TITLE: HIGH-RATE MATERIAL MODELING AND VALIDATION USING THE TAYLOR CYLINDER IMPACT TEST

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High-Rate Material Modeling and Validation Using the Taylor Cylinder Impact Test

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ABSTRACT

Taylor Cylinder impact testing is used to validate anisotropic elastoplastic constitutive modeling by comparing polycrystal simulated yield surface shapes (topography) to measured shapes from post-test Taylor impact specimens and quasistatic compression specimens. Measured yield surface shapes are extracted from the experimental post-test geometries using classical r-value definitions modified for arbitrary stress state and specimen orientation. Rolled tantalum (body-centered-cubic metal) plate and clock-rolled zirconium (hexagonal-close-packed metal) plate are both investigated. The results indicate that an assumption of topography invariance with respect to strain-rate is justifiable for tantalum. However, a strong sensitivity of topography with respect to strain-rate for zirconium was observed, implying that some accounting for a deformation mechanism rate-dependence associated with lower-symmetry materials should be included in the constitutive modeling. Discussion of the importance of this topography rate-dependence and texture evolution in formulating constitutive models appropriate for FEM applications is provided.

I. Introduction

The importance of an accurate constitutive description for large deformation involving anisotropic metallic materials has been demonstrated in many applications; the earring of deep-drawn cups is a classic low-strain-rate example. Our interest is to develop more accurate descriptions of material strength for high-rate forming applications, and to integrate such descriptions into the appropriate continuum mechanics codes. Over the last decade the computing power (i.e., memory, processor speed and number of processors) available for numerical analysis has increased substantially. As a result, the computational tools available for simulating high deformation processes have
recently evolved to accommodate more complex descriptions of material behavior. However, even with state-of-the-art computing power there is still a need to be cognizant of the cost of using advanced material modeling in the codes and balancing this cost with the realized accuracy improvement in predictive capability.

Our elastoplastic modeling combines an appropriate elastic stiffness, a physically based flow stress model describing rate and thermally dependent hardening, and a yield surface representation again physically-based on experimental measurements of the crystallographic texture and polycrystal simulations. This elastoplastic property information is utilized in classical associative flow constitutive formulations using unrotated (material frame) tensors, with emphasis on cubic and hexagonal materials. This approach attempts to bridge the gap between single crystal and continuum length scales in order to address high-rate deformation processes with more physical fidelity.

Taylor cylinder impact testing [1-5] has been utilized to validate constitutive modeling due to the gradients of stress, strain, and strain-rate which this integrated test affords. For example, an investigation of plastic wave propagation in a Taylor test comparing time-resolved experimental data using high-speed photography with two-dimensional dynamic simulations is given in Ref. [3]. Reference [4] presents a static comparison of calculated three-dimensional final shapes with measured shapes of post-test specimens for an orthotropic material. In this effort r-values (straining ratios) are extracted from quasistatic compression data and high-rate Taylor impact specimens, and compared to polycrystal simulations using yield surface shape as the basis for comparison. Using this approach, inferences can be made as to the evolution and rate dependence of yield surface shape (topography) for a given material. Results from such comparisons are presented here. Examples and counter-examples of
the importance of yield surface topography and the effect of texture evolution on topography are discussed.

II. Theory

Constitutive modeling appropriate for the anisotropic elastic-plastic flow of metal is first reviewed, followed by an extension of Hill's classic definition of r-value [6] to accommodate arbitrary stress state and material orientation. The relationship between r-value and yield surface shape is then developed as a basis for comparison to experimental data.

II.A. Elastoplastic Constitutive Modeling

We begin with a continuum level constitutive description that uses the rate form of Hooke's law, i.e., hypoelasticity, which is a very good approximation for metals that exhibit small elastic strains:

\[ \dot{\sigma} = E : \dot{D}^e \quad (1) \]

This relationship assumes the unrotated Cauchy stress \(\sigma\) as a stress measure and the unrotated rate-of-deformation tensor \(D\) (symmetric part of the velocity gradient tensor) as an appropriate work conjugate rate-of-strain measure. Tensor order is denoted here by the number of underbars. The quantity \(D^e\) is the elastic part of \(D\) that follows from a partition assumption for the elastic and plastic rates-of-strain, i.e.,

\[ D = D^e + D^p \quad (2) \]

Deviatoric versions of Eqs. (1) and (2), which are more convenient for incompressible materials, can be derived as:

\[ \dot{\sigma} = \overline{\xi} : \dot{d}^e \quad (3) \]
and
\[ \bar{d} = d^e + d^p \]  
where \( \bar{d} \) is the deviator of the fourth order elastic stiffness tensor \( \bar{E} \).

