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HOMOGENEITY AND HETEROGENEITY OF SINGLE CRYSTALSIN CHANNEL-DIE COMPRESSION; REPRESENTATION OF THE YIELD LOCUS¹⁾

JEDNORODNOŚĆ I NIEJEDNORODNOŚĆ MONOKRYSZTAŁÓW W PROCESIE ŚCISKANIA W KANALE PROSTYM; REPREZENTACJA ODKSZTAŁCENIA PLASTYCZNEGO

A polynomial approximation of the flow surface of single crystals deforming plastically on various slip systems is considered. Because it involves an exponent n, it is known as the power law. It is shown that, by introducing deviations from the Schmid law (but deviations not discernible by measurement), an extension of the normality rule can be proposed: not only the flow direction, but also the rate of rotation due to the glide on the slip systems are obtained in a single algebraic formula. The validity of all this is assessed by comparing its predictions with the results of the compression of single crystals in channel-die. The lateral reactions and the lattice rotations have been measured in typical rolling orientations and found in good agreement with the calculations.

Key words: plastic deformation, normality rule, single crystal, flow surface.

Przedmiotem pracy jest wielomianowa aproksymacja powierzchni płynięcia monokryształów odkształcanych plastycznie na różnych systemach poślizgu, która ze względu na występujący wykładnik *n* nazywana jest 'prawem wykładniczym'. Pokazano, że wprowadzając mierzalne odchylenia od prawa Schmidta, można zaproponować pewne rozszerzenie reguły normalizacji: nie tylko kierunek płynięcia, ale także prędkość rotacji spowodowanej poślizgiem w danym systemie są uzyskane w pojedynczej formule algebraicznej. Zasadność tych spostrzeżwń oceniono poprzez porównanie odpowiednich wartości oczekiwanych z wynikami ściskania monokryształów w kanale kątowym.

I. Introduction

Experiments have repeatedly shown the validity of the Schmid law [1], which determines that the flow surface of a plastically deformed single crystal is a polyhedron with

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faces, edges and vertices. Nevertheless, when introduced in the calculations, it leads to a piecewise linear law of behaviour which is more complicated than a unique analytical formulation [2]. So scientists have considered algebraic approximations of the yield polyhedron, thus replacing the vertices by smooth surfaces. Various examples can be found in [3], in which it is shown that this substitution has a physical basis, i.e. that real crystals or grains present some scatter around their ideal crystallographic orientations.

The best approximation seems the so-called power law studied for example in [4]. Let a single crystal deform on G slip systems, the unit vectors of their slip directions being \mathbf{b}^g g = 1...G and the unit normals to their slip planes \mathbf{n}_g . This defines the usual symmetrized Schmid factor $\mathbf{M}^g = \frac{1}{2} (\mathbf{b}^g \otimes \mathbf{n}^{\cdot g} + \mathbf{n}^g \otimes \mathbf{b}^g) g = 1...G$ and the unsymmetrized one $\overline{\mathbf{M}}^g = \mathbf{b}^g \otimes \mathbf{n}^g$. Each system has a critical resolved shear stress τ_c^g . If **T** is the applied Cauchy stress, the power law can be written as:

$$f_n(\mathbf{T}) = \left[\sum_{g=1}^{G} \left(\frac{|\mathbf{M}^g : \mathbf{T}|}{\tau_c^g}\right)^n\right]^{\frac{1}{n}} - 1 = 0.$$
(1)

It easy to demonstrate that $f_n(T)$ is as close to the flow polyhedron as whished if $\rightarrow +\infty$. It must be noticed that, since T is a symmetrical tensor, an entirely equivalent formulation using the unsymmetrized Schmid tensors \overline{M}^g is:

$$\mathbf{f}_{n}^{*}(\mathbf{T}) = \left[\sum_{g=1}^{G} \left(\frac{|\overline{\mathbf{M}}^{g}:\mathbf{T}|}{\tau_{c}^{g}}\right)^{n}\right]^{\frac{1}{n}} - 1 = 0.$$
(2)

The deviatoric part S of T can be substituted to T in Eqs (1,2) since M^g and \overline{M}^g are symmetrical tensors.

2. Extended form of the normality rule

On the yield polyhedron, the symmetrical tensor of the plastic deformation rates D^p is normal to the faces (where one slip system is active) and undetermined within the flow cone of the edges and the vertices (several active systems). So if $f_n(T)$ or $f_n(S)$ approximates the polyhedron, the normality rule is applied and is written classically as:

$$\mathbf{D}^{\mathbf{p}} = \lambda \sum_{g=1}^{G} \frac{|\mathbf{M}^{g} : \mathbf{T}|^{n-1}}{(\tau_{c}^{g})} \mathbf{M}^{g} = \lambda \frac{\partial f_{n}(\mathbf{T})}{\partial \mathbf{T}},$$
(3)

where $\hat{\lambda}$ is the plastic multiplier. This can be put in parallel with:

