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Yield criterion of an fcc polycrystal under combined loadings

C. R. CHIANG
Department of Power Mechanical Engineering, National Tsing Hua University, Hsinchu 30043, Taiwan

The yield criterion of an fcc polycrystal under combined loadings is derived based on a newly proposed polycrystal model. The single crystal is assumed to be non-hardening. Cases of biaxial tension and tension–torsion tests are all studied. It is shown that the macro yield stress component of the polycrystal can always be identified with the critical resolved shear stress τ_0 multiplied by some orientation factor *M*. A Monte Carlo procedure is used to evaluate *M*. The results of the present model are found in reasonable agreement with those of the Taylor–Bishop–Hill model, and in excellent agreement with the Mises' criterion.

1. Introduction

The inception of the plastic flow in a material under combined stresses is conventionally characterized by postulating the existence of a yield criterion, i.e.

$$F(\sigma_{ij}) = 0 \tag{1}$$

where F is a scalar function of the stress state of the material such that no plastic deformation occurs as $F < 0$ and plastic deformation takes place only when $F = 0$. Most of various yield criteria that were proposed in the past are now only of historic interest, since they usually conflict with later experiments [1]. For polycrystalline metals, the yield criteria of Tresca and von Mises are the two so far most frequently used. Tresca's criterion is known as the maximum shear stress criterion and von Mises' criterion is known as the maximum shear strain energy or the maximum octahedral shear stress criterion. However, there was no physical reason why the plastic behaviour of a polycrystalline metal should depend on the maximum shear stress or the maximum octahedral shear stress. On the other hand it has been experimentally confirmed that within a certain range of temperatures the plastic deformation of single crystals is a result of slip over certain crystallographic plane [2]. Furthermore, slip usually takes place on the slip system for which the resolved shear stress reaches some critical value known as the critical resolved shear stress τ_0. Therefore, in principle it is possible to derive the yield criterion of a polycrystalline metal on the basis of crystallographic slips of the single crystal. Pioneering works of Sachs [3] and Taylor [4] laid the firm foundation for further developments (see the review articles of Kocks [5] and Lin [6]).

The purpose of the present study is to investigate the yield criterion of an fcc polycrystalline metal under combined stresses based on the polycrystal model which was developed by Chiang and Weng [7]. In order to compare with the classical Taylor–Bishop–Hill (TBH) model [8], it is assumed that the single crystal is non-hardening. In other words, the critical resolved shear stress of the active slip systems does not change during plastic deformation. This assumption greatly simplifies the analysis carried out in the next section. The present results are shown in reasonable agreement with those of the TBH model. Furthermore, the excellent agreement between the present predictions and the Mises criterion indicates that as far as the initial yielding is concerned, the Mises criterion is physically justified to be used for the low strain hardening fcc polycrystalline metal. Detailed discussion is given in the final section.

For easy reference, in this paper the capital letter represents the macro state variable; the lower-case letter denotes the micro state variable; the lower-case letter with bar over it signifies the averaged micro state variable.

2. Polycrystal model

Before developing the present polycrystal model, it is worth indicating some crucial simplifying assumptions involved in the following derivation. The assumptions include:

(1) The polycrystal is composed of perfectly plastic single crystals. No deformation is allowed until the critical stress states (depending on how many and which slip systems are activated) of all the single crystals are reached. The average of these critical stress states is defined as the yield stress of the polycrystal.

(2) Experimental evidence shows that the plastic behaviour of the grain boundary regions is different from that of the grain interior. But in this paper it is assumed that the influence of the grain boundaries can be safely ignored.

(3) The ratios among the dominant stress components of the single crystals is the same as those of the polycrystal. Assumptions (1) and (2) are similar to the TBH model, but Taylor's other assumptions such as uniform strains among all grains and the least slip hypothesis are replaced by assumption (3).

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For the purpose of brevity, we shall assume in the following derivation that the polycrystal is under biaxial tension state, i.e., Σ_{11} and Σ_{22} are the only non-vanishing stress components (the dominant stress components). Let σ_{ij} denote the (micro) stress tensor of the single crystal grain (in fact, it is better to view σ_{ij} as the ensemble average of the stress state of the same crystal orientation). According to assumption (1), we conclude that

$$v_{ij}^{(k)}\sigma_{ij} = \tau_0 \qquad k = 1, 2, \ldots, n \qquad (2)$$

where $v_{ij}^{(k)} = \frac{1}{2}(b_i^{(k)}n_j^{(k)} + b_j^{(k)}n_i^{(k)})$ is the Schmid tensor of the kth active slip system, $b_i^{(k)}$ and $n_i^{(k)}$ being the unit vectors of the slip direction and the slip plane normal respectively.

