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Plastic stress–strain relations of polycrystalline metals

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Plastic deformation of polycrystals is investigated on the basis of single-crystal deformation. Slip is assumed to be the only deformation mechanism. Accordingly, an explicit tensile plastic stress–strain relation which contains the relevant microstructure parameters is obtained. As a simple application of the theoretical model, the effect of grain size on the flow stresses of polycrystals is studied. Finally, the general features of the present polycrystal model are summarized. Numerical results are obtained for face-centred cubic polycrystals, and the theoretical predictions are found to be in reasonable agreement with those of Taylor, Bishop, Hill and Hutchinson.

1. Introduction

When the physical mechanisms for the generation and interaction of dislocations within single crystals and those within polycrystals are similar, we expect that the plastic stress–strain curve of a polycrystal derived from the shear stress–slip strain curve of its constituent single crystal, based on Taylor's approach [1], should be reasonably accurate, especially when material constants of the single crystal are taken from the experimental results obtained under multi-slip conditions [2]. On the other hand, it has been observed that the yield stress, as well as the flow stress, of a polycrystal are significantly influenced by its grain size d. The well-known Hall–Petch relation [3, 4] states that

$$\sigma = \sigma_{\bar{\varepsilon}}^{0} + k_{\bar{\varepsilon}} d^{-1/2} \quad (1)$$

where $\sigma_{\bar{\varepsilon}}^{0}$ and $k_{\bar{\varepsilon}}$ are material constants. The subscript $\bar{\varepsilon}$ is to signify their dependence on the strain. It is noted that a different grain-size dependence has been observed and proposed [5, 6], but Equation 1 seems to be valid for a wide range of materials. In any event, the classical Taylor model cannot predict this grain-size influence. Even the more sophisticated models developed later such as the KBW model [7, 8] or Hill's model [9], which take into account the elastic/plastic strain, fail to reveal this size influence. This is partly due to the inherent assumption of homogeneous strain within the spherical grains embedded in an infinite polycrystal matrix.

To overcome this difficulty, Armstrong *et al.* [10] and Weng [11] assumed an inherent size dependence in the shear stress–slip strain curve of single crystals in order to bring out this phenomenon. An alternative approach was proposed by Chiang [12]. Basically, the later distinguishes two different regions in a polycrystal, i.e. grain interiors and grain boundary regions. It was assumed that the grain interiors can be treated by the conventional Taylor approach (or its variations and generalizations), while the influence of the grain boundary regions is accounted for by a suitable interaction law.

The objective of the present study is two-fold. First, a polycrystal model developed by Chiang and Weng [13] which is restricted to linear-hardening materials is to be generalized to take into consideration a non-linear (power type) hardening. The derivation of the new model is, in general, parallel to that outlined previously [13]. Secondly, based on this polycrystal model in conjunction with the two-phase approach proposed by Chiang [12], a fairly general explicit expression for the flow stress of the polycrystal in terms of the relevant microstructure parameters is then obtained. In the final section, a summary of the features of this polycrystal is given.

2. Theoretical model

2.1. Deformation of single crystals

The plastic behaviour of a single crystal is most appropriately expressed as the relationship between the resolved shear stress τ and the slip strain γ in the active slip system, i.e.

$$\tau = f(\gamma) \quad (2)$$

In general, a threshold value τ_0 can be identified at which extensive plastic deformation begins, i.e. the so-called Schmid law. Consequently, Equation 2 can usually be put into the form

$$\tau = \tau_0 + g(\gamma) \quad (3)$$

where τ_0 is the critical resolved shear stress. To be specific, we shall assume here that the function g can be adequately represented by a power-type form in conjunction with Taylor's isotropic hardening rule, so that the resolved shear stress $\overset{(i)}{\tau}$ on the ith currently active slip system relates to the total sum of the slip strains of all the independent slip systems within the

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grain as

$$\overset{(i)}{\tau} = \tau_0 + h\left(\sum_{j=1}^{n} \overset{(j)}{\gamma}\right)^{\beta} = \tau_0 + h(n\bar{\gamma})^{\beta} \quad (4)$$

where n is the number of the active slip system, $\bar{\gamma} \equiv (\Sigma_{j=1}^{n} \overset{(i)}{\gamma})/n$ and h and β are material constants. From the dislocation viewpoint, several theories have been proposed to determine the values of τ_0, h and β in terms of more fundamental parameters (see e.g. [14]). However, the discussion of these theories is outside the scope of the present study and we shall omit it here. Instead, we treat these material constants as empirical constants which can be obtained by suitable experiments. It is also to be noted that Equation 4 is slightly different from that used by Weng [15].