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$$\mathbf{D}^{\mathbf{g}} = \sum_{g=1}^{G} \dot{\gamma}_{g} \mathbf{M}^{g} \quad \text{and} \quad \mathbf{L}^{\mathbf{P}} = \sum_{g=1}^{G} \dot{\gamma} \overline{\mathbf{M}}^{g}, \quad (4, 5)$$

where $\mathbf{L}^{\mathbf{P}}$ is the gradient of the plastic deformation rates $\left(\mathbf{D}^{\mathbf{P}} = \frac{1}{2}(\mathbf{L}^{\mathbf{P}} + \mathbf{L}^{\mathbf{pT}})\right)$ and $\dot{\gamma}$ the shear rates. Hence the quantities $\dot{\lambda} \frac{|\mathbf{M}^{g}: \mathbf{T}|^{n-1}}{(\tau_{c}^{g})^{n}}$ can be reinterpreted as:

$$\dot{\gamma} = \dot{\lambda} \frac{|\mathbf{M}^{g} : \mathbf{T}|^{n-1}}{(\tau_{c}^{g})^{n}} = \dot{\lambda} \frac{|\mathbf{\overline{M}}^{g} : \mathbf{T}|^{n-1}}{(\tau_{c}^{g})}.$$
(6)

By doing this, an approach slightly different from the S c h m i d law is taken for the representation of the plastic flow of the crystal. A critical shear stress is still postulated on the slip systems with $\forall g \mid M^g : T \mid \leq \tau_c^g$, but all of them glide with a shear rate given by Eq (6). When the exponent n is large (n > 6), which is usually the case, the less favoured systems have very small shear rates, so that the deviation from the S c h m i d law (for which it would be zero) is not discernible by measurement. Combining Eqs (4, 5 and 6) leads to:

$$\mathbf{D}^{\mathbf{P}} = \hat{\lambda} \frac{\partial f_n(\mathbf{T})}{\partial \mathbf{T}}$$
 and $\mathbf{L}^{\mathbf{P}} = \hat{\lambda} \frac{\partial f_n^*(\mathbf{T})}{\partial \mathbf{T}}$ (7, 8)

Thus, when $f_n^*(T)$ is used, an extended form of normality rule allows not only to deduce the flow rates from the yield locus, but also the rotation rates due to the glide on the slip systems. Although mathematically close to rate sensitive formulations [5], it has completely different physical basis, and applies mainly to cold working. The measurements made in order to check the validity of Eqs (2, 7) are presented in the following section.

3. Single crystal experiments

Al 1% Mn single crystals of initial height h0 were compressed in a channel-die at room temperature down to h, reaching a logarithmic $\overline{\epsilon}_{ln} = Ln (h_0/h)$ of 1.3 (Fig. 1a). The samples had the initial orientations Goss {110}<001>, Brass {110}<112≥, Copper {112}<111> and Strange {123}<634>. Deformation was conducted by steps of about $\overline{\epsilon}_{ln} = 0.1$ and at each step, the TEFLONTM wrapping was changed so that friction was at a minimum. Although the experimental evidence of the heterogeneity of the deformation is well documented [6], these precautions authorize a homogeneous mechanical analysis at the macroscopic scale in which the samples remain parallelepiped, the initially right angles inclining of α and β (Fig. 1b).





The analysis was conducted using the formalism of large deformations [7] in which point M, initially $M(X_J) J = 1..3$, becomes $m(x_i) i = 1..3$:

$$\begin{aligned} x_1 &= \frac{h_0}{h} X_1 + \tan \alpha X_2 + \tan \beta X_3 \\ x_2 &= X_2 \\ x_3 &= \frac{h}{h_0} X_3. \end{aligned}$$
 (9)

1 is the elongation direction (ED), 2 the transverse one (TD) and 3 the normal one (ND). Hence, since $\mathbf{F}_{iJ} = \begin{bmatrix} \frac{\partial \mathbf{x}_i}{\partial \mathbf{X}_J} \end{bmatrix}$ and $\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1}$, if the elastic part of the deformation is neglected:

$$\mathbf{L}^{\mathbf{P}} = \begin{bmatrix} -\frac{\dot{\mathbf{h}}}{\mathbf{h}} & \frac{\dot{\mathbf{h}}}{\mathbf{h}} \tan \alpha + \frac{\dot{\alpha}}{\cos^2 \alpha} & 2\frac{\dot{\mathbf{h}}}{\mathbf{h}} \tan \beta + \frac{\dot{\beta}}{\cos^2 \beta} \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\dot{\mathbf{h}}}{\mathbf{h}} \end{bmatrix}$$
(10)

 $D_{12}^{P} = \frac{1}{2} \left(\frac{\dot{h}}{H} \tan \alpha + \frac{\dot{\alpha}}{\cos^{2} \alpha} \right)$ and $D_{13}^{P} = \frac{\dot{h}}{h} \tan \beta + \frac{\dot{\beta}}{2\cos^{2}\beta}$. The α and β angles have been measured by profile projector, as shown for Brass (Fig. 2a), for which $\beta = 0$ and Copper (Fig. 2b), for which $\alpha = 0$. Similar results have been obtained for Strange ($\alpha \neq 0, \beta \neq 0$). For Goss, $\alpha = \beta = 0$. The corresponding D_{12}^{P} and D_{13}^{P} have been calculated (Fig. 2c and 2d).



