce zero resultant strain. Of the 384 independent sets of five shears, 216 have two shears on each of two planes, and 168 have two shears on one plane only (the latter were apparently thought by Taylor to be dependent sets).

If the components of a stress applied to the crystal are σ_{ij} referred to the cubic axes, the shear stress components, multiplied by $\sqrt{6}$, are equal to

$$\left.\begin{array}{lll} A-G+H\ (a_1), & B+F-H\ (a_2), & C-F+G\ (a_3), \\ A+G+H\ (b_1), & B-F-H\ (b_2), & C+F-G\ (b_3), \\ A+G-H\ (c_1), & B+F+H\ (c_2), & C-F-G\ (c_3), \\ A-G-H\ (d_1), & B-F+H\ (d_2), & C+F+G\ (d_3), \end{array}\right\} \qquad (10)$$

where

$$A=\sigma_{22}-\sigma_{33}, \quad B=\sigma_{33}-\sigma_{11}, \quad C=\sigma_{11}-\sigma_{22},$$
$$F=\sigma_{23} \quad , \quad G=\sigma_{31} \quad , \quad H=\sigma_{12}.$$

It will be observed that the 12×6 matrix of coefficients in the relations (10) between the 12 shear stress components and the 6 applied stress components is just the transpose of the 6×12 matrix of coefficients in (9). This is a simple consequence of the virtual work equation $\sigma_{ij}\, d\epsilon_{ij}=\Sigma\tau\, d\gamma$, and does not depend on any particular lattice geometry. It follows that we can always find a stress for which the component shear stresses attain the critical values in prescribed senses in a given set of five independent slip-directions (the respective minors being identical and non-zero). The critical value would usually be exceeded in one or more of the other seven directions, but, for any given strain, it is always possible to find at least one of the independent sets for which there exists a physically possible stress to operate the constituent shears. However, in evaluating the expression (8) there is no need to determine a physically possible combination of shears which are equivalent to the strain. It is necessary merely to calculate the works done in the given strain by stresses not violating the yield condition, and to select from these works the greatest. In fact it is only necessary to make the choice from the works done by 56 particular stresses, which correspond to the "vertices" of the polyhedral surface in stress space representing the yield criterion for the crystal. Proofs of these statements are left to a subsequent paper.

The 56 stresses may be classified in five groups, in which the typical values of $(A, B, C, F, G, H)/\sqrt{6}\tau$ are as follows when the critical shear stress τ is the same in all the slip-directions:

(i.) $(1, -1, 0, 0, 0, 0)$. Tension or compression of amount $\sqrt{6}\tau$ along a cubic axis.

(ii.) $(0, 0, 0, 1, 0, 0)$. A pure shear of amount $\sqrt{6}\tau$ in a cubic plane and parallel to a cubic axis.

(iii.) $(\frac{1}{2}, \frac{1}{2}, -1, 0, 0, \pm\frac{1}{2})$. A pure shear of amount $\sqrt{3}\tau$ in a cubic plane and at $22\frac{1}{2}°$ to the cubic axes.

(iv.) $(\frac{1}{2}, -\frac{1}{2}, 0, \pm\frac{1}{2}, \pm\frac{1}{2}, 0)$. Principal stresses $\pm\sqrt{6}\tau(1, -\frac{1}{2}, 0)$ with the second normal to an octahedral plane and the third along a slip-direction in that plane.

(v.) $(0, 0, 0, \frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2})$. Tension or compression of amount $\frac{3}{2}\sqrt{6}\tau$ normal to an octahedral plane.

The 56 stresses have 6 members in each of (i.) and (ii.), 12 in (iii.), 24 in (iv.), and 8 in (v.). The critical shear-stress is attained in 8 slip-directions for (i.), (ii.), and (iii.), and in 6 slip-directions for (iv.) and (v.).

§ 5. The Numerical Method.