2.2. The polycrystalline deformation model

The polycrystal model developed by Chiang and Weng [13] will be reviewed. In particular, the emphasis will be placed on its extension to account for the cases where $\beta \neq 1$. For more detailed analysis and discussion, especially in the transition state, interested readers are referred to Chiang and Weng [13].

We first replace Equation 4 with a linear form

$$\overset{(i)}{\tau} = \tau_0 + h_s(n\bar{\gamma}) \quad (5)$$

where h_s is chosen as

$$h_s = h(n\bar{\gamma})^{\beta-1} \quad (5')$$

so that Equation 5 is identical to Equation 4. However, it is noted that h_s is no longer a material constant but depends on the strain.

Kinematically, the strain of a single crystal can be related to the slip magnitude by

$$\varepsilon_{kl} = \sum_{j=1}^{n} \overset{(i)}{\nu}_{kl} \overset{(j)}{\gamma} \quad (6)$$

where ν_{kl} is the Schmid factor tensor. For the (1 1) component we have

$$\varepsilon_{11} = \sum_{j=1}^{n} \overset{(j)}{\nu}_{11} \overset{(j)}{\gamma} = n\bar{\nu}_{11}\bar{\gamma} + \sum_{j=1}^{n} \overset{(j)}{\nu}_{11} \overset{(j)}{\gamma}' \quad (7)$$

where $\overset{(j)}{\gamma} = \bar{\gamma} + \overset{(j)}{\gamma}'$ has been used. Proceeding in parallel with the analysis carried out by Chiang and Weng [13], we conclude that in the grain considered, the micro-constitutive equation can be represented by

$$\sigma_{11} = \frac{(1-\eta)}{\bar{\nu}_{11}}\tau_0 + \frac{h_s(1-\delta)}{\bar{\nu}_{11}}\varepsilon_{11} \quad (8)$$

where n is the contribution from the non-dominant stress components and $\delta \equiv (\Sigma_{j=1}^{n} \overset{(j)}{\nu}_{11} \overset{(j)}{\gamma})/\varepsilon_{11}$. In comparison with other rigorous numerical treatments, the errors due to neglecting η and δ are found to be quite small. We conclude that such approximations are, in fact, "compatible" with the self-consistent formulation which accounts for the interaction of the grains by assuming

$$\sigma_{11} = \bar{\sigma}_{11} + A\mu(\bar{\varepsilon}_{11} - \varepsilon_{11}) \quad (9)$$

where σ_{11} and $\bar{\sigma}_{11}$ are the (1 1) components of stress tensors of grains and the polycrystal, respectively; ε_{11} and $\bar{\varepsilon}_{11}$ are their respective plastic strains, μ is the shear modulus and A is the constraint tensor [16].

Following the solution method previously developed [13], with $c = 1$, i.e. in the fully plastic state, we arrive at

$$\bar{\sigma}_{11} = (1-\psi)^{-1}(\phi\tau_0 + \psi A\mu\bar{\varepsilon}_{11}) \quad (10)$$

where

$$\psi \equiv \sum_{i=0}^{\infty} \left\langle (-1)^i \left(\frac{1}{\bar{\nu}_{11}^2}\frac{h_s}{A\mu}\right)^{i+1} \right\rangle$$
$$\phi \equiv \sum_{i=0}^{\infty} \left\langle (-1)^i \frac{1}{\bar{\nu}_{11}} \left(\frac{1}{\bar{\nu}_{11}^2}\frac{h_s}{A\mu}\right)^{i} \right\rangle \quad (10')$$

and $\langle\ \rangle$ denotes the average over all grain orientations. It is noted that deviations (such as δ and η) from the dominant component (here the (1 1) component) have been omitted in the derivation.