If σ_{22}/σ_{11} is denoted by λ, Equation 2 can be expanded as

$$(v_{11}^{(k)} + \lambda v_{22}^{(k)})\sigma_{11} + \xi^{(k)} = \tau_0 \qquad (3)$$

where

$$\xi^{(k)} = v_{33}^{(k)}\sigma_{33} + 2v_{12}^{(k)}\sigma_{12} + 2v_{23}^{(k)}\sigma_{23} + 2v_{31}^{(k)}\sigma_{31}$$

representing the contribution from non-dominant stress components. Summing up n simultaneous equations in Equation 3, we obtain

$$\sum_k (v_{11}^{(k)} + \lambda v_{22}^{(k)})\sigma_{11} + \sum_k \xi^{(k)} = n\tau_0 \qquad (4a)$$

or more concisely

$$n(\bar{v}_{11} + \lambda\bar{v}_{22})\sigma_{11} + n\bar{\xi} = n\tau_0 \qquad (4b)$$

where

$$\bar{v}_{11} = \frac{1}{n}\sum_k v_{11}^{(k)}, \quad \bar{v}_{22} = \frac{1}{n}\sum_k v_{22}^{(k)}, \quad \bar{\xi} = \frac{1}{n}\sum_k \xi^{(k)}$$

We may rewrite Equation 4b as

$$\sigma_{11} = \frac{1}{\bar{v}_{11} + \lambda\bar{v}_{22}}\tau_0 - \frac{\bar{\xi}}{\bar{v}_{11} + \lambda\bar{v}_{22}} \qquad (5)$$

Upon taking an average over all grain orientations, we find that

$$\Sigma_{11} = \langle\sigma_{11}\rangle = \left\langle\frac{1}{\bar{v}_{11} + \lambda\bar{v}_{22}}\right\rangle\tau_0 - \left\langle\frac{\bar{\xi}}{\bar{v}_{11} + \lambda\bar{v}_{22}}\right\rangle \qquad (6)$$

The last term of Equation 6 is negligible. This can be justified as follows. Consider, for instance, the contribution of σ_{12}. Since the magnitude of $\bar{v}_{12}/(\bar{v}_{11} + \lambda\bar{v}_{22})$ is around O (1) and it is unlikely that σ_{12} could be surprisingly large, with $\Sigma_{12} = \langle\sigma_{12}\rangle = 0$ we expect that $\langle\bar{v}_{12}\sigma_{12}(\bar{v}_{11} + \lambda\bar{v}_{22})\rangle$ would remain small in comparison with the first term of the right hand side of Equation 6. The arguments hold true for other non-dominant stress components. Therefore we can ignore the last term of Equation 6 without causing much error. We believe that this assumption is quite mild in comparison with other assumptions mentioned in the above. Accordingly we reach the conclusion that

$$\Sigma_{11} = \left\langle\frac{1}{\bar{v}_{11} + \lambda\bar{v}_{22}}\right\rangle\tau_0 \qquad (7a)$$

and

$$\Sigma_{22} = \left\langle\frac{\lambda}{\bar{v}_{11} + \lambda\bar{v}_{22}}\right\rangle\tau_0 \qquad (7b)$$

In general, λ is not a constant. As a matter of fact, any *a priori* assumed grain interaction law (for example, the self consistent models [9, 10]) would impose some λ distribution implicitly. But the *actual* λ distribution seems to be difficult to obtain, if not impossible. According to the assumption (3), in this paper λ is taken to be a constant so that

$$\Sigma_{22}/\Sigma_{11} = \lambda = \Lambda \qquad (8)$$

and Equation 7 can further be simplified as

$$\Sigma_{11} = \left\langle\frac{1}{\bar{v}_{11} + \Lambda\bar{v}_{22}}\right\rangle\tau_0 = M_\Lambda\tau_0 \qquad (9a)$$

$$\Sigma_{22} = \Lambda\Sigma_{11} = \Lambda M_\Lambda\tau_0 \qquad (9b)$$

By the same procedure, it can be obtained that the results for the cases of combined tension and torsion are

$$\Sigma_{11} = \left\langle\frac{1}{\bar{v}_{11} + 2\Omega\bar{v}_{12}}\right\rangle\tau_0 = M_\Omega\tau_0 \qquad (10a)$$

$$\Sigma_{12} = \Omega\Sigma_{11} = \Omega M_\Omega\tau_0 \qquad (10b)$$

where

$$\Omega = \Sigma_{12}/\Sigma_{11}$$

Generalization to cases of other combined loadings is possible.