For a calculation of the yield function of an isotropic aggregate in which there is no Bauschinger effect, it is only necessary to consider macroscopic strains dE_{ij} whose principal values are $(1, -\lambda, \lambda-1)\,dE$ where $\frac{1}{2}\leqslant\lambda\leqslant 1$ (Hill 1950, p. 17 *et seq.*). The work done in such a strain of a free crystal has to be computed for each orientation of the strain axes to the cubic axes. If (θ, ϕ, ψ) are the Eulerian angles of the strain axes with respect to the cubic axes, all essentially distinct orientations occur once only in the intervals

$$0\leqslant\phi\leqslant\pi/4, \qquad 0\leqslant\cot\theta\leqslant\sin\phi, \qquad 0\leqslant\psi\leqslant\pi,$$

in view of the lattice symmetry and the assumption of equally hardened slip-directions. In other words, it is sufficient to restrict the major strain axis to one of the 48 identical spherical triangles in the stereographic projection, and allow the other axes to rotate through half a revolution. If dW is the work done on unit volume of crystal in a strain defined by given values of λ, θ, ϕ and ψ ($\bar{\tau}$ being the average critical shear stress), then, from (7),

$$S_{ij}\,dE_{ij}(\lambda)=\iiint dW\sin\theta\,d\theta\,d\phi\,d\psi/\iiint\sin\theta\,d\theta\,d\phi\,d\psi.$$

In the computation, net points were taken at 5° intervals of θ and ϕ, and 18° intervals in ψ. Five values of λ were taken in steps of $\frac{1}{8}$ between $\frac{1}{2}$ and 1. It was found convenient to express dW in terms of the principal values of the 56 stresses and the angles between the stress and strain axes. The angles were read from a stereographic net on which were marked the axes of the 56 stresses.

If p denotes the perpendicular (8) from the origin to a tangent plane of the yield surface in principal stress space, the results of the calculations are

λ	$\frac{1}{2}$	$\frac{5}{8}$	$\frac{3}{4}$	$\frac{7}{8}$	1
$\sqrt{(\frac{3}{2})}p/\tau$	3·06	3·04	2·98	2·91	2·86

The error involved in the integration is estimated to be not more than one unit in the second decimal place.

§ 6. Discussion of Results.

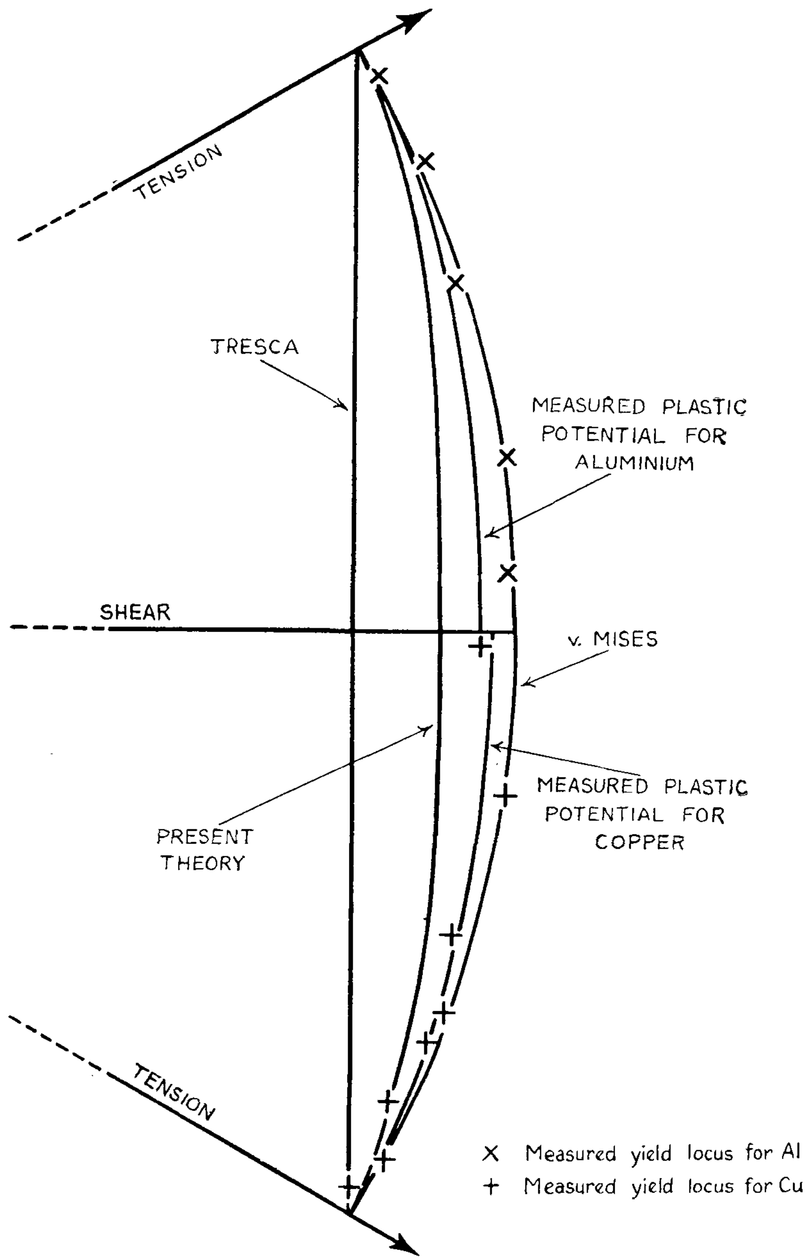
Fig. 1 shows a typical 60° sector of the cross-section of the yield surface, obtained from the values of p as described in § 3. The calculated curve cuts orthogonally the radii corresponding to pure shear and to pure tension, and lies between the Tresca hexagon and the von Mises circle when all are made to coincide for tension. In particular, the ratio of the yield stress in shear to that in tension is $2{\cdot}86/(\sqrt{3}\times 3{\cdot}06)=0{\cdot}540$, compared with 0·500 and 0·577 for the Tresca and Mises criteria.

