J. Mech. Phys. Solids, 1964, Vol. 12, pp. 25 to 33. Pergamon Press Ltd. Printed in Great Britain.

PLASTIC DEFORMATION OF B.C.C. POLYCRYSTALS*

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(*Received 1st August*, 1963)

SUMMARY

PLASTIC deformation of b.c.c. polycrystals is investigated on the basis of a single-crystal deformation model. Many of the calculations previously only presented for f.c.c. polycrystals are given here for the b.c.c. structure. In particular, stress–strain curves in tension and simple shear are presented along with the b.c.c. limit yield surface and the polycrystalline Bauschinger effect. The model employed is one suggested by BUDIANSKY and WU (1962) and KRÖNER (1961). Many of the results correspond to those which would be obtained from Taylor's model, or Lin's extension to the Taylor model.

1. INTRODUCTION

PREVIOUS theoretical investigations of plastic polycrystalline deformation on the basis of single-crystal deformation models have been limited almost exclusively to the face-centred cubic (f.c.c.) crystalline structure. Here calculations are presented which are relevant to body-centred cubic (b.c.c.) polycrystals and are examined in the light of the numerous results which have been obtained for f.c.c. polycrystals since TAYLOR's (1938) rigid-plastic model. BISHOP and HILL (1951) simplified the calculation procedure associated with Taylor's model and extended this analysis to polyaxial stress states and calculated the limit yield surface for f.c.c. polycrystals comprised of perfectly plastic single crystals. LIN (1957) further extended Taylor's model by including the elastic strain, and thus the extended model was capable of predicting polycrystalline stress–strain behaviour for both large and small plastic strains. Later, KRÖNER (1961) and BUDIANSKY and WU (1962) suggested another polycrystalline deformation model which was also constructed to be valid for the entire stress–strain range. The calculations presented here are based on the latter model, but the stress–strain relations as predicted by the two theories, Lin's and that used here, are simply related.

Some uncertainty exists with respect to the crystallographic slip planes of b.c.c. single crystals; but, as TAYLOR (1955) suggests, a precise knowledge of the slip system is not necessary for determining macroscopic polycrystalline deformation. Accordingly, Taylor's suggestion, now widely accepted, is that slip can occur on any plane associated with any of the four (111) type slip directors. Polycrystalline strain hardening is investigated by assuming, somewhat arbitrarily, that the single crystals harden according to Taylor's rule, $\tau_y = F\,(\Sigma|\gamma|)$. In the following sections the equations of the deformation model suggested by Budiansky–Wu and Kröner are first briefly reviewed, and then the calculations for the b.c.c.

*This work was supported by Advanced Research Projects Agency under contract SD-88 with Harvard University.

structure—stress–strain curves in tension and simple shear, the polycrystalline Bauschinger effect, the limit yield surface, and the Lode diagram—are contrasted with the previous f.c.c. predictions.

2. POLYCRYSTALLINE DEFORMATION MODEL

The equations of the present model have been developed at length by BUDIANSKY and WU (1962) or HUTCHINSON (1964). Here the equations are listed for easy reference. The stress in any crystal is obtained by assuming the crystal is spherical, elastically isotropic, and surrounded by an elastic-plastic matrix which has the same elastic moduli as the single crystal. A stress, S^o_{ij}, applied to the matrix at infinity is the macroscopic aggregate stress and a plastic strain, E^p_{ij}, the aggregate plastic strain, is imposed throughout the matrix. If ϵ^p_{ij}, the plastic strain in the spherical crystal is uniform, the stress in the crystal, s_{ij}, is also uniform and is

$$s_{ij} = S^o_{ij} - \frac{2\,(7 - 5\nu)}{15\,(1 - \nu)}\, G\,(\epsilon^p_{ij} - E^p_{ij}) \tag{1}$$

where ν and G are the Poisson ratio and the elastic shear modulus. All the tensors in the above equation are deviators; the hydrostatic component of the stress tensor does not contribute to the plastic strain. The polycrystalline stress and plastic strain are the average of these quantities over all the grains; or equivalently, the average of these quantities over all the possible orientations of the grain axes with respect to the specimen axes. Since $(s_{ij})_{ave} = S^o_{ij}$, equation (1) is consistent with the identification of S^o_{ij} as the polycrystalline stress.