Furthermore, it is noted that

$$h_s = h\left(\sum_{j=1}^{n} \overset{(j)}{\gamma}\right)^{\beta-1} = h(n\bar{\gamma})^{\beta-1}$$
$$= h\left(\frac{\varepsilon_{11}}{\bar{\nu}_{11}} - \frac{\Sigma\, \nu_{11}\gamma'}{\bar{\nu}_{11}}\right)^{\beta-1} = h\left[\frac{\varepsilon_{11}}{\bar{\nu}_{11}}(1-\delta)\right]^{\beta-1} \quad (11)$$

On the other hand, ε_{11} can be resolved into two components, i.e. $\bar{\varepsilon}_{11}$ and ε'_{11}. We write $\varepsilon_{11} = \bar{\varepsilon}_{11} + \varepsilon'_{11}$ where $\langle\varepsilon'_{11}\rangle = 0$. Therefore

$$\varepsilon_{11} = \bar{\varepsilon}_{11}(1+\omega) \quad (12)$$

where $\omega \equiv \varepsilon'_{11}/\bar{\varepsilon}_{11}$. Note the $\langle 1+\omega\rangle = 1$, so Equation 11 becomes

$$h_s = h\left(\frac{\bar{\varepsilon}_{11}}{\bar{\nu}_{11}}\right)^{\beta-1}(1-\delta)^{\beta-1}(1+\omega)^{\beta-1}$$
$$\approx h\left(\frac{\bar{\varepsilon}_{11}}{\bar{\nu}_{11}}\right)^{\beta-1} \quad (13)$$

The error due to the above approximation can be roughly estimated by considering the difference of the energy dissipated between the actual deformation path, i.e. Equation 4, and the assumed linear path, i.e. Equation 5. When $\beta = 0.6$, it has been found that the error is within 5% for $\bar{\varepsilon} < 0.1$ and is within 12% for $\bar{\varepsilon} < 0.2$ [17]. From Equation 13 with definitions of ψ and ϕ from Equation 10′, we then find that

$$\psi \equiv \sum_{i=0}^{\infty} \left\langle (-1)^i \left(\frac{1}{\bar{\nu}_{11}^2}\frac{h_s}{A\mu}\right)^{i+1} \right\rangle$$
$$= \left\langle \frac{h_s}{\bar{\nu}_{11}^2} \right\rangle \frac{1}{A\mu} - \left\langle \frac{h_s^2}{\bar{\nu}_{11}^4} \right\rangle \left(\frac{1}{A\mu}\right)^2 + \cdots$$
$$\approx \left\langle \frac{1}{\bar{\nu}_{11}^{1+\beta}} \right\rangle \left(\frac{h}{A\mu}\right)\bar{\varepsilon}^{\beta-1}$$
$$- \left\langle \frac{1}{\bar{\nu}_{11}^{2(1+\beta)}} \right\rangle \left(\frac{h}{A\mu}\right)^2 \bar{\varepsilon}^{2(\beta-1)} + \cdots$$
$$= \left\langle \frac{1}{\bar{\nu}_{11}^{1+\beta}} \right\rangle \left(\frac{h}{A\mu}\right)\bar{\varepsilon}^{\beta-1}(1-\psi)$$

TABLE I Values of $\langle 1/\bar{v}_{11}^{1+\beta}\rangle$ (upper) and $\langle 1/\bar{v}_{11}\rangle^{1+\beta}$ (lower) for fcc polycrystals

