Calculation of the Taylor Factor and Lattice Rotations for Bcc Metals Deforming by Pencil Glide

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Values of the Taylor factor M and the corresponding lattice rotations for tension or compression have been computed for grains of various orientations postulated to slip on arbitrary planes in ⟨111⟩ directions. The stresses in each grain were first obtained by numerically maximizing the work expression subject to the constraints of the pencil-glide yield expressions. The derived value of M_{ave} = 2.733 is slightly lower than in the case of mixed {110}, {112}, and {123} ⟨111⟩ slip and the computed rotations are in reasonable agreement with experiments on iron. In compression, 26 pct of the grains are predicted to rotate toward ⟨100⟩, although the ⟨111⟩ texture component develops faster. The computational method used can easily be applied to the determination of the mechanics of texture generation for arbitrary deformations.

PREDICTIONS of texture development and the variation of uniaxial yield stress with orientation of bcc crystals subjected to axisymmetric flow have previously been performed for a number of assumed modes of deformation.[1-4]

All of these deformation modes—{110}⟨111⟩ slip, {112}⟨111⟩ slip, {123}⟨111⟩ slip, {112}⟨111⟩ twinning, and various combinations of these four—produce crystallographic shear on a restricted number of systems. We have now performed similar calculations for the pencil-glide model first proposed by Taylor,[5] in which slip can occur on any plane containing a ⟨111⟩ direction. For a given ⟨111⟩ slip direction, the operative slip plane is that on which the resolved shear stress is a maximum.

We assume that deformation occurs only by slip and that the critical resolved shear stress k is the same for each of the four ⟨111⟩ slip systems. The stress state in a crystal of given orientation will then be that which operates enough slip systems to accommodate the imposed strain and at the same time maximizes the incremental external work done, $dW = \Sigma\sigma_{ij}d\epsilon_{ij}$.[6] The Taylor factor M is customarily defined as

$$M = \frac{\sum_l d\gamma_l}{d\epsilon}$$

where $d\gamma_l$ are the magnitudes of the incremental amounts of slip on the four systems and $d\epsilon$ is the magnitude of the applied tensile or compressive strain. Because of the equivalence of the maximum work and minimum shear criteria,[7] it is easier to compute M as $(1/k)(dW/d\epsilon)$. We have computed values of M throughout the stereographic triangle by applying computer minimization techniques to $-dW$ expressed as a function of the stresses, subject to the constraints of the yield criteria for pencil glide, Ref. 8, Table III. The values of σ_{ij} obtained through this process were then used to compute the associated rotations of the tensile axis.

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COMPUTATIONAL METHODS

Given an imposed shape change to be accommodated by pencil glide, there is no immediate way of telling whether it will require the operation of three or four ⟨111⟩ slip systems. Thus, it is necessary to consider both possibilities. The case of four active slip directions presents no problem, since all possible stress states for this case have been tabulated, Ref. 8, Table IV. However, the quadratic yield expressions for pencil glide on only three ⟨111⟩ slip systems are too involved to be handled analytically, even by the method of Lagrange multipliers. We therefore employed a pattern-search minimization program[9] capable of dealing with multimodal functions and nonlinear constraints. For each grain orientation, we minimized the expression for $-dW$ as a function of stress state under each of the four possible assumptions that the critical resolved shear stress is not reached on one ⟨111⟩ system, and then selected the lowest of the four. In cases where maximum work would be achieved by operating all four systems, this procedure yielded the same result for each assumed combination, and this proved to be almost identical to the known analytical expression for the stresses.

It was found that this process, while not difficult to carry out for the limited number of grain orientations shown in Fig. 2 would be prohibitively expensive in terms of computer time if applied to complicated problems involving thousands of grains. We therefore developed a faster approximate method capable of dealing with more lengthy pencil-glide texture problems. By means of the pattern-search program with the strains unspecified, we generated a large number of solutions to the yield equations selected at random from five-dimensional stress space. Because of the symmetry of the yield expressions for the four systems and the fact that each stress state could have positive or negative signs, each of the solutions actually corresponded to eight stress states. For a grain of given orientation subjected to a given strain, we then examined only a limited number of stress states to find that which would produce maximum work. In terms of the stress state notation of Ref. 8, we tested only the stress states in Groups I, II, III (the only ones that operate all four systems), and V (the only ones operating three systems and yielding zero shear stress on the remaining system), plus a specified number of the stress states randomly selected from Group IV.