The fourfold-infinity slip model suggested by Taylor for b.c.c. single crystals is modified, for calculation purposes, by permitting slip to occur on only a finite number of planes associated with each direction. For a sufficiently large number of systems, the polycrystalline predictions are essentially independent of the number of systems and thus identical with the fourfold-infinity model. With m_i as any one of the four slip directions and n_j as the normal to one of the slip planes associated with this direction, the plastic strain in the crystal resulting from a slip, γ, on this system is

$$\epsilon^p_{ij} = \tfrac{1}{2}\,\gamma\,(n_i\, m_j + n_j\, m_i) = \gamma\alpha_{ij}.$$

The total slip in any crystal is the sum of the slips on all the systems,

$$\epsilon^p_{ij} = \sum_n \gamma^{(n)}\,\alpha_{ij}{}^{(n)} \tag{2}$$

Slip occurs on the n^{th} system when the resolved shear stress on that system, $s_{ij}\,\alpha_{ij}{}^{(n)}$, equals the yield stress τ_y of that system. We will specifically be interested in solutions obtained under the assumptions of either ideally plastic single crystals or crystals hardening according to a linear version of Taylor's hardening rule. Thus, the yield stresses on all systems are assumed equal and given by

$$\tau_y = \tau^o{}_y + b \sum_n \left|\gamma^{(n)}\right|. \tag{3}$$

Equations (1), (2), and (3) are now combined to give the equations for obtaining the slips, $\gamma^{(n)}$'s, for the deforming crystals. An active system, $s_{ij}\,\alpha_{ij}^{(n)} = \pm\,\tau_y$, either remains active, in which case (dots indicate incremental quantities)

$$\dot{s}_{ij}\,\alpha_{ij}^{(n)} = \pm\,\dot{\tau}_y \tag{4}$$

with $\dot{\gamma}^{(n)} \geqslant 0$, if the resolved shear stress is positive and $\dot{\gamma}^{(n)} \leqslant 0$, if it is negative, or it unloads and

$$\left|\dot{s}_{ij}\,a_{ij}\right| < \dot{\tau}_y \text{ and } \dot{\gamma}^{(n)} = 0.$$

An inactive system, $\left|s_{ij}\,a_{ij}^{(n)}\right| < \tau_y$, contributes no slip until it is activated. Equation (4) written in terms of the unknown incremental $\dot{\gamma}^{(n)}$'s is

$$\dot{R}^o{}_{ij}\,a_{ij}{}^{(n)} - \frac{2\,(7-5\nu)}{15\,(1-\nu)}\,G \sum_m \dot{\gamma}^{(m)}\,a_{ij}{}^{(m)}\,a_{ij}{}^{(n)} = \pm\,b \sum_m \left|\dot{\gamma}^{(m)}\right| \tag{5}$$

where $R^o{}_{ij}$, the independent variable in the calculation, is defined by

$$R^o{}_{ij} = S^o{}_{ij} + \frac{2\,(7-5\nu)}{15\,(1-\nu)}\,G\,E^p{}_{ij}. \tag{6}$$

In general, this tensor cannot be specified so as to obtain, say, a prescribed stress history; but for both tension and simple shear the tensors $S^o{}_{ij}$ and $E^o{}_{ij}$ are proportional and $R^o{}_{ij}$ can be specified to give either of these two histories.

We now consider some of the details of the deformation of the single crystal which are peculiar to the b.c.c. structure; in particular, let us look at the perfect plasticity solution. As $R^o{}_{ij}$ increases from zero, the stress in the crystal increases with no slip taking place until the resolved shear stress on some slip system reaches the yield stress. This system slips and continue to remain active until a second slip system, associated with one of the three inactive directions, is activated; both these systems slip simultaneously. These two systems remain active until either (i) another system associated with the remaining two inactive directions is activated or (ii) as often occurred, a system associated with one of the active directions and adjacent to one of the active planes is activated. With an infinite number of planes per slip direction only one slip plane per direction could be active at any stage. The active system rotates about the slip direction with a continuous distribution of slip over the 'fan' of slip planes which have been active. It is possible for two adjacent slip systems associated with a given slip direction to be active in a crystal with only a finite number of systems, and possibility (ii) would be expected. Unloading, as one might suspect, takes place frequently : in most cases an active system unloads as an adjacent system associated with the same directions becomes active. Thus, as the crystal deforms, three, four, and five slip systems become active. When five independent slip systems are active, the stress in the crystal has reached a fixed value and no further slip system is activated.