Next consider the classical associated flow rule for evolving the plastic rate-of-strain \( d^p \):
\[ d^p = \lambda \frac{\partial f}{\partial \bar{d}} \]  
where \( f \) is a continuous yield function that is assumed to be known either from polycrystal predictions [see Refs. 7 and 8] or from experimental interrogation [6]. The quantity \( \lambda \) in Eq. (5) is a time dependent scalar. The function \( f \) is five dimensional in terms of independent deviatoric stress components \( (s_{11}, s_{22}, s_{23}, s_{31}, s_{12}) \), and physically constrains the magnitude of \( \bar{d} \) during plastic flow. The stress gradient of \( f \) determines the direction of the plastic rate-of-strain tensor \( d^p \) as indicated in Eq. (5). A general quadratic form for \( f \) can be written:
\[ f = \frac{1}{2} \bar{d} : \bar{\alpha} : \bar{d} - \sigma^2 = 0 \]  
where \( \bar{\alpha} \) is a fourth-order major and minor symmetric shape tensor and \( \sigma \) is a flow stress scalar assumed to be a function of strain, strain-rate and temperature invariants. For orthotropic materials (mirror plane symmetry where the deviator tensor \( \bar{\alpha} \) has six independent constants), Eq. (6) simplifies to the Hill [6] quadratic function:
\[ f = \frac{1}{2} \left[ (G + H)s_{11}^2 + (F + H)s_{22}^2 + (F + G)s_{23}^2 - 2Hs_{11}s_{22} - 2Gs_{11}s_{33} - 2Fs_{22}s_{33} \right. \\
+ 2Ls_{23}^2 + 2Ms_{31}^2 + 2Ns_{12}^2] - \sigma^2 = 0 \]  
(7)
and the shape tensor $\alpha$ written in Voigt-Mandel components can be expressed in terms of the Hill coefficients of Eq. (7):

$$VM(\alpha)_{\text{Hill48}} = \begin{pmatrix} G + H & -H & -G & 0 & 0 & 0 \\ -H & F + H & -F & 0 & 0 & 0 \\ -G & -F & F + G & 0 & 0 & 0 \\ 0 & 0 & 0 & L & 0 & 0 \\ 0 & 0 & 0 & 0 & M & 0 \\ 0 & 0 & 0 & 0 & 0 & N \end{pmatrix}$$

(8)

A von Mises yield function can be recovered from Eq. (6) using the following matrix for $\alpha$:

$$VM(\alpha)_{\text{von Mises}} = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

(9)

To achieve a final constitutive relationship in rate form (useful for explicit continuum code computations), we substitute Eqs. (4), (5) and (6) back into Eq. (3), giving the unrotated stress rate used for finite element computations discussed in other efforts [see for example Refs. 4,9]:

$$\dot{s} = \dot{\xi} : (d - \lambda \alpha : s)$$

(10)
II.B. Classical and Generalized r-Values

Following the classic work of Hill [6] we define an r-value ($r$) as a ratio of orthogonal plastic strain-rates realized in a metal specimen of rectangular cross-section loaded in a state of uniaxial stress (tension or compression). These straining rates are logically in directions perpendicular to the direction of loading and the free surfaces. For example, if "1" is the direction of uniaxial loading, it follows from the boundary conditions that $s_{11} = -2s_{22} = -2s_{33} = 2/3 \sigma$ in the laboratory test frame, and the corresponding r-value definition is:

$$r_1 = \frac{e_2 \cdot \frac{d\epsilon}{dt} \cdot e_2}{e_3 \cdot \frac{d\epsilon}{dt} \cdot e_3}$$

(11a)

Here the $e_i$ are Cartesian base vectors for the laboratory reference frame, and the r-value subscript designates the loading direction. Similar r-value definitions for loading in the other two directions, i.e., 2 and 3 respectively, follow as:

$$r_2 = \frac{e_1 \cdot \frac{d\epsilon}{dt} \cdot e_2}{e_3 \cdot \frac{d\epsilon}{dt} \cdot e_3} \quad \text{and} \quad r_3 = \frac{e_1 \cdot \frac{d\epsilon}{dt} \cdot e_1}{e_2 \cdot \frac{d\epsilon}{dt} \cdot e_2}$$

(11b)

The definition of r-value can be generalized into a second-order tensor having the form:

$$\Gamma = \begin{pmatrix}
1 & r_{12} & r_{13} \\
 r_{21} & 1 & r_{23} \\
 r_{31} & r_{32} & 1
\end{pmatrix} \quad \text{where} \quad r_{ij} = \frac{e_i \cdot \frac{d\epsilon}{dt} \left( Q^T \cdot \frac{\mathbf{s}}{\mathbf{s}} \right) \cdot e_j}{e_j \cdot \frac{d\epsilon}{dt} \left( Q^T \cdot \frac{\mathbf{s}}{\mathbf{s}} \right) \cdot e_i} \quad \text{no sum on I, J} \quad (12)$$

where the tensor $Q$ is a proper orthogonal rotation that properly aligns the direction of loading for each value of $r_{ij}$.
Here \( \varepsilon_{uk} \) is the third-order alternator tensor. For clarity, the functional dependence of the rate-of-straining tensor \( \dot{D} \) on \( Q \) is shown explicitly in Eq. (12). Also note that the tensor definition of \( r \)-value contains only three independent coefficients: \( r_{12}, r_{13}, r_{23} \); the relationship \( r_{ij} = -1/r_{ji} \) holds between transposed components and obviously \( r_{ii} = 1 \) (no sum on \( I \)) from inspection of Eq. (12).