With an imput of a sufficiently large number of Group IV stress states, this latter technique gave essentially the same results as the former in much less computer time. Using 40 "random stress states" with Groups I, II, III, and V, lattice rotation and M values were computed for about fifty orientations on a UNIVAC 1108 in 17 sec. Noticeable discrepancies between rotations found by the two methods were observed only near border zones where the mode of deformation changes from the operating of three systems to four; even here only the magnitude, not the direction, of rotation was much different. When 125 Group IV solutions were used, the two methods were almost indistinguishable. Thus, in more complicated problems where only the approximate method could be used, the resulting inaccuracies would be expected to be small.

RESULTS AND DISCUSSION

M Factor

Contours of constant M within the basic triangle are shown in Fig. 1. The coordinates θ and φ (the same as those used by Taylor) represent the colatitude and longitude, respectively, of the tensile or compressive axis with respect to the crystallographic axes. The four marked regions in the diagram are areas within which the stress states of one particular group operate. The stress states of Groups I and IIIb operate all four systems; those of IVa operate all but the [111] system; those of IVd operate all but the $[\bar{1}11]$ system. As would be expected from symmetry considerations alone, the [111] slip direction cannot be activated by tension along an axis close to the [111], but all four $\langle 111 \rangle$ directions are activated by tension along axes near the [100] or [101] directions.

The constant-M contours within the triangle closely resemble those previously computed by a rough approximate method[10] and for mixed $\{110\}\langle 111 \rangle$, $\{112\}\langle 111 \rangle$, and $\{123\}\langle 111 \rangle$ slip. Furthermore, the average value of M according to the present calculations, 2.733, is not much less than values computed by restricted-glide models with large numbers of slip systems. Chin and Mammel obtained a value of 2.754 for their mixed slip model; Hutchinson computed a value of 2.748 for the case of twenty equally spaced planes for each $\langle 111 \rangle$ slip direction.[11] The magnitude of the difference between pencil glide (the limiting case of an infinite number of possible slip planes) and Hutchinson's model is less than the 1 pct he estimated. These results are summarized in Table I.

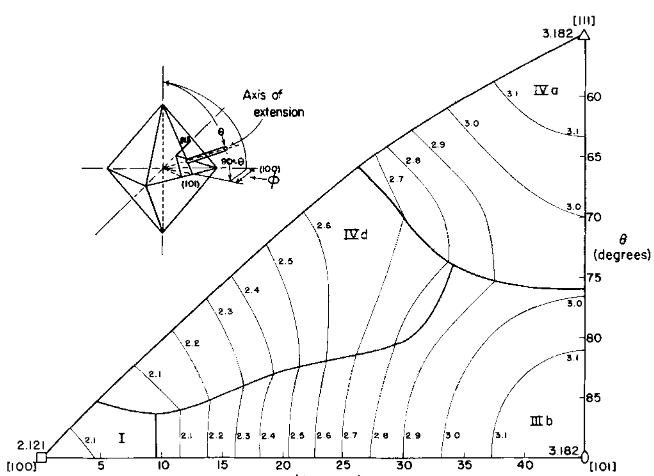

Fig. 1—Contours of constant M for pencil glide. The heavy solid lines separate regions within which stress states of one group operate. Roman numerals refer to the stress state groups.