The plastic strain is an average of $\epsilon^p{}_{ij}$ over all the orientations of the grain axes relative to the specimen axes. As the symmetry of the b.c.c. single crystal is similar to that of the f.c.c. crystal, the same reduced regions employed in the f.c.c. calculation are valid for the b.c.c. investigations. Two identical tensile calculations, each a numerical integration over ninety-one orientations of the grain axes relative to the tensile axis but one with twenty slip planes per slip direction and the other with only ten, differed nowhere by more than 0·7 per cent. In addition, two calculations, both with ten slip systems per direction but with ninety-one and twenty-eight orientation stations respectively, showed less than 0·5 per cent divergence. In the calculation for the polycrystalline simple shear relation the third Euler angle variation, from 0 to $\frac{1}{2}\pi$, was divided into ten equal divisions; 280 orientation stations were used for this calculation. It was necessary to include a variation of the third Euler angle from 0 to π for the calculation of the limit yield surface. This variation was divided into twelve equal divisions with 336 orientations in all. The error of the tensile calculation, compared to an exact calculation using the Taylor fourfold-infinity slip model, with twenty slip planes per direction should be less than 1 per cent, while that of the other calculations, performed with ten slip plane per direction should be less than 2 per cent. All the calculations were performed by a 7090 IBM computer with $\nu = \frac{1}{3}$.

3. TENSILE AND SIMPLE SHEAR STRESS-STRAIN RELATIONS

COX and SOPWITH (1937) calculated the lower bound of the tensile yield stress of a b.c.c. polycrystal of ideally plastic single crystals. They assumed each grain

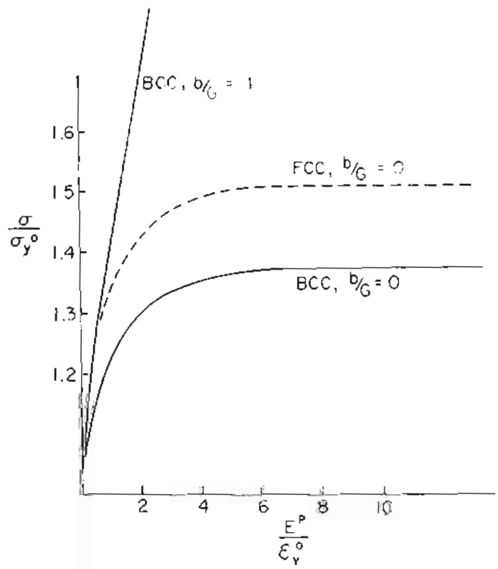

FIG. 1. Tensile stress-plastic strain curves. $\sigma^0{}_y$ and $\epsilon^0{}_y$ are the stress and strain at the initial elastic limit. $\nu = 1/3$ for both b.c.c. and f.c.c.