$1+\beta$	n				
	1	2	3	4	5
1	2.232	2.336	2.510	2.673	2.898
	2.232	2.336	2.510	2.673	2.898
1.1	2.420	2.545	2.754	2.951	3.225
	2.419	2.543	2.752	2.949	3.223
1.2	2.624	2.772	3.021	3.259	3.590
	2.621	2.768	3.017	3.255	3.585
1.3	2.846	3.020	3.315	3.599	3.997
	2.840	3.013	3.308	3.590	3.988
1.4	3.087	3.290	3.638	3.975	4.451
	3.077	3.280	3.627	3.961	4.435
1.5	3.348	3.585	3.993	4.391	4.957
	3.335	3.570	3.977	4.370	4.933
1.6	3.633	3.907	4.383	4.851	5.520
	3.613	3.886	4.360	4.822	5.487
1.7	3.941	4.259	4.812	5.359	6.150
	3.915	4.231	4.780	5.320	6.103
1.8	4.277	4.643	5.283	5.922	6.852
	4.243	4.605	5.241	5.869	6.789
1.9	4.634	5.062	5.800	6.545	7.634
	4.597	5.013	5.746	6.476	7.551
2	5.039	5.520	6.370	7.235	8.508
	4.982	5.457	6.300	7.145	8.398

$$\begin{aligned}\phi &\equiv \sum_{i=0}^{\infty}\left\langle (-1)^i \frac{1}{\bar{v}_{11}}\left(\frac{1}{\bar{v}_{11}^2}\frac{h_s}{A\mu}\right)^i\right\rangle \\ &= \left\langle\frac{1}{\bar{v}_{11}}\right\rangle - \left\langle\frac{h_s}{\bar{v}_{11}^3}\right\rangle\frac{1}{A\mu} + \left\langle\frac{h_s^2}{\bar{v}_{11}^5}\right\rangle\left(\frac{1}{A\mu}\right)^2 - \cdots \\ &\approx \left\langle\frac{1}{\bar{v}_{11}}\right\rangle - \left\langle\frac{1}{\bar{v}_{11}^{2+\beta}}\right\rangle\left(\frac{h}{A\mu}\right)\bar{\varepsilon}^{\beta-1} \\ &\quad + \left\langle\frac{1}{\bar{v}_{11}^{3+2\beta}}\right\rangle\left(\frac{h}{A\mu}\right)^2\bar{\varepsilon}^{2(\beta-1)} - \cdots \\ &= \left\langle\frac{1}{\bar{v}_{11}}\right\rangle(1-\psi) \end{aligned} \tag{14}$$

It is noted that the following approximations for fcc polycrystals have been observed, i.e.

$$\begin{aligned}&\left\langle\left(\frac{1}{\bar{v}_{11}^{1+\beta}}\right)\left(\frac{1}{\bar{v}_{11}^{1+\beta}}\right)^N\right\rangle \approx \left\langle\frac{1}{\bar{v}_{11}^{1+\beta}}\right\rangle\left\langle\left(\frac{1}{\bar{v}_{11}^{1+\beta}}\right)^N\right\rangle \\ &\qquad N = 1, 2, \ldots \\ &\left\langle\left(\frac{1}{\bar{v}_{11}}\right)\left(\frac{1}{\bar{v}_{11}^{1+\beta}}\right)^N\right\rangle \approx \left\langle\frac{1}{\bar{v}_{11}}\right\rangle\left\langle\left(\frac{1}{\bar{v}_{11}^{1+\beta}}\right)^N\right\rangle \\ &\qquad N = 1, 2, \ldots \end{aligned} \tag{15}$$

Finally, Equation 10 becomes

$$\begin{aligned}\bar{\sigma}_{11} &= \left\langle\frac{1}{\bar{v}_{11}}\right\rangle\tau_0 + \left[\left\langle\frac{1}{\bar{v}_{11}^{1+\beta}}\right\rangle\left(\frac{h}{A\mu}\right)\bar{\varepsilon}^{\beta-1}\right]A\mu\bar{\varepsilon}_{11} \\ &= \left\langle\frac{1}{\bar{v}_{11}}\right\rangle\tau_0 + \left\langle\frac{1}{\bar{v}_{11}^{1+\beta}}\right\rangle h\bar{\varepsilon}^{\beta} \end{aligned} \tag{16}$$

Table I shows values of $\langle 1/\bar{v}_{11}^{1+\beta}\rangle$ and $(\langle 1/\bar{v}_{11}\rangle)^{1+\beta}$ for fcc crystals. Now we shall introduce a more concise notation $\bar{m}$ to replace the cumbersome expression $\langle 1/\bar{v}_{11}\rangle$, so Equation 16 can be written as

$$\bar{\sigma}_{11} = \bar{m}\tau_0 + \bar{m}^{1+\beta}h\bar{\varepsilon}^{\beta} \tag{17}$$

It should be emphasized that the constraint factor A does not explicitly appear in the final macroconstitutive equation (Equations 16 or 17). However, this does not mean that A has no influence on the flow stress of the polycrystal. Its influence, in fact, indirectly affects the average number of active slip systems, n.