Texture Prediction

Predicted lattice rotations for compression of orientations again represented in the $\theta-\varphi$ coordinate system are shown in Fig. 2. The pencil-glide hypothesis uniquely predicts lattice rotations without recourse to any additional assumptions except the principle of maximum work. In this respect, pencil glide differs considerably from restricted glide, for even the assumption of mixed $\{110\}\langle 111 \rangle$ $\{112\}\langle 111 \rangle$, and $\{123\}\langle 111 \rangle$ slip fails to predict unique slip combinations over half the stereographic triangle.[2,3] The reasons for this have been pointed out by Piehler and Backofen.[8]

As expected, the results show that, in compression, $\langle 110 \rangle$ is a point of unstable equilibrium and all grains rotate to $\langle 111 \rangle$ or $\langle 100 \rangle$. Since the slip process is assumed to be reversible, the results for tension are exactly the reverse of those for compression and all grains tend to rotate toward $\langle 110 \rangle$. Where unique results are predicted for mixed $\{110, 112,$ and $123\}\langle 111 \rangle$ slip,[3] the lattice rotations are almost exactly the same as those calculated here. The data of Ref. 3 predict a

Table I. Average Values of M for Various Slip Modes

Slip Mode	No. of Slip Planes per <111> Direction	M_{ave}	Ref.
{110} <111>	3	3.067	6, 2
{112} <111>	3	2.954	2
{123} <111>	6	2.803	2
mixed {110, 112, and 123} <111>	12	2.754	2
approximate pencil glide	20	2.748	11
pencil glide	∞	2.733	present work

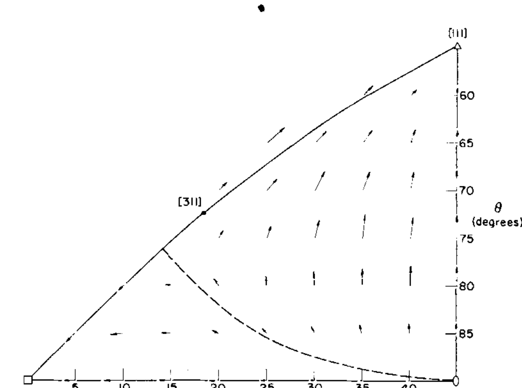

Fig. 2—Computed rotations of the compressive axis for 5 pct compression. The dotted line separates those grains that rotate toward $\langle 100 \rangle$ from those that rotate toward $\langle 111 \rangle$.

final texture that is 24 pct ⟨100⟩, 76 pct ⟨111⟩; Fig. 2 predicts a 26 pct ⟨100⟩, 74 pct ⟨111⟩ texture, which is not significantly different.

Experimental texture determinations for compression might therefore be able to determine how accurate the pencil-glide model is for various metals. However, any data are necessarily complicated by the fact that different texture components develop at different rates. Thus, findings of large ratios of ⟨111⟩ to ⟨100⟩ components may be due to the faster development of ⟨111⟩ textures. It would be interesting to see if the relative strength of the ⟨100⟩ component actually increases with the total amount of compression.

Single crystal experiments could also be used to check these findings, but not many have been performed to date.[12] Our Fig. 2 and Fig. 4 of Ref. 3 agree about equally with the rotations measured by Mayer and Backofen for iron.[10]

SUMMARY AND CONCLUSIONS

Values of M and lattice rotations for grains of various orientations subjected to axisymmetric flow have been computed on the basis of Taylor's pencil-glide model for bcc metals. The results are generally similar to those obtained under the mixed {110} ⟨111⟩, {112} ⟨111⟩, and {123} ⟨111⟩ slip assumption, with the exception that values of the rotations are necessarily unique. The calculated rotations seem to be in good agreement with single-crystal experiments. The computed value of M_{ave}, 2.733, is necessarily a lower value than that computed from previous models, since it represents the limiting case of an infinite number of slip planes for each ⟨111⟩ slip direction.

The numerical method used to compute the stress state in a grain is fast and general enough to be applied to the prediction of texture in any material subjected to any shape change, provided that the pencil-glide approximation is a good one. If twinning could be incorporated into the model, this technique could be expected to yield even more realistic information about texture development in bcc metals. We are currently engaged in making texture calculations for rolling, cross-rolling, and simple shear and comparing the results with the known textures of iron and other bcc metals. We hope also to suggest means of deforming bcc metals to produce textured aggregates with desired anisotropic properties.

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