was subject to a uniaxial stress, parallel to the specimen axis, sufficient to produce slipping on the most highly stressed slip system. These uniaxial stresses were averaged over all orientations to give for the limit yield stress $\sigma_{\text{lim}}/\sigma^0{}_y = 1{\cdot}068$, where $\sigma^0{}_y$ is the initial elastic limit. A similar calculation gives a lower bound of $\sigma_{\text{lim}}/\sigma^0{}_y = 1{\cdot}116$ for f.c.c. polycrystals. TAYLOR (1938) obtained what is a much more realistic approximation to the limit yield stress of f.c.c. polycrystals under simple tension : $\sigma_{\lim}/\sigma^o{}_y = 1{\cdot}53$. TAYLOR (1955) described a procedure for calculating the limit yield stress of a polycrystal of ideally plastic single crystals on the basis of the fourfold-infinity b.c.c. slip model. He made, however, no calculations. The limit yield stress as predicted by the present model can be shown to be identical with that predicted by the Taylor model, as well as Lin's extension. Thus, the value of the limit yield stress in simple tension for the b.c.c. structure, $\sigma_{\lim}/\sigma^o{}_y = 1{\cdot}374$ (from the calculation with twenty slip planes), and the limit yield stress in simple shear, $\tau_{\lim}/\sigma^o{}_y = 0{\cdot}771$, and the corresponding values associated with the f.c.c. structure, $\sigma_{\lim}/\sigma^o{}_y = 1{\cdot}536$ and $\tau_{\lim}/\sigma^o{}_y = 0{\cdot}828$, are appropriate for each of these three deformation models. The significance of these numbers is discussed in the following section. The stress–strain relations in tension and simple shear are given in Table 1 for $b = 0$ and one non-zero value of b. Fig. 1 is a plot of the tension stress–strain curves with the perfectly plastic f.c.c. curve included for comparison. As was pointed out by HUTCHINSON (1964), the stress–strain curves as predicted by Lin's extension to Taylor's model and the Budiansky and Wu model are simply related. For example, in simple tension for ideal plasticity with $\nu = \frac{1}{3}$ the plastic strain predicted by the Lin model is 8/15 of that predicted by the present model.

TABLE 1

$b/G = 0$		$b/G = 0{\cdot}10$	
$\sigma/\sigma^o{}_y$	$E^p/\epsilon^o{}_y$	$\sigma/\sigma^o{}_y$	$E^p/\epsilon^o{}_y$
1·087	0·188	1·109	0·151
1·139	0·435	1·189	0·352
1·200	0·834	1·367	0·881
1·279	1·702	1·465	1·223
1·350	3·91	1·591	1·674
1·367	7·88	1·814	2·476
1·372	16·21	2·953	6·91
1·374	∞	4·430	12·78

The strain hardening relations listed in Table 1 are the results of exact calculations. For reasonably small values of the strain hardening parameter, say $b/G < 0{\cdot}05$, the following formulae give very close approximations to the exact calculations (HUTCHINSON 1964). With bars denoting the ideally plastic polycrystalline quantities, the polycrystalline strain hardening quantities are given by

$$\sigma = \frac{1}{1 - \dfrac{b}{\tau^o{}_y} m_{ave} \bar{E}^p} \bar{\sigma}, \quad E^p = \frac{1}{1 - \dfrac{b}{\tau^o{}_y} m_{ave} \bar{E}^p} \bar{E}^p,$$

where m_{ave} is 3·06 for the f.c.c. structure and 2·75 for the b.c.c. structure. TAYLOR's (1938) formulae relating the tensile stress and plastic strain, valid for large plastic strains is

$$\sigma = F\,(m_{ave}\,E^p)\,m_{ave} \tag{7}$$

where F is the hardening function of the single crystal and, as above, m_{ave} is either 3·06 or 2·75 depending on the crystalline structure. Note that from (7) the limit yield stress of a polycrystal perfectly plastic single crystal is exactly $\frac{1}{2}m_{ave}$; the number m_{ave} appropriate to b.c.c. polycrystals was obtained from the present calculations. It is of interest to compare the final slope of the stress–strain curve as predicted by a linear version of (7), $\sigma = b\,(m_{ave})^2\,E^p$, with the predictions of the present model. These results are shown in Fig. 2. For small values strain hardening the agreement is very good but Taylor formula gives larger estimates of the final slope with increasing strain hardening. Noting that the slope of the stress–strain curve for large plastic strains as predicted by the Taylor formula (7) for linear hardening is dependent on $(m_{ave})^2$, it is seen that for equal single crystal hardening the slope for the f.c.c. polycrystal is 1·24 times that for the b.c.c. polycrystal.