The experimental data of Taylor and Quinney (1931) for copper and aluminium are also shown in the figure, and tend to lie between the Mises circle and the theoretical curve. The small discrepancy may be due to defects in the theory such as the approximation involved in equation (6), unequal hardening of slip-directions in individual crystals, or microscopic modes of distortion other than slip in the 12 directions. On the other hand, the experimental data may not be completely reliable, due to anisotropy or to a slight uncertainty in the extrapolation used to circumvent the hysteresis loop.

Also shown in the figure are the plastic potential curves computed from Taylor and Quinney's measured relation between the directions of the stress and strain-increment vectors ; Taylor's (1947) calculations for copper have been corrected in some instances. The agreement of the plastic potential curves with the directly measured yield loci suggests the substantial validity of (3), the theoretical derivation of which does not involve the further assumptions made in the present computation of the actual form of f.

The comparison can also be made in terms of Lode's diagram, but in our opinion, this over-magnifies small variations in the stress–strain relations, and is responsible for frequent statements that the Lévy–Mises equations are merely a moderate approximation. Thus, to the uncritical eye, a typical observed pair of Lode variables (0·5, 0·4), compared with the Lévy–Mises prediction (0·5, 0·5) might suggest an error of 20 per cent. However, it can be seen from the figure that the maximum difference in direction between the normals to the Mises circle and the measured plastic potential curves for copper and aluminium is only about 4° : without any theory at all the strain-increment vector could be anywhere in the 360° range.

Fig. 1.



§ 7. Influence of Residual Stresses.

When the external loads are removed from a plastically-deformed aggregate, a residual distribution of internal stress remains. According to the maximum work principle for the aggregate (BH, equation (16)), the yield function for the aggregate does not depend in any way on these internal stresses, but only upon the intrinsic hardening of the grains (as specified by the current values of the critical shear stresses in the slip directions). This conclusion is directly due to the neglect of elasticity in the present theory. In effect, the theory assumes that the elastic moduli are indefinitely large, so that a single crystal remains rigid under increasing load until it yields plastically. Similarly, an aggregate remains rigid until all grains are stressed to their individual yield points, and there is therefore no hysteresis loop. During loading, the weakest grain becomes plastically stressed under a load which may be termed the elastic limit of the aggregate. The elastic limit is generally appreciably lower than the yield-point load of the aggregate and clearly depends directly on the residual stresses. With increasing load other grains in turn are plastically stressed, but are prevented from deforming (or hardening) by the remaining non-plastic, and therefore rigid, grains. Hence, apart from the restricted possibilities of a stress adjustment within the individual yield surfaces of such plastically stressed grains, the greater part of further increments of load is borne by the non-plastic grains.