From Equations (9) and (10), it is obvious that the problem now is reduced to the determination of M_Λ and M_Ω. The same numerical procedure developed in [11] is used to evaluate M_Λ and M_Ω. Each sample polycrystal containing 2000 single crystal grains of randomly distributed orientations is numerically generated. The mean values of M_Λ and M_Ω of 12 such fcc polycrystals are calculated. It is noted that deviations of M_Λ and M_Ω from the mean values are within 1.5%. In the next section the numerical results are presented and compared with other theoretical predictions.

3. Numerical results and comparisons

For the purpose of comparison, we use the following notations. Y and k denote the polycrystal yield stresses in uniaxial tension and pure torsion respectively. In the combined loadings cases, q and p denote the ratios of Σ_{11}/Y and Σ_{12}/Y respectively. Accordingly, the Mises criterion gives

$$k^{VM} = 0.577Y,$$

$$q^{VM} = 1/\sqrt{(1 - \Lambda + \Lambda^2)}, \quad p^{VM} = \Omega/\sqrt{(1 + 3\Omega^2)}$$

While the present model predicts that

$$k = \lim_{\Omega\to\infty}\frac{\Omega M_\Omega}{M_{\Omega=0}}Y,$$

$$q = M_\Lambda/M_{\Lambda=0}, \quad p = \Omega M_\Omega/M_{\Omega=0}$$

Since the values of M_Λ and M_Ω depend on n (the number of active slip systems), q and p will be varied for different n. In Tables I to X, the numerical results

TABLE I Results of biaxial tension tests. $n = 1$

Λ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
M_Λ	2.232	2.334	2.422	2.493	2.542	2.563	2.541	2.493	2.423	2.335	2.232
ΛM_Λ	0	0.2334	0.4884	0.7479	1.017	1.282	1.525	1.745	1.938	2.102	2.322
q	1	1.046	1.085	1.117	1.139	1.148	1.138	1.117	1.086	1.046	1
q^{VM}	1	1.048	1.091	1.125	1.147	1.155	1.147	1.125	1.091	1.048	1

TABLE II Results of combined tension–torsion tests. $n = 1$

Ω	0	0.1	0.3	0.5	0.7	1	1.5	2	5	10	∞
M_Ω	2.232	2.203	1.984	1.683	1.414	1.106	0.7940	0.6128	0.2537	0.1276	0
ΩM_Ω	0	0.2203	0.5952	0.8415	0.9877	1.106	1.191	1.226	1.269	1.276	1.281
p	0	0.099	0.267	0.377	0.443	0.496	0.534	0.549	0.569	0.572	0.574
p^{VM}	0	0.099	0.266	0.378	0.445	0.500	0.539	0.554	0.575	0.576	0.577

TABLE III Results of biaxial tension tests. $n = 2$

Λ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
M_Λ	2.336	2.453	2.568	2.676	2.762	2.797	2.762	2.677	2.569	2.454	2.336
ΛM_Λ	0	0.2453	0.5136	0.8028	1.105	1.399	1.657	1.874	2.055	2.209	2.336
q	1	1.050	1.099	1.146	1.182	1.197	1.182	1.146	1.100	1.051	1
q^{VM}	1	1.048	1.091	1.125	1.147	1.155	1.147	1.125	1.091	1.048	1

TABLE IV Results of combined tension–torsion tests. $n = 2$

Ω	0	0.1	0.3	0.5	0.7	1	1.5	2	5	10	∞
M_Ω	2.336	2.306	2.080	1.775	1.499	1.184	0.8565	0.6640	0.2766	0.1392	0
ΩM_Ω	0	0.2306	0.6240	0.8875	1.049	1.184	1.285	1.328	1.383	1.392	1.397
p	0	0.099	0.267	0.380	0.449	0.507	0.550	0.568	0.592	0.596	0.598
p^{VM}	0	0.099	0.266	0.378	0.445	0.500	0.539	0.554	0.575	0.576	0.577

TABLE V Results of biaxial tension tests. $n = 3$

Λ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
M_Λ	2.510	2.635	2.757	2.869	2.958	3.000	2.959	2.870	2.758	2.635	2.510
ΛM_Λ	0	0.2635	0.5514	0.8607	1.183	1.500	1.775	2.009	2.206	2.372	2.510
q	1	1.050	1.098	1.143	1.178	1.195	1.179	1.143	1.099	1.050	1
q^{VM}	1	1.048	1.091	1.125	1.147	1.155	1.147	1.125	1.091	1.048	1