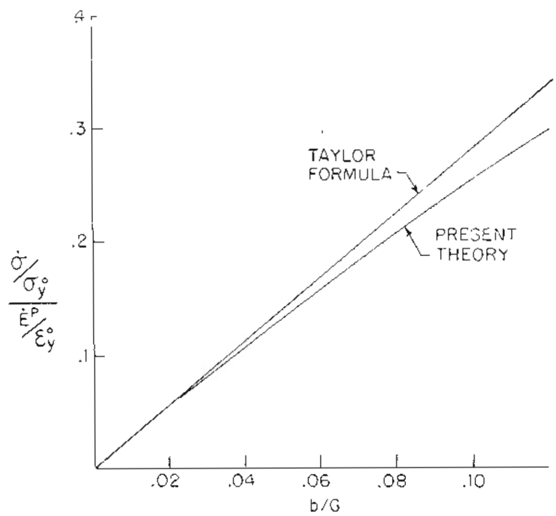

FIG. 2.

4. LIMIT YIELD SURFACE

The limit yield stress in tension is defined as the maximum tensile stress which the polycrystal of perfectly plastic single crystals can sustain, and similarly for the limit yield stress in simple shear. Knowledge of the yield surface in σ_x, σ_y space for $0 \leqslant \sigma_y \leqslant \frac{1}{2}\sigma_x$ completely characterizes the yield surface for all stress states. BISHOP and HILL (1951) calculated the limit yield surface for f.c.c. polycrystals. We have used the calculation framework of the present model to determine the yield surface for b.c.c. polycrystals. Although this procedure is somewhat different from the scheme of Bishop and Hill, it is equivalent. In calculating a typical point on the surface, $R^o{}_{ij}$ was arbitrarily chosen, and a procedure similar to that described in Section 3 was used to determine the final stress in each crystal, and then these stresses were averaged to obtain the limit yield stress associated with the particular choice of $R^o{}_{ij}$. From (6) $\dot{E}^p{}_{ij} \approx \dot{R}^o{}_{ij}$ once the stress has reached the yield surface.

The results of these calculations are listed in Table 2. Both the yield surface and the Lode (μ, ν) diagram have been plotted. To facilitate comparison with

TABLE 2

$\dot{E}^p_{ij}/\dot{\epsilon}^0_y \approx (1, \lambda - \frac{1}{2}, -\lambda - \frac{1}{2}, 0, 0, 0)$		
σ_x/σ_y^0	σ_y/σ^0_y	λ
1·38	0	0
1·44	0·142	0·125
1·49	0·308	0·250
1·53	0·510	0·375
1·54	0·771	0·500

Bishop and Hill's results for f.c.c. polycrystals, all points on the yield surface were normalized by dividing their co-ordinates by the value of the tensile yield stress. The normalized f.c.c. and b.c.c. yield surfaces are plotted in Fig. 3 along with the predictions of the τ_{max} vs. γ^p_{max} theory and the J_2 theory, both phenomenological.

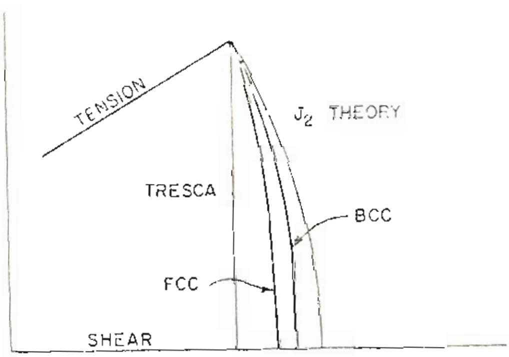

FIG. 3. Normalized limit yield surface; f.c.c. curve from Bishop and Hill.

The plane of the trace of the yield surface is identical to that given by Bishop and Hill. In this plane the J_2 (or von Mises) curve is a circle and the τ_{max} vs. γ^p_{max} (or Tresca) curve is a straight line. The two phenomenological curves bracket the f.c.c. and b.c.c. yield surfaces; yet, while the f.c.c. surface lies more or less midway between the two curves, the b.c.c. yield surface lies much closer to the J_2 curve. This suggests that the J_2 theory is preferable to the τ_{max} vs. γ^p_{max} theory when applied to b.c.c. polycrystals. This is further borne out when the entire simple shear and tensile stress–strain curves of the present calculations are brought into comparison through the two phenomenological theories.