In an actual aggregate, elasticity permits plastic distortion and hardening of the weakest grains as soon as the elastic limit is reached. The immediate consequence is a hysteresis loop, greatly dependent on residual stresses (and correspondingly removable by a mild annealing), and with a breadth equivalent to a strain of elastic magnitude. When the hardening during the loop is small, it is naturally to be expected (in accord with observation) that the reloading branch of the loop will bend over fairly sharply to rejoin, virtually, the continuation of the previous stress–strain curve. Moreover, the local ordinate of the curve should be effectively identical with the yield-point stress calculated for a plastic-rigid aggregate. Many parallels might be instanced in stress analyses of structural parts on the basis of the macroscopic theory for a plastic-elastic homogeneous solid.

Similar considerations apply to the hysteresis loop during reverse loading, and to the tendency of the residual stresses to act so as to lower the elastic limit (Bauschinger effect). However, a further distinction must be made here. When the sign of dE_{ij} is reversed, the value of S_{ij} calculated from equation (6) would not be merely reversed when there is a *microscopic* Bauschinger effect; that is, when the critical shear stress on a slip-plane depends on the sense of slip. Thus, even for the plastic-rigid model, one would expect in such circumstances a macroscopic Bauschinger effect on the *yield-point*.

§ 8. Work Hardening of an Aggregate.

The calculated value of the tensile yield stress is $3{\cdot}06\tau$. This agrees closely with the value obtained by Taylor (1938 b), who assumed that an aggregate *actually* deforms uniformly (whereas we have conjectured that the work done is *as if* it did). Taylor was able to determine the yield stress directly from the work done in a pure extension since, for an isotropic aggregate, it follows from symmetry alone that the stress is uniaxial. In general, of course, it is also necessary to know the relations between the directions of the stress and strain-increment vectors.

Taylor computed the work from the minimum shear principle. As we have proved (BH, equation (11)), this leads to the same result as the maximum work principle, but the latter is much more convenient. Taylor's values for the works done in the individual orientations agree closely with ours (even though he selected the shears from only 216 of the 384 independent sets).

As Taylor showed, the formula $S=m\tau(mE)$ for the tensile stress–strain curve of an aggregate, where $\tau(\gamma)$ is the shear-hardening curve for a crystal, is in fairly good agreement with observation (when $m=3{\cdot}06$, in the case of aluminium). It is assumed in the derivation that the virtual work equation $S\,dE=\bar{\tau}\,d\bar{\gamma}$ can be written for an aggregate, where the averaged quantities $\bar{\tau}$ and $\bar{\gamma}$ actually *correspond* on the shear-hardening curve.

In general, however,

$$dW=S_{ij}\,dE_{ij}=\int\tau\Sigma\,|\,d\gamma\,|\,dV \quad \text{and} \quad d\bar{\tau}=\int(d\tau)\,dV=\int r(\tau)\Sigma\,|\,d\gamma\,|\,dV$$

if hardening in multi-slip is a function only of the sum of the shears. Here $r(\tau)$ denotes the rate of hardening $d\tau/d\gamma$. Assuming that there is no correlation between τ and $\Sigma\,|\,d\gamma\,|$,

$$dW=\bar{\tau}\int\Sigma\,|\,d\gamma\,|\,dV \quad \text{and} \quad d\bar{\tau}=\overline{r(\tau)}\int\Sigma\,|\,d\gamma\,|\,dV.$$

Hence

$$dW=\bar{\tau}\,d\bar{\tau}/\overline{r(\tau)}. \qquad (11)$$

If all grains are equally hardened, $\overline{r(\tau)}=r(\bar{\tau})$ and $dW=\bar{\tau}\,d\bar{\gamma}\,.\,\tau$ and the hardening of the aggregate (*i. e.* the scale of the yield surface) are then functions only of the total plastic work. The unequal hardening of the grains in such a way that $\overline{r(\tau)}\neq r(\bar{\tau})$ is presumably responsible for the observed departures from this functional relation and from the formula $S=m\tau(mE)$.

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