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TITLE: **INTRODUCTION OF POLYCRYSTAL CONSTITUTIVE
LAWS IN A FINITE ELEMENT CODE WITH
APPLICATIONS TO ZIRCONIUM FORMING**

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ABSTRACT: In this work we simulate the compressive deformation of heavily textured zirconium sheet using a finite element code with the constitutive response given by a polycrystal self-consistent model. We show that the strong anisotropy of the response can be explained in terms of the texture and the relative activity of prismatic (easy) and pyramidal (hard) slip modes. Our simulations capture the yield anisotropy observed for so-called "through-thickness" and "in-plane" compression tests in terms of the loading curves and final specimen geometries.

1 INTRODUCTION

Simulating the forming of anisotropic polycrystals, such as zirconium, requires a description of the anisotropy of the aggregate and the single crystal, and also of their evolution with deformation (texture development and hardening). The anisotropy of the single crystal requires the use of polycrystalline models that account for inhomogeneous deformation depending on grain orientation. Self-consistent models have demonstrated that they are up to the task in both respects.

Using polycrystal models to describe the constitutive response of a material within the framework of a finite element codes represents a considerable improvement over using empirical constitutive laws, since they provide a physical basis to anisotropy and its evolution. Such an approach, however, has the disadvantage of being time consuming, and even more so when self-consistent instead of upper-bound models are used.

We have implemented a self-consistent polycrystal model (Lebensohn and Tomé 1993) into the explicit Finite Element (FE) code EPIC-97 (Johnson et al. 1997), and then applied this methodology to the prediction of uniaxial compression deformation. The polycrystal constitutive modeling is spatially applied at each FE integration point. However, for uniaxial compression the deformation is practically homogeneous and a single polycrystal calculation is representative of the response for the entire compression specimen. As a matter of fact, this case was chosen because it provides a simple benchmark for testing the mechanics of interfacing the FE code with the polycrystal code. The FE code imposes the

computed velocity gradient on the polycrystal, updates the orientation and the hardening of the individual grains as deformation proceeds, and predicts the macroscopic stress state for subsequent use in solution of the continuum conservation equations. The advantage of this approach is that it accurately accounts for material anisotropy including texture development; however these calculations are computationally intensive.

In this work the main focus is to gauge the accuracy of the constitutive modeling by comparing numerical FE results to Zr compression data; both final deformed specimen geometries and associated loading curves are compared.

2 MATERIAL AND EXPERIMENTS

Uniaxial compression testing was conducted on a high-purity zirconium plate obtained from Teledyne. This material contained (by weight) approximately 54 ppm Hf and 40 ppm O, and had a mean grain size of approximately 25 μm . The Zr plate had been clock-rolled at room temperature and then annealed at 823 K for one hour, producing an equiaxed grain structure with a strong in-plane isotropic basal texture (Kaschner, Gray and Chen 1997).

In the discussion below, we consider the Zr plate to have a right-handed material (sample) coordinate system with axes 1, 2, 3. The 1-2 plane corresponds to the original rolling plane and the 3 axis is through-thickness.

To examine the influence of loading orientation, and thereby texture, on the mechanical response of this strongly basal textured Zr-plate, compression

samples were cut from both the through-thickness (TT, equivalent to the 3 direction) and in-plane (IP, equivalent to the 1, 2 or at any angle in-between directions) plate directions. Cylindrical compression samples (nominally 5 mm diameter by 5 mm height) were first electro-discharge machined (EDM) normal to the plane of the plate (i.e., TT); this orientation, relative to the plate texture, fixed the compression axis of the samples to be nominally 20 degrees to the c-axis orientation of the grains. Samples were also EDM machined in the IP plate direction to evaluate texture effects on constitutive behavior and possible substructure evolution. In-plane samples were machined at 0°, 45°, and 90° relative to an arbitrary direction in the plate.

Mechanical tests were performed in compression at 76 and 298 K, and quasistatic strain rates of 0.001 and 0.1 s⁻¹ using an Instron screw-drive load frame (Kaschner, Gray and Chen 1997). Results for IP samples produced very similar stress-strain curves along the three IP directions, with small variations in stress of about ±10 MPa about the mean value for a given set of conditions. This finding validates the expectation of in-plane isotropy.

Figure 1. Zirconium stress-strain loading curves for quasistatic, room temperature, uniaxial compression tests using in-plane and through-thickness specimens.

Table 1. Compression Specimen Data for Zirconium

Sample	L ₀	L _f	D ₀	χ	ε _{xx}	ε _{yy}	ε _{zz}	ε _{eq}
TT	5.103	4.093	5.103	1	11.0%	11.0%	-22.1%	22.1%
IP-90°	5.098	3.830	5.101	1.17	22.1%	6.4%	-28.6%	30.0%
IP-0°	5.096	4.093	5.109	1.17	18.8%	3.1%	-21.9%	23.7%
IP-45°	5.090	4.023	5.096	1.17	19.6%	3.9%	-23.5%	25.2%

Table 2. Voce Law Coefficients for Zirconium

Slip Mode	τ ₀	τ ₁	Θ ₀	Θ ₁	γ̇ ₀	n
Prismatic	15. MPa	40. MPa	2000. MPa	100. MPa	1.0 s ⁻¹	20
Pyramidal	100. MPa	250. MPa	3000. MPa	0. MPa	1.0 s ⁻¹	20

Also shown are single crystal hardening curves in terms of the critically-resolved-shear-stress versus system shear strain for the pyramidal and prismatic slip modes.