The theoretical (μ, ν) diagram (Fig. 4) agrees with the experimental findings of b.c.c. metals reported by LODE (1926) and TAYLOR (1931). The Lode parameters for this plot are

$$\mu = 2\,\frac{\sigma_y}{\sigma_x} - 1, \quad \text{and} \quad \nu = 2\,\frac{E^p{}_y - E^p{}_z}{E^p{}_x - E^p{}_z} - 1.$$

The line $\mu = \nu$ corresponds to agreement with the J_2 flow theory.

There is by no means concurrence in the reportings of the experimental Lode diagrams. This is especially true for f.c.c. investigations for which experimental curves have been found to lie to the right as well as the left of the line $\mu = \nu$. ELLINGTON (1958) found the experimental (μ, ν) curve to be considerably to the

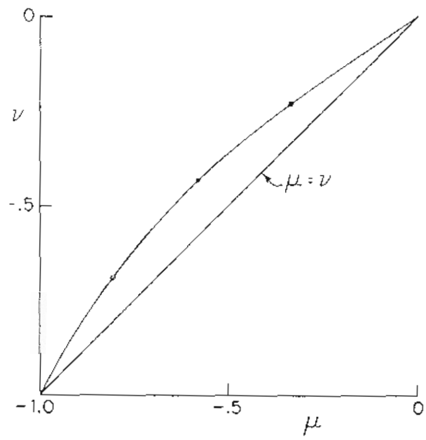

FIG. 4.

right of the line $\mu = \nu$ for polycrystalline copper and along the line $\mu = \nu$ for α-brass. While Taylor's specimens displayed little strain hardening, Ellington's had a high rate of work hardening. The possibility that the difference in findings can be accounted for by including strain hardening is currently being considered.

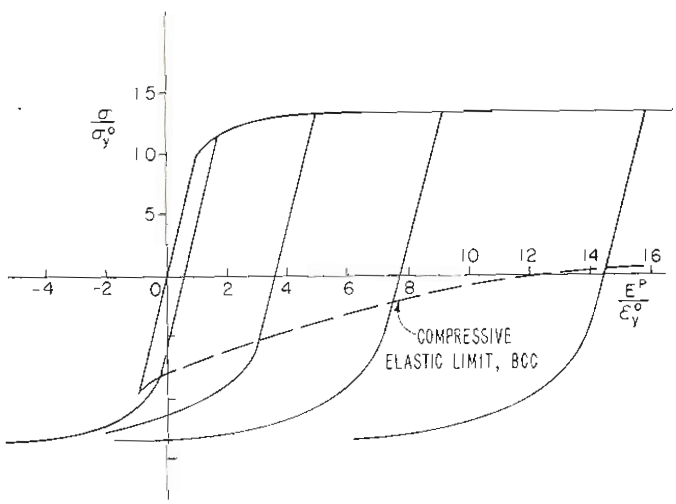

FIG. 5.

5. B.C.C. POLYCRYSTALLINE BAUSCHINGER EFFECT

Here a polycrystalline Bauschinger effect is demonstrated assuming the b.c.c. single crystals display no hardening. As in the calculations we have discussed, it is interesting to draw comparison with previously obtained results for the f.c.c. structure. A typical calculation paralleled the following conceptual experiment : the specimen was given an initial tensile elongation, the tensile load was reduced, and the specimen was deformed in compression. Several such calculations, corresponding to different initial plastic strains, are shown in Fig. 5. No plastic strain is predicted when the tensile load is diminished from its initial value, as was reported for f.c.c. polycrystals [see CZYZAK, BOW and PAYNE (1957) or HUTCHINSON (1964)]. The nominal compressive elastic limit of an f.c.c. specimen after a large initial plastic extension is $\sigma/\sigma^0{}_y = 0{\cdot}17$, while for b.c.c. specimen the compressive elastic limit is actually positive : $\sigma/\sigma^0{}_y = 0{\cdot}08$. The b.c.c. structure displays a stronger polycrystalline Bauschinger effect.

ACKNOWLEDGMENT

The author is grateful to Professor B. Budiansky who suggested the work and who gave considerable helpful advice.

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