We now substitute the associated flow rule given by Eq. (5) into Eq. (12), obtaining an \( r \)-value involving only yield surface stress gradients \( \partial f/\partial \mathbf{S} \) after cancellation of \( \dot{\lambda} \). Recalling from Eq. (10) the evaluation of \( \partial f/\partial \mathbf{S} \) for a quadratic yield function, and now incorporating \( Q \) to impose the direction of loading gives:

\[
\frac{\partial f}{\partial \mathbf{S}} = \alpha \cdot \mathbf{Q}^T \cdot \mathbf{S} \cdot \mathbf{Q} \quad \text{or in indicial notation} \quad \frac{\partial f}{\partial s_{ij}} = \alpha_{ijkl} \mathbf{Q}^T_{km} s_{mn} Q_{nl}
\]

and after substitution of Eq. (14) back into Eq. (12) we obtain the final \( r \)-value result:

\[
r_{ij} = \frac{\varepsilon_I \cdot \varepsilon_I : \mathbf{Q}^T \cdot \mathbf{S} \cdot \mathbf{Q} \cdot \varepsilon_I}{\varepsilon_I \cdot \varepsilon_I : \mathbf{Q}^T \cdot \mathbf{S} \cdot \mathbf{Q} \cdot \varepsilon_I} \quad \text{or} \quad r_{ij} = \frac{\alpha_{ijkl} \mathbf{Q}^T_{km} s_{mn} Q_{nl}}{\alpha_{jlpq} \mathbf{Q}^T_{pr} s_{rs} Q_{sq}} \quad \text{no sum on } I, J
\]

As an example, consider the case of uniaxial stress in the 1-direction \( Q_{kk} = 1 \) where the stress deviator simplifies to
The yield function gradient given by Eq. (14) becomes

$$\frac{\partial f}{\partial s_{ij}} = s_{11} \left[ \alpha_{i11} - \frac{1}{2} \alpha_{i22} - \frac{1}{2} \alpha_{i33} \right]$$

(17)

Evaluation of the r-value (specifically \(r_{23}\)) follows from Eq. (15) as just a ratio of the normal shape coefficients:

$$r_{23} = \frac{\alpha_{122}}{\alpha_{133}}$$

(18)

In like manner, uniaxial stress loading in the 2 (\(Q_{k=2}\)) and 3 (\(Q_{k=3}\)) directions results in similar expressions for the other orthogonal \(r_{ij}\), and thus we obtain for the r-value tensor:

$$r = \begin{bmatrix}
1 & \frac{\alpha_{113}}{\alpha_{133}} & \frac{\alpha_{122}}{\alpha_{133}} \\
\frac{\alpha_{223}}{\alpha_{233}} & 1 & \frac{\alpha_{223}}{\alpha_{233}} \\
\frac{\alpha_{223}}{\alpha_{233}} & \frac{\alpha_{223}}{\alpha_{233}} & 1
\end{bmatrix}$$

(19)

Expressions for the normal shape coefficients (and hence the \(r_{ij}\)) as functions of the deviator stress are next derived by solving a system of six equations for the six unknowns \(\alpha_{ijk}\delta_{kl}\delta_{ij}\), where \(\delta_{ij}\) is the Kronecker delta function. Three equations are consecutively generated by substituting the condition of uniaxial stress (e.g., Eq. (16)) into the yield function Eq. (6) for each of the three Cartesian directions \(\varepsilon_i\). Three additional equations are
available given that \( \alpha \) is a deviator tensor and the six coefficients \( \alpha_{ijk} \delta_{ki} \delta_{ij} \) are dependent, i.e., each row (or column) of \( \alpha \) must sum to zero:

\[
\begin{align*}
\alpha_{11i} &= 0 \\
\alpha_{22i} &= 0 \\
\alpha_{33i} &= 0
\end{align*}
\] (20a, 20b, 20c)