3. Grain size effects

In this section the two-phase model proposed by Chiang [12] will be used to discuss the grain size influence. Basically, we distinguish two regions in a polycrystal: (a) grain interiors V_c and (b) grain boundary regions V_{gb}. We assume that the analysis in the previous section is valid for V_c, so

$$\bar{\sigma}_c = \bar{m}\tau_0 + \bar{m}^{1+\beta}h\bar{\varepsilon}^{\beta} \tag{18}$$

where $\bar{\sigma}_c$ denotes the average stress in V_c. Furthermore, the average stress in V_{gb} can be accounted for through an "interaction" law similar to Equation 9, so

$$\bar{\sigma}_{gb} = \bar{\sigma} + A\mu(\bar{\varepsilon} - \bar{\varepsilon}_{gb}) \tag{19}$$

Now, if we further assume that no plastic strain is allowed to relax the high stress concentration accumulated within V_{gb}, then $\bar{\varepsilon}_{gb} = 0$, i.e.

$$\bar{\sigma}_{gb} = \bar{\sigma} + A\mu\bar{\varepsilon} \tag{20}$$

Moreover, since $\bar{\sigma} = f_c\bar{\sigma}_c + f_{gb}\bar{\sigma}_{gb}$ and $f_c + f_{gb} = 1$ where f_c and f_{gb} are the volume fractions of V_c and V_{gb}, respectively, so we obtain

$$\bar{\sigma} = f_c\bar{\sigma}_c + f_{gb}(\bar{\sigma} + A\mu\bar{\varepsilon})$$

or

$$\bar{\sigma} = \bar{\sigma}_c + \frac{f_{gb}}{f_c}A\mu\bar{\varepsilon}$$

It is noted that, in Equation 21, the only possible size-dependence factor is contained in the last term. To conform with the Hall–Petch relation, phenomenologically we assume

$$\frac{f_{gb}}{f_c}A = \alpha d^{-1/2} \tag{22}$$

where α is a constant independent of grain size. Consequently, from Equations 18, 21 and 22 we conclude that

$$\bar{\sigma} = \bar{m}\tau_0 + \bar{m}^{1+\beta}h\bar{\varepsilon}^{\beta} + \alpha\mu\bar{\varepsilon}d^{-1/2} \tag{23}$$

Comparing Equation 23 to Equation 1, we find that the Hall–Petch parameters are

$$\sigma_{\bar{\varepsilon}}^0 = \bar{m}\tau_0 + \bar{m}^{1+\beta}h\bar{\varepsilon}^{\beta}$$

and

$$k_{\bar{\varepsilon}} = \alpha\mu\bar{\varepsilon} \tag{24}$$

It is worth comparing the theoretical findings with available experimental results. For example, Gupta and Garofalo [18] have reported some experimental data for the Fe–Ti alloys. It is found that

$$k_{\bar{\varepsilon}} \sim \bar{\varepsilon}^{1/2} \tag{25}$$

In this case, from Equation 24 it is required that

$$\alpha \sim \bar{\varepsilon}^{-1/2} \tag{26}$$

To the contrary, the experimental results of Jago and

Hassen [19] for polycrystalline iron reveal that $k_{\bar{\varepsilon}}$ decreases with strain. Nevertheless several experimental results [20] including those of Jago and Hassen seem to support the conclusion that, above a certain range of plastic strain, $k_{\bar{\varepsilon}}$ is relatively insensitive to strain. This suggests that asymptotically

$$\alpha \sim \bar{\varepsilon}^{-1} \tag{27}$$

At present, we are unable to settle this question. This is because of the phenomenological approach adopted in Equation 22. To resolve this problem, a consideration of the different micro-mechanisms operating in V_{gb} and V_c and their respective contributions to the macro-stress during plastic deformation (particularly the influence of temperature and solute atoms) cannot be avoided. Nevertheless, different dependences of α upon $\bar{\varepsilon}$ indicate that different micro-mechanisms must be responsible for such discrepancies.