TABLE VI Results of combined tension–torsion test. $n = 3$

Ω	0	0.1	0.3	0.5	0.7	1	1.5	2	5	10	∞
M_Ω	2.510	2.478	2.236	1.905	1.609	1.270	0.918	0.712	0.297	0.149	0
ΩM_Ω	0	0.2478	0.6708	0.9525	1.126	1.270	1.377	1.424	1.485	1.490	1.500
p	0	0.099	0.267	0.379	0.449	0.506	0.549	0.567	0.592	0.594	0.598
p^{VM}	0	0.099	0.266	0.378	0.445	0.500	0.539	0.554	0.575	0.576	0.577

TABLE VII Results of biaxial tension tests. $n = 4$

Λ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
M_Λ	2.673	2.809	2.945	3.062	3.158	3.197	3.159	3.067	2.945	2.809	2.673
ΛM_Λ	0	0.2809	0.5890	0.9186	1.263	1.599	1.895	2.147	2.356	2.528	2.673
q	1	1.051	1.102	1.146	1.181	1.196	1.182	1.147	1.102	1.051	1
q^{VM}	1	1.048	1.091	1.125	1.147	1.155	1.147	1.125	1.091	1.048	1

TABLE VIII Results of combined tension–torsion tests. $n = 4$

Ω	0	0.1	0.3	0.5	0.7	1	1.5	2	5	10	∞
M_Ω	2.673	2.639	2.378	2.033	1.718	1.358	0.981	0.760	0.316	0.159	0
ΛM_Ω	0	0.2639	0.7134	1.017	1.203	1.358	1.472	1.520	1.580	1.590	1.597
p	0	0.099	0.267	0.380	0.450	0.508	0.551	0.569	0.591	0.595	0.597
p^{VM}	0	0.099	0.266	0.378	0.445	0.500	0.539	0.554	0.575	0.576	0.577

TABLE IX Results of biaxial tension tests. $n = 5$

Λ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
M_Λ	2.898	3.040	3.171	3.284	3.368	3.400	3.369	3.284	3.171	3.039	2.898
ΛM_Λ	0	0.3040	0.6342	0.9852	1.347	1.700	2.021	2.299	2.537	2.735	2.898
q	1	1.049	1.094	1.133	1.162	1.173	1.163	1.133	1.094	1.049	1
q^{VM}	1	1.048	1.091	1.125	1.147	1.155	1.147	1.125	1.091	1.048	1

TABLE X Results of combined tension–torsion tests. $n = 5$

Ω	0	0.1	0.3	0.5	0.7	1	1.5	2	5	10	∞
M_Ω	2.898	2.861	2.575	2.196	1.850	1.457	1.049	0.8116	0.3367	0.1690	0
ΩM_Ω	0	0.2861	0.7725	1.098	1.295	1.457	1.574	1.623	1.684	1.690	1.699
p	0	0.099	0.267	0.379	0.447	0.503	0.543	0.560	0.580	0.583	0.586
p^{VM}	0	0.099	0.266	0.378	0.445	0.500	0.539	0.554	0.575	0.576	0.577

for a variety of combinations of Λ (and Ω) and n are presented. For easy comparison, q^{VM} and p^{VM} are also included in all tables. The yield surfaces predicted by the present theory are accordingly plotted in Figs 1 and 2. It is seen that the present results are in excellent agreement with the von Mises' yield surfaces. In Fig. 3, the present prediction for $n = 5$ is compared with the yield surface predicted by the TBH model. It is found that reasonable agreement is observed.

4. Discussion and conclusions

The yield surface of the f c c polycrystal derived in this paper is on the basis of the rigid perfect plasticity of the single crystal. Accordingly, the ambiguity in the definition of yielding is avoided, otherwise it is known that if strain hardening effect is present, the observed yield surface will be dependent on the offset plastic strain level (e.g. [12]). Nevertheless, it is believed that the present results should be valid for investigating the f c c polycrystal of low strain hardening. The close agreement between the present predictions and the Mises criterion implies the following. The reason for the Mises criterion being so fit with the experimental data is neither that the material yields because the shear strain energy attains the critical value nor that the material yields because the octahedral shear stress reaches the threshold value. The actual physical reason is simply because the polycrystal is made of single