Specimens for optical metallography were sectioned, parallel to the loading axis, from the initial as-recrystallized and deformed samples. The initial microstructure of both forms may be characterized as having equiaxed grains, a relatively broad grain size distribution, and few residual twinned grains.

Loading curves from the quasistatic test conducted at room temperature are shown in Figure 1 for the TT and IP cases. True measures of stress and strain are used to display these results. Note the difference in flow stress and hardening rate between the TT and IP orientations in Figure 1: at 10% strain the flow stress differs by a factor of 2.9 and the hardening by a factor of 2.3.

Figure 2. Photographs of the final compression shapes for quasistatic, room temperature, uniaxial stress tests for zirconium specimens machined (a) through-thickness and (b) in-plane at 90°.

Figure 2 presents photographs of the deformed specimens for the orientations discussed above. The final dimensions for these specimens are given in Table 1, in addition to eccentricity (ratio of major to minor diameters), total strains in component form and equivalent strain. Note in Table 1 that the final deformations realized by the IP samples are all very similar, with the IP-90° case deformed to the largest equivalent strain of 30%.

3 MECHANICAL BEHAVIOR

A self-consistent polycrystal methodology (Lebensohn and Tomé 1993) incorporated into the EPIC code was used to predict the constitutive response of the Zr compression samples tested as described above. The form of the single-crystal constitutive relationship is

$$\underline{d}^p = \dot{\gamma}_0 \sum_i \left(\frac{\underline{m}_i : \underline{s}}{\tau_{ci}} \right)^n \underline{m}_i \quad (1)$$

where the plastic strain rate $\underline{d}^p$ and deviator stress $\underline{s}$ are calculated for each crystal, satisfying strain compatibility and stress equilibrium with respect to the average behavior of the crystal aggregate. The index "i" designates slip system, $\underline{m}_i$ is the symmetric part of the Schmid tensor and the constants n and $\dot{\gamma}_0$ appearing in Eqn. (1) are given in Table 2.

The main characteristic of this self-consistent polycrystal model is that each grain is treated as an ellipsoidal viscoplastic inclusion embedded in, and interacting with, a Homogeneous Effective Medium (HEM) that describes the crystal aggregate. Both the inclusion and the HEM represent anisotropic viscoplastic media, and their interaction accounts for the directional anisotropy of the polycrystal. As a consequence of this interaction, the deformation varies from grain to grain depending on the crystallographic orientation. Specifically, grains tend to accommodate deformation along their "soft" directions.

Prismatic and pyramidal slip modes were assumed to be active for each grain, i.e., $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$ and $\{10\bar{1}1\}\langle 11\bar{2}3 \rangle$, having three and twelve independent slip systems, respectively. Each slip mode is weighted differently with a value of the Critical Resolved Shear Stress (CRSS) τ_c that hardens according to an extended Voce law (Tomé et al. 1984):

$$\tau_c = \tau_0 + (\tau_1 + \Theta_1 \Gamma) \left[1 - e^{-\Theta_0 \Gamma / \tau_1} \right] \quad (2)$$

where Γ is the accumulated single-crystal shear strain, and τ_0 is the initial CRSS. This law exhibits an asymptotic slope Θ_1 which back-extrapolates to $\tau_0 + \tau_1$. Prismatic slip is relatively easy in zirconium at room temperature but has the limitation that it cannot accommodate deformation perpendicular to the basal plane. As a consequence, pyramidal slip was introduced, although with a CRSS much larger than that for the prismatic mode. The numerical values of the hardening parameters appearing in Eqn. (2) for each system are given in Table 2. They were adjusted to replicate the IP and TT compression curves of

Figure 1 using the polycrystal model and the distribution of orientations (see Figure 3a) that reproduces the basal pole distribution for the rolled sheet. This parameter fitting should be regarded valid for strains exceeding 1%, for which elastoplastic effects, not accounted for by the model, become negligible.

Stress-strain prismatic and pyramidal curves illustrating the hardening behavior represented by Eqn (2) are also shown in Figure 1. Note the much harder response of the pyramidal systems compared to the prismatic systems.

Figure 3. An equal-area pole figure for (a) the initial zirconium clock-rolled plate as measured from an areal patch on the rolling plane, and (b) the final deformed state as calculated from the polycrystal simulation for the through-thickness deformation.

The ODF calculated from the experimental Basal texture represented by Figure 3a was discretized by weighting a set of random orientations by the method of Kocks, Kallend, and Biondo 1991. Those orientations with negligible weights were eliminated to improve computational efficiency, resulting in a representative set of 478 grains. This set was used in the polycrystal model for the EPIC calculational results presented in Figure 4, and in the yield-surface probes to construct the upper-bound Taylor and self-consistent envelopes presented in Figure 6.