Solving this 6x6 system of equations for \( \alpha_{ijk} \delta_{ki} \delta_{ij} \) produces the solution:

\[
\begin{align*}
\alpha_{1111} &= \frac{8}{9} \sigma^2 \\
\alpha_{2222} &= \frac{8}{9} \sigma^2 \\
\alpha_{3333} &= \frac{8}{9} \sigma^2 \\
\alpha_{2233} &= \frac{4}{9} \sigma^2 \left( \frac{1}{s_{11}^2} - \frac{1}{s_{33}^2} - \frac{1}{s_{22}^2} \right) \\
\alpha_{1133} &= \frac{4}{9} \sigma^2 \left( \frac{1}{s_{22}^2} - \frac{1}{s_{11}^2} - \frac{1}{s_{33}^2} \right) \\
\alpha_{1122} &= \frac{4}{9} \sigma^2 \left( \frac{1}{s_{33}^2} - \frac{1}{s_{11}^2} - \frac{1}{s_{22}^2} \right)
\end{align*}
\] (21a, 21b, 21c, 21d, 21e, 21f)

The deviatoric stress components \( (s_{11}, s_{22}, s_{33}) \) in Eqs. (21) are uniaxial values as measured in three independent orthogonal tests. These relationships assume that the flow stress \( \sigma \) is a known function characterized from uniaxial stress data in a specific \( \varepsilon_i \) direction.

Recalling the relationship between \( \alpha \) and \( F, G, H \) as given by Eq. (8), a similar set of equations for \( F, G, H \) as a function of deviatoric stress can be obtained by inspection of Eqs. (21):

\[
\begin{align*}
F &= \frac{4}{9} \sigma^2 \left( \frac{1}{s_{22}^2} + \frac{1}{s_{33}^2} - \frac{1}{s_{11}^2} \right) \\
G &= \frac{4}{9} \sigma^2 \left( \frac{1}{s_{33}^2} + \frac{1}{s_{11}^2} - \frac{1}{s_{22}^2} \right)
\end{align*}
\] (22a, 22b)
The above formulations assume that the material reference frame (where \( f \) is characterized) and the laboratory test frame are coincident. However, if the two differ by some three-dimensional rigid body rotation, then the derivation for the \( r \)-values is somewhat more complicated. Physically, this situation would arise when the material frame (which is based on the microstructural symmetry of the material) differs in orientation from the laboratory test frame where some geometrical specimen is loaded. An example of this situation is given below. For clarity in the subsequent discussion, we associate the Cartesian base vectors \( \bar{\epsilon}_i \) with the material frame and, as stated above, the Cartesian base vectors \( \epsilon_i \) with the laboratory frame.

In order to derive a more general \( r \)-value definition, recall that the yield function \( f \) as given by Eq. (6) is a function of deviatoric stress as observed with respect to the material frame. It therefore depends on the unrotated stress state \( \bar{s} \) (the overbar designates unrotated material frame tensors). This unrotated stress differs from the laboratory stress \( s \) by a rigid body rotation described by the proper orthogonal tensor \( R \) (where \( \epsilon_i = R \cdot \bar{\epsilon}_i \)):

\[
\bar{s} = R^T \cdot s \cdot R \quad \text{or in indicial notation} \quad \bar{s}_{ij} = R_{ik}^T s_{kl} R_{lj}
\]

Noting the \( r \)-value relationship given by Eq. (15), the stress gradient given by Eq. (14) is expanded using the chain rule such that:

\[
\frac{\partial f}{\partial \bar{s}} = \frac{\partial f}{\partial s} \cdot \frac{\partial s}{\partial \bar{s}} = \alpha : Q^T \cdot \bar{s} : Q = \sum_{k=1}^n \sum_{l=1}^n \alpha_{klnm} Q_{mp}^T \bar{s}_{pq} Q_{nq} \frac{\partial s_{kl}}{\partial \bar{s}_{ij}}
\]

and the stress derivative \( \partial \bar{s}/\partial \bar{s} \) follows from Eq. (23) as:
The r-value expression then has a form that contains the unrotated stress:

$$r_U = \frac{e_i \cdot \alpha : Q^T \cdot \bar{s} \cdot Q : R^T \otimes R \cdot e_j}{e_j \cdot \alpha : Q^T \cdot \bar{s} \cdot Q : R^T \otimes R \cdot e_j} \quad \text{no sum on } I, J \quad (26a)$$

or

$$r_U = \alpha_{klnm} Q^T_{np} R_{aq} R^T_{kl} R_{nj} \quad \text{no sum on } I, J \quad (26b)$$

If the unrotated stress is replaced with the laboratory stress via Eq. (23), we obtain the more useful, albeit more complicated, laboratory form:

$$r_U = \frac{e_i \cdot \alpha : Q^T \cdot R^T \cdot \bar{s} \cdot Q : R^T \otimes R \cdot e_j}{e_j \cdot \alpha : Q^T \cdot R^T \cdot \bar{s} \cdot Q : R^T \otimes R \cdot e_j} \quad \text{no sum on } I, J \quad (27a)$$

or

$$r_U = \frac{\alpha_{ijkl} Q^T_{np} R_{aq} R^T_{kl} R_{nj}}{\alpha_{rsuv} Q^T_{ws} R_{yz} R^T_{uv} R_{ij}} \quad \text{no sum on } I, J \quad (27b)$$