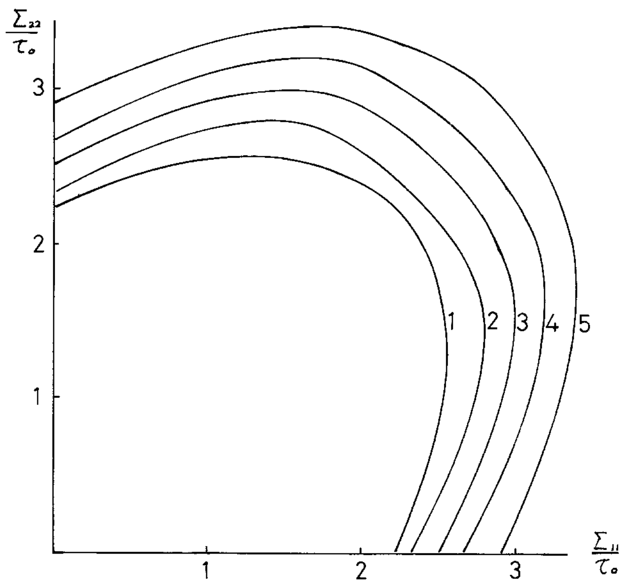

Figure 1 Under biaxial tension tests, the theoretical yield surfaces of an f c c polycrystal for different values of n where n is the number of the active slip systems per grain.

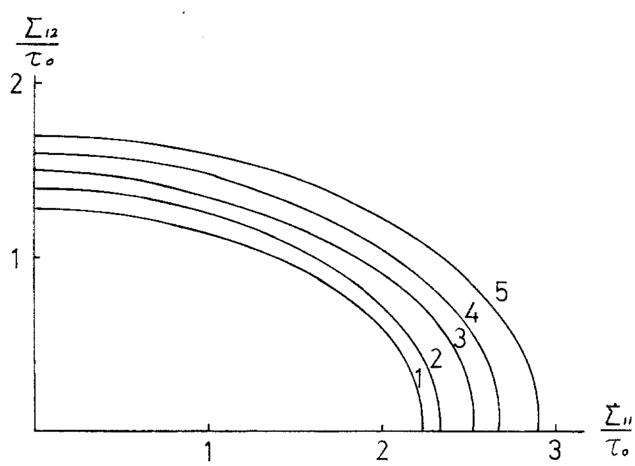

Figure 2 Under combined tension–torsion tests, the theoretical yield surfaces of an f c c polycrystal for different values of n where n is the number of the active slip systems per grain.

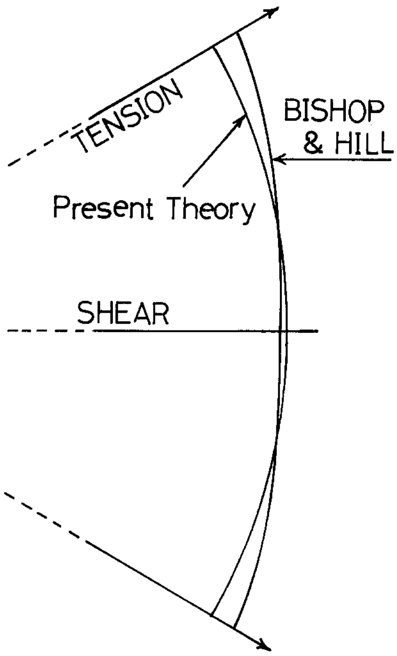

Figure 3 Comparison of the present model with the Taylor–Bishop–Hill model.

crystal grains which follow the well-defined Schmid law.

The reasonable agreement between the TBH model and the present model (for $n = 5$) further implies that the yield surface of the polycrystal depends strongly on how many and which slip systems are activated but negligibly on the detailed grain–grain or grain–matrix interactions. This fact partially justifies the assumption (3) pointed out in Section 2, i.e. the assumption of $\lambda = \Lambda$ made in Equation 8.

The present model can be extended to incorporate the effect of strain hardening. As the experiences gained in the previous investigations on strain hardening [7, 11], it is concluded that, under pure tension test or pure torsion test, the predictions of the present model turn out to be in reasonable agreement with those of the Mises theory. Therefore, it is reasonable to expect that, at least for radial loading in the presence of strain hardening, the present approach should still be in accord with the deformation theory based on the Mises criterion. Although we do not address other important metallurgical factors that influence the yield surface such as grain size in this paper, the approach adopted in [13, 14] may be useful in this respect.

In summary, we have derived the yield criterion of a polycrystal on the basis of slip mechanism of the single crystal grain. Specific results for the fcc polycrystal with $\{1\,1\,1\}\langle 1\,\bar{1}\,0\rangle$ slip systems have been calculated and compared with the TBH model and the Mises phenomenological criterion. It is concluded that the present approach is feasible and the results are accurate.

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