Fig. 2. Geometric evolution of the sample: (2a) Orientation Brass {110}<112>, measured α and corresponding D^P₁₂, (2b) Orientation Copper {112}<111>, measured β and corresponding D^P₁₃

X-ray analysis gave pole figures in the (1, 3) plane, the compressive stress T_{33} was measured and so was the lateral reaction T_{22} with the help of an original device shown in Fig. 3. The sample was poised on a holder, which allowed to measure the micrometric deflection of the walls of the channel-die, which deform only in the elastic range, outside the sample. The ratio lateral reaction / compression stress, which would be 0.5 if the material was isotropic, can be seen for the orientation Goss on Fig. 4a and Brass on Fig. 4b. Copper and Strange are presented further (Fig. 5d and 6f), all clearly anisotropic.



Fig. 3. Device for measuring the lateral reaction

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Fig. 4. Ratio lateral reaction / compression stress: (4a) orientation Goss $\{110\}<001>$, (4b) orientation Brass $\{110\}<112>$. The same for orientations Copper and Strange can be seen on Fig. 5d and 6f

4. Test of the validity of the power law

Since the macroscopic deformation D^p of the test pieces is completely known, the power law allows to calculate the applied Cauchy stress T within the plastic multiplier $\hat{\lambda}$, when the strain hardening and the crystallographic orientation are given. Since little is known of the former, it was assumed to be isotropic. The latter is known at the beginning of the deformation and its variation can be calculated step by step, as becomes clear below. Eq (3) provides a system of five independent equations with five unknowns which yields S, and consequently T (T₁₁ = 0), through a numerical resolution using the Newton-Raphston method. Hence the ratio T₂₂/T₃₃. The $\dot{\gamma}$ are calculated through Eq (6) and the value of the

imposed $\mathbf{D}_{33} = \sum_{g=1}^{N} \dot{\gamma}_g \mathbf{M}_{33}^g$ (it was 5. 10⁻³ s⁻¹ in the conditions of the experience). The tensor of the rotation rates due to the glide on the slip systems is:

$$\mathbf{\Omega} = \frac{1}{2} \sum_{g=1}^{N} \dot{\gamma}_{g} (\overline{\mathbf{M}}^{g} - \overline{\mathbf{M}}^{gT})$$
(11)

and the tensor giving the rates of rotation of the lattice is:

$$\boldsymbol{\omega} = \frac{1}{2} (\mathbf{L} - \mathbf{L}^{\mathrm{T}}) - \boldsymbol{\Omega}$$
 (12)

hence the evolution of the Euler angles φ_1 , Φ and φ_2 which define the orientation of the lattice.

The (1, 3) plane being a {111} symmetry plane for Copper, the lattice rotates around the axis 2. The evolution of the corresponding angle Φ is given on Fig. 5a. It shows the evolution of the crystal towards the stable D {4 4 11}<1111 $\bar{8}$ > orientation, as documented in [8]. The ratio T₂₂/T₃₃ depends little on the exponent n and is overestimated by the calculations (0.6 instead of 0.4).

Experiments and calculations fit better for the orientation Strange and show that after $\bar{\epsilon}_{in}$ > 0.5 it moves towards a rather stable position close to {135}<211>, for which T₂₂/T₃₃ is about 0.4 (Fig. 6). The results for Goss and Brass are not presented here for lack of space, but they are quite satisfactory.



Fig. 5. Orientation Copper {112}<111>. Comparison between: (5a) Simulated evolution of the angle Φ of rotation of the crystal lattice, (5b) Pole figure showing the lattice evolution (taken at Ln/h₀/h) = 1.3), (5c) Simulated evolution of the ratio lateral reaction / stress compression, (5d) Measured evolution of the same

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Fig. 6. Orientation Strange $\{123\}<634>$. Comparison between: (6a) Simulated evolution of the angle φ_1 of rotation of the crystal lattice, (6b) Same, with Φ , (6c) Same, with φ_2 , (6d) Pole figure showing the lattice evolution (taken at Ln(h₀/h) = 1.3), (6e) Simulated evolution of the ratio lateral reaction / stress compression, (6f) Measured evolution of the same

5. Conclusion

In spite of strong hypotheses of homogeneity, a good agreement was found between the experiments and the calculations using the power law and the extended normality rule. This shows that they form a robust instrument to predict the plastic behaviour of single crystals and prompts to do further use of it, namely:

- introduce them in a finite element code, and take full account of the effects of the friction,

- calculate the corresponding incremental law of behaviour and use it in bifurcation criteria such as Rice's, for the prediction of shear bands.

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