4 NUMERICAL SIMULATIONS

The yield behavior based on self-consistent polycrystal calculations was used in 3D EPIC-97 FE simulations of the Zr compression tests. In-plane and through-thickness compression were simulated imposing a true strain rate of 10^{-3} s^{-1} in the constitutive modeling along these same directions. In particular the compression tests IP-90° and TT were simulated using 5182 tetrahedral elements (quadrature points) and 2168 time cycles out to the equivalent strains show in Table 1. Texture updates were performed after every increment of 1.0% strain. The yield response of the entire compression specimen is consistent with the condition of homogeneous deformation.

Figure 4. Comparison of final Zr compression shapes showing: (a) the initial EPIC finite element mesh of the uniaxial compression test, (b) a photograph of the through-thickness experimental shape, and (c) the calculated through-thickness FE shape, (d) a photograph of the in-plane experimental shape, and (e) the calculated in-plane FE shape. For both (b) and (d) the outer circumference of the calculated FE shape has been superimposed over the experimental shape as depicted by the white dashed curve.

Results from the EPIC simulations are shown in Figures 4. The initial finite element geometry illustrating the steel platens and compression specimen is depicted in Figure 4a. For TT compression, the final calculated shape of Figure 4c (compression face is normal to the 3-axis) is in good agreement to the experimental shape of Figure 4b

Figure 5. Prismatic and pyramidal slip mode activity shown evolving as a function of equivalent plastic strain. Note the IP compression produces no significant pyramidal activity.

In this TT orientation the plate is fairly isotropic in the 1-2 plane and remains so throughout the deformation, as the final texture depicted in Figure 3b testifies. Since the c-axes are practically aligned with the compression axis, roughly 70% of the deformation is accommodated by "hard" pyramidal slip and, as a consequence, the flow stress is large as indicated in Figure 1. The relative contribution of prismatic and pyramidal systems is illustrated in the activity diagram of Figure 5.

Figures 4d and e present similar EPIC results for the IP-90° case, where now 2-3 plane anisotropy produces a very elliptical footprint, that is also in good agreement to the experimental shape. Deformation is completely accommodated by prismatic slip (see Figure 5), which explains the near plane-strain deformation induced by the compression (prism slip doesn't occur parallel to the c-axis), and also the low value of flow stress (see Figure 1).

Finally, related calculations were performed to test the effect of hardening, texture and texture evolution, and the loading path upon the plastic properties of the specimens. For the IP compression test, successive polycrystal yield-surface π -planes were calculated by probing the aggregate after every increment of 5% strain using both upper-bound Taylor and the self-consistent models; the results are presented in Figure 6 in terms of normalized stress.

Figure 6a presents an upper-bound rather asymmetric family of π -plane sections (zero shear stress) shown as a function of increasing equivalent plastic strain. These curves are observed to harden and seem to be close to saturation by 20% strain. The bulging along the direction of the 2-axis is related to the lack of full symmetry in the texture (see Figure 3a), and the fact that the upper-bound Taylor calculation is very sensitive to these asymmetries in the initial texture and will force the use of the hard pyramidal systems.

Figure 6b, on the other hand, presents similar π -plane curves constructed from self-consistent polycrystal calculations that show symmetric stress envelopes (because mostly prism slip is being activated) hardening to magnitudes of normalized stress that do not appear to be close to saturation by 20% strain.

Figure 6. Family of Zr π -plane yield envelopes (only half of the π -plane is depicted, mirror plane symmetry has been assumed) shown evolving as a function of equivalent plastic strain. These normalized curves were produced using a series of polycrystal plasticity calculations involving both pyramidal and prismatic slip modes; both (a) the Taylor (upper bound) assumption and (b) self-consistent results are shown. The asymmetry in the Taylor curves is the result of an asymmetry in the initial texture and the sensitivity of the Taylor simulation (hard pyramidal slip) to this initial texture.

5 CONCLUSIONS

A self-consistent polycrystal model for a strongly textured clock-rolled zirconium plate material was successfully used as the constitutive description in three-dimensional finite-element simulations of quasistatic uniaxial-stress compression tests. These calculational results were in good agreement with the experimental stress-strain loading curves and the final deformed specimen shapes.

Two slip system modes each with unique Voce Law hardening parameters were used at the grain length scale in the FE calculations. For the TT compression hard pyramidal systems (see Figure 1) accounted for most of the slip activity, whereas for the IP compression, only soft prism slip was active. This slip mode selectivity in conjunction with the initial orientation distribution of grains explains the macroscopic loading curve observation of hard TT versus soft IP behavior seen in Figure 1.

A timing analysis of the FE simulations presented above is rather vexatious (using 478 grains) in that the self-consistent algorithm is roughly a factor of 20 slower than a Taylor upper-bound approach, and the Taylor algorithm will adversely impact the FE simulation by a factor of 4 or 5 when compared to classical elastoplastic (continuum level) constitutive modeling. Clearly additional development of the algorithms is needed to establish polycrystal plasticity as a viable physical-based alternative in large-scale 3D application calculations.

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