It is also a particular interest to note that the experimental data reviewed by Armstrong *et al.* [10] show that, at a specific strain, k/μ is a constant (particularly for f c c crystals such as copper, aluminium and silver). This phenomenon can be inferred from Equation 24, since α depends on plastic strain only.

4. Discussion and conclusions

The original polycrystal model developed by Chiang and Weng has been extended to account for non-linear hardening and the grain-size effect. The specific features of this model are as follows.

1. The final macro-constitutive Equation 23 is given explicitly in terms of the important micro-parameters such as the Taylor factor $\bar{m}$, slip modulus h, hardening exponent β and grain size d. The advantage of the present model over other purely numerical approaches lies in the fact that general qualitative and quantitative information can be analytically derived once and for all without repeatedly doing the same numerical studies for each and every case.

2. For f c c crystals without hardening, assuming $n = 5$, the present model predicts that the yield stress in pure tension and pure shear are [21]

$$\bar{\sigma} = 2.898\tau_0 \qquad \bar{\tau} = 1.699\tau_0 \tag{28}$$

respectively. On the other hand, the results of Bishop and Hill [22] give

$$\bar{\sigma} = 3.06\tau_0 \qquad \bar{\tau} = 1.656\tau_0 \tag{29}$$

The agreement between two theories is within 6%. For linear hardening, i.e. $\beta = 1$, it is easy to deduce the hardening rate H of the polycrystal according to Equation 23. Assuming that the grain size effect is negligible and $n = 5$, we find that

$$H = 8.508h$$

The result is compared with that obtained by Hutchinson [23] in Fig. 1. The difference between the two predictions over a wide range of h/μ is within 5%. From the above comparisons, the present model is judged to be reasonably accurate.

3. The accuracy of the present model indicates that the assumption of a negligible effect of deviation terms such as η, δ and ω made in this model is justified. In particular, this fact implies that the presence of η, δ and ω introduces only a secondary effect on the macro-plastic behaviour (especially in the fully plastic state) of the polycrystal.

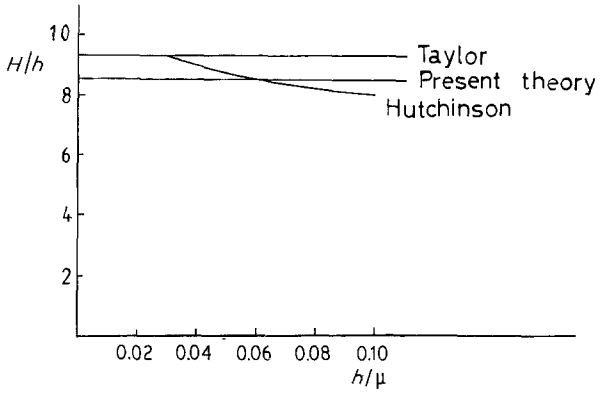

Figure 1 Ratio of the polycrystal hardening rate H to the single-crystal hardening rate h as a function of h/μ with μ being the shear modulus; linear hardening assumed; Poisson's ratio $\nu = 1/3$ used for Hutchinson's curve and $n = 5$ used for the present model.

4. If the Hall-Petch parameter $k_{\bar{\varepsilon}}$ is normalized with respect to the shear modulus μ, according to Equation 24 at a specific plastic strain, k/μ should be a constant for the same class of crystalline structure since the relationship between α and $\bar{\varepsilon}$ is probably identical for materials of the same crystallinity. The experimental data compiled by Armstrong *et al.* [10] seem to support this conclusion.

5. It must be emphasized that although only f c c polycrystalline metals are specifically considered in this paper and, in fact, the numerical results are calculated and presented only for this class of materials, the theoretical formulation and general analysis are believed to be valid for all types of crystallinity, particularly for materials in which the slip mechanism is responsible for the major plastic deformation.

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