Equation (27) represents a general r-value expression for an arbitrary stress state (not restricted to just uniaxial stress) and for an arbitrary orientation difference between the material and laboratory reference frames. Therefore stress states other than uniaxial can be accommodated, and $\bar{s}$ still retains its basic definition as a ratio of normal straining rates realized in two orthogonal directions. Note that for an arbitrary orientation difference between the material and laboratory frames $\bar{s}$ assumes the three-dimensional form:
\[
\mathbf{R} = \begin{pmatrix}
\cos \phi & -\sin \phi & 0 \\
\sin \phi & \cos \phi & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
1 & 0 & 0 \\
0 & \cos \theta & -\sin \theta \\
0 & \sin \theta & \cos \theta
\end{pmatrix}
\begin{pmatrix}
\cos \psi & -\sin \psi & 0 \\
\sin \psi & \cos \psi & 0 \\
0 & 0 & 1
\end{pmatrix}
\] (28)

Here the Euler angles \( \psi, \theta, \phi \) represent right-hand-rule rotations as per the convention described in Ref. [15].

As an example of Eqs. (27), assume plane rotation around the 3-axis such that \( \mathbf{R} \) becomes

\[
\mathbf{R} = \begin{pmatrix}
\cos \psi & -\sin \psi & 0 \\
\sin \psi & \cos \psi & 0 \\
0 & 0 & 1
\end{pmatrix}
\] (29)

and the laboratory observed stress is again uniaxial in the 1-direction as given by Eq. (16). Expanding the summations of Eq. (27b), substituting in Eqs. (16) and (29), and noting the deviator relationships given by Eqs. (20) gives:

\[
\begin{align*}
\tau_{23} &= \alpha_{1111} + (\alpha_{1111} + \alpha_{2222} - 2\alpha_{1112} \cos^2 \psi) \sin^2 \psi \cos^2 \psi \sin \psi \cos \psi + \alpha_{1113} \cos^2 \psi \sin \psi \cos \psi \\
&= \alpha_{2222} - 4\alpha_{1112} \cos^2 \psi \sin \psi \cos \psi + \alpha_{1113} \cos^2 \psi \sin \psi \cos \psi
\end{align*}
\] (30)

Replacing the tensor components \( \alpha_{ij} \) in Eq. (30) with Hill coefficients from Eq. (8) gives the classic Hill result [6] for an \( r \)-value specimen cut from sheet metal at an arbitrary orientation \( \psi \) with respect to the rolling direction:

\[
\tau_{23} = \frac{H + (2N - F - G - 4H) \sin^2 \psi \cos^2 \psi}{F \sin^2 \psi + G \cos^2 \psi}
\] (31)

III. Low-Rate Yield Surface Comparisons

Experimental data sets are presented for both tantalum and zirconium metals: Stress-strain loading curves were produced for compression specimens subjected to a state of uniaxial stress This information is converted
into yield surface shape coefficients which are compared subsequently to polycrystal simulations.

III.A. Tantalum

Consider a plate of unidirectional rolled body-centered-cubic (BCC) tantalum from which compression specimen "blocks" are cut as depicted in Fig. 1. These blocks have an associated material coordinate system (basis $\vec{e}_i$) as shown in Fig. 1, where $\vec{e}_1$ is transverse to the rolling direction, $\vec{e}_2$ corresponds to the rolling direction and $\vec{e}_3$ is through-thickness (TT). The manufacturing process for this plate produced a near-orthotropic, mild rolling texture discussed in some detail in Refs. [4, 5].
Figure 1: Hexahedral compression test specimen cut from a unidirectional rolled plate of tantalum.

A set of yield stress points mapping out a $\pi$-plane yield envelope can be generated by repetitive plastic straining probes of an orientation distribution function as discussed by Ref. [8]. For each arbitrary straining direction, a yield stress point is computed via a Bishop-Hill polycrystal calculation using the upper bound option of the LApp (Los Alamos polycrystal plasticity) code (see Refs. [10, 11]) with the slip deformation modes \{110\}(111) and \{112\}(111). Such a $\pi$-plane yield surface is presented in Fig. 2,
showing a LApp simulated yield surface and also a quadratic fit to the Lapp piece-wise function; this quadratic interpolates the Lapp results at the horizontal and vertical axis intercepts. The shape coefficients associated with the quadratic fit are given in Row 1 of Table I along with the associated $r_{ij}$ that are easily computed using Eq. (19).

Figure 2: A two-dimensional π-plane subspace showing a polycrystal generated piece-wise yield surface (line segments and points) being compared with a quadratic fit (solid curve) interpolating the piece-wise function at the horizontal and vertical axis intercepts.

The blocks of Fig. 1 were compressed quasi-statically at room temperature in a state of uniaxial stress along each material axis $\bar{\varepsilon}_i$ producing the loading curves presented in Fig. 3. These curves show the TT $\bar{\varepsilon}_3$ direction to produce the hardest response, with the other in-plane (IP) directions producing roughly 20% softer but similar responses. The apparent
discontinuities at 4% and 8% strains in these curves represent unload/reload steps in the compression testing in order to minimize surface friction.

Figure 3: Uniaxial stress/strain curves for a unidirectional rolled Ta plate compressed along each of the material axes $\xi_i$.

Conversion of the uniaxial stress-strain data of Fig. 3 into $\alpha_{ijkl}\delta_{kl}\delta_{ij}$ using Eqs. (21) gives the results presented in Fig. 4. These curves quantify material anisotropy in terms of yield surface shape coefficients shown as a function of true strain. As confirmed by Fig. 4, after only 12% strain one would not expect significant texture evolution and thus the $\alpha_{ijkl}\delta_{kl}\delta_{ij}$ remain relatively constant. Values for the $\alpha_{1122}, \alpha_{1133}, \alpha_{2233}$ at 12% strain are given in
Row 2 of Table I along with the corresponding r-values as computed using Eq. (19).

Figure 4: Quadratic shape coefficients evolving as a function of true strain. These coefficients were evaluated using Eqs. (21) and the loading curves of Fig. 3.

Table I: Tantalum R-Values and Shape Coefficients

<table>
<thead>
<tr>
<th>Experiment or Simulation</th>
<th>$r_{23}$</th>
<th>$r_{13}$</th>
<th>$r_{12}$</th>
<th>$\alpha_{1122}$</th>
<th>$\alpha_{1133}$</th>
<th>$\alpha_{2233}$</th>
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</thead>
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<tr>
<td>Polycrystal Simulations (LApp)</td>
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<td>1.52</td>
<td>1.22</td>
<td>1.37</td>
<td>1.10</td>
<td>0.90</td>
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<td>Low-Rate Compression</td>
<td>1.32</td>
<td>1.46</td>
<td>1.10</td>
<td>1.39</td>
<td>1.05</td>
<td>0.95</td>
</tr>
<tr>
<td>Taylor Cylinder Impact (175 m/s)</td>
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<td>1.25</td>
<td>1.00</td>
<td>1.25</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>
III.B. Zirconium

Uniaxial compression testing was conducted on a high-purity crystal-bar zirconium plate as discussed in detail in Ref. [12]. Zirconium is a hexagonal-close-packed (HCP) metal. This Zr 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 as further discussed in Refs. [12,13]. Next we associate a material reference frame (basis $\xi_i$) with the Zr plate where the $\xi_1 \times \xi_2$ plane corresponds to the original rolling plane, and the $\xi_3$ direction is through-thickness. Right-circular-cylinder compression samples (nominally 5 mm in diameter by 5 mm in height) were cut from the plate in all three $\xi_i$ orientations, i.e., TT ($\xi_3$) and IP ($\xi_1$ or $\xi_2$) specimens. The IP specimens were machined at 0°, 45°, and 90° relative to the $\xi_i$ axis [12].

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 as described by Ref. [12]. Figure 5 presents photographs of final geometries for these tests featuring TT and IP ($\xi_2$) specimens strained to values of 22% and 30% equivalent plastic strain, respectively.

A $\pi$-plane yield envelope for this Zr material was again generated by repetitive plastic straining probes of the texture orientation distribution function presented in Ref. [13]. For each arbitrary straining direction, a yield stress point was computed via a self-consistent polycrystal simulation using the code VPSC [14]. Prismatic and pyramidal slip deformation modes were
assumed. The resulting π-plane yield surface is presented in Fig. 6 presenting a VPSC simulation of a 10% strained, shape-hardened yield surface [additional detail is given in Ref. 13]. Also shown in Fig. 6 is a quadratic fit to the polycrystal results, again interpolating the VPSC piece-wise curve at the horizontal and vertical axis intercepts. This quadratic fit to the polycrystal results is reasonably accurate (depending on the finite element (FE) application of this information) but does miss the stress corners in the VPSC shape. A yield function with the stress components raised to fractional powers would better fit the corners apparent in the Fig. 6 results [16]. The shape coefficients associated with the quadratic fit are given in Row 1 of Table II along with the corresponding $r_0$.

![Figure 5: Photographs of the final compression shapes for quasistatic, room temperature, uniaxial stress tests for zirconium specimens machined (a) through-thickness ($\bar{e}_1\bar{e}_2$ plane) and (b) in-plane ($\bar{e}_2\bar{e}_3$ plane).](image)
Loading curves for the TT and IP samples are presented in Fig. 7. The IP compressions produced very similar stress-strain curves along the two IP directions $\bar{\varepsilon}_1$ and $\bar{\varepsilon}_2$, with small variations in stress of about $\pm 10$ MPa about the mean value for a given set of conditions. This finding supports the expectation of in-plane isotropy for this clock rolled material.

Figure 6: A two-dimensional $\pi$-plane subspace showing a piece-wise yield surface (line segments and points) being compared with a quadratic fit (solid curve) interpolating the piece-wise function at the horizontal and vertical axis intercepts.
Table II: Zirconium R-Values and Shape Coefficients

<table>
<thead>
<tr>
<th>Experiment or Simulation</th>
<th>( r_{23} )</th>
<th>( r_{13} )</th>
<th>( r_{12} )</th>
<th>(-\alpha_{1122})</th>
<th>(-\alpha_{1133})</th>
<th>(-\alpha_{2233})</th>
</tr>
</thead>
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<tr>
<td>Polycrystal Simulations (VPSC)</td>
<td>7.30</td>
<td>7.30</td>
<td>1.00</td>
<td>7.30</td>
<td>1.00</td>
<td>1.00</td>
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<td>7.03</td>
<td>0.63</td>
<td>8.65</td>
<td>0.78</td>
<td>1.22</td>
</tr>
<tr>
<td>Taylor Cylinder Impact (243 m/s)</td>
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<td>1.31</td>
<td>1.00</td>
<td>1.31</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Figure 7: Uniaxial stress/strain curves for a crystal bar clock-rolled Zr material compressed quasistatically along each of the material axes \( \tilde{c}_1 \).

As performed for the tantalum, we converted the uniaxial stress-strain data of Fig. 7 into \( \alpha_{ijkl}\delta_{ij}\delta_{kl} \) using Eqs. (21), giving the results presented in Fig. 8. These shape coefficient curves quantify strong plastic anisotropy and also demonstrate strong texture evolution as a function of strain. For example, the TT coefficient \( \alpha_{1122} \) has a value of 15 at 10% strain decreasing to about 8 at 22%
strain. The other IP coefficients $\alpha_{1133}$ and $\alpha_{2233}$ evolve also from their initially rather large values, and approach unity at large strain. Values for $\alpha_{1122}, \alpha_{1133}, \alpha_{2233}$ at 22% strain are given in Row 2 of Table II for these quasistatic compression tests, along with the corresponding $r$-values as computed using Eqs. (19).

![Graph showing quadratic shape coefficients evolving as a function of strain.](image)

**Figure 8:** Quadratic shape coefficients evolving as a function of strain. These coefficients were evaluated using Eqs. (21) and the loading curves of Fig. 7.

IV. High Rate Yield Surface Comparisons

Taylor test profile data sets are presented for both tantalum and zirconium metals: Three-dimensional post-impact specimen shapes were digitized in order to estimate the spatial distribution of strain. This
information is converted into yield surface shape coefficients which are compared subsequently to polycrystal simulations.

IV.A. Tantalum

Taylor cylinder impact specimens were cut from the same tantalum plate described above for the compression blocks producing two IP cylinder orientations, i.e., the cylindrical axes are coincident with either the $\bar{e}_1$ (transverse) or the $\bar{e}_2$ (rolling) material directions. The Taylor specimens were caliber 30 (7.62 mm diameter) cylinders with a length of 1.5 inch (38.1 mm) having the length-to-diameter ratio $L/D = 5$.

Taylor tests were conducted at Eglin Air Force Base as described in Ref. [4], producing three good post-test geometries (designated SC-11, SC-12 and SC-21 in Ref. [4]) all having the general appearance portrayed in Fig. 9. The cylinders were launched using a caliber 30 Mann powder gun. The velocity of the projectiles was measured using both pressure transducers and parallel laser beams crossing the flight path. Velocities determined from the two systems were about 175 m/s, agreeing to within ± 3.0 m/s. The anvil target was AF1410 steel heat treated to a surface hardness of Rc 58.
After testing, geometric profile data for the deformed specimens was generated using an optical comparator. As discussed in Ref. [4], the data set consists of three digitized side profiles for the minor dimension, three digitized side profiles for the major dimension and three digitized footprints (the cross-sectional area at the impact interface, i.e., the $\bar{e}_1 x_3$ or $\bar{e}_2 x_3$ plane). All three tests indicated good comparability in terms of the post-test shapes. The digitized footprints, in particular, are nearly identical in shape. Eccentricities (ratio of major to minor diameters) of the footprints range from 1.18 to 1.23 (say an average value of 1.20). Approximate r-values are extracted from these footprint geometries using an integrated form of Eqs. (11):

$$r_{ij} \equiv \frac{\int_{R_0}^{\infty} \frac{dR^P}{dR^P} dR}{\int_{R_0}^{\infty} \frac{dR^P}{dR} dR} = \frac{\ln(R_j/R_o)}{\ln(R_j/R_o)} \quad \text{no sum on } I, J$$

(32)

where $R$ is the specimen radius. Applying Eq. (32) to the Taylor footprint data gives the r-values estimates in Row 3 of Table I, along with the inferred shape
coefficients. These coefficients were obtained by solving Eq. (19) for the \( \alpha_{122}, \alpha_{133}, \alpha_{2233} \), and noting that the resulting set of three linear equations is homogeneous and thus does not represent a system of three independent equations. An extra equation is needed to obtain a non-trivial unique solution. This is a consequence of the fact that the yield function given by Eq. (6) has an implied normalization. If the flow stress \( \sigma \) had been characterized from uniaxial stress data in a specific direction, say in the \( \bar{e}_i \) direction, then the normalization relationship \(-\alpha_{iii} - \alpha_{2ii} = 2\) must hold in order to recapture the uniaxial stress state from the yield function. This normalization in conjunction with Eq. (19) will produce a unique set of \( \alpha_{ijkl} \delta_{kl} \delta_{ij} \). The use of Eq. (19) to compute \( \alpha_{ijkl} \delta_{kl} \delta_{ij} \) from Taylor test r-values assumes that a state of uniaxial stress existed in the specimen during deformation. As discussed in Ref. [17], this is actually a good assumption. Specimen r-values extracted from test geometries that did not realize uniaxial stress during deformation require the use of an inverted Eq. (27) to compute \( \alpha_{ijkl} \delta_{kl} \delta_{ij} \).

Further analysis of the digitized side profiles for these Taylor shots is useful to better understand plastic anisotropy and texture evolution. Axial strain profiles for both the major and minor sides of the deformed specimens are presented in Fig. 10. The ordinate is true strain \( \ln(R/R_o) \) for the various tests plotted as a function of axial position \( z \), where \( z \) is measured relative to the impact interface. The major and minor strains, which are both zero at large \( z \), accumulate at different rates as \( z \) decreases. Their maximum values of 87% and 70% are obviously realized at \( z = 0 \), respectively.
Recasting the Fig. 10 strain profiles in terms of r-value (via Eq. (32)) expressed as a function of minor-side strain gives the very interesting results shown in Fig. 11. Despite the footprint r-values from Row 3 of Table I, the r-value from the Taylor specimen profiles actually varies from 1.25 at the impact interface to a peak value of 2.4 at a strain slightly greater than 20%, indicating rather strong microstructural evolution. Note that all three curves in Fig. 11 are nearly identical from the impact interface down to approximately 15% strain, and then diverge at smaller strain (perhaps due to geometric measurement uncertainties). Since r-values are related to yield surface shape coefficients and shape coefficients reflect the crystallographic
texture of the material, one may conclude from the Fig. 11 results that grain reorientation jumps sharply between 15% and 20% strain; at strains greater than 20% the yield topography evolves rather monotonically back towards the original shape as strains accumulate to 72%.

![Graph](image)

**Figure 11**: Tantalum Taylor cylinder r-value profiles shown as a function of minor-side true strain for three Taylor shots.

### IV.B. Zirconium

Taylor cylinder impact specimens were cut from the zirconium plate described above for the cylindrical compression specimens producing two IP cylinder orientations, i.e., the cylindrical axes are coincident with either the $\bar{e}_1$ or $\bar{e}_2$ plate directions. The Taylor specimens were caliber 30 (7.62 mm...
diameter) cylinders with a length of 2 inch (50.8 mm) having the length-to-diameter ratio L/D = 6.67.

Taylor tests were conducted at Los Alamos National Laboratory at various velocities: 50, 101, 170 and 243 m/s. The 243 m/s Taylor shot is portrayed in Fig. 12 in terms of major- and minor-side profiles and the impact footprint. These cylinders were launched using a caliber 30 He gas-driven gun. The velocity of the projectiles was measured using parallel laser beams crossing the flight path. The anvil target was AF1410 steel heat treated to a surface hardness of Rc 58 and lapped to a mirror finish.

![Figure 12: Photographs of the post-test geometry for a zirconium Taylor specimen.](image)

Post-test geometric profile data for the 243 m/s specimen was generated using interface reconstruction software from the National Institute of Health. Thus the data set consists of digitized side profiles for the major and minor dimension, and a digitized footprint (the cross-sectional area at the impact
interface, i.e., the $\xi_2\xi_3$ plane). The digitized footprint showed an eccentricity (ratio of major to minor diameters) value of 1.10. Approximate $r$-values extracted from the footprint geometry of Fig. 12 using Eq. (32) are given in Row 3 of Table II, along with the inferred shape coefficients. Comparing the rows of Table II, note the large differences in plastic anisotropy implied by these shape coefficients.

V. Discussion of Results

Review of Tables I and II indicates variability in the values for the Ta and Zr quadratic shape coefficients, but the important question from an applications point-of-view is how significant are these differences. Figure 13 illustrates the Table I shape coefficients as $\pi$-plane ellipses using Eq. (6). It is interesting to note from this figure that of the above discussed methodologies for estimating yield topography, i.e., polycrystal simulations, low strain-rate compression testing ($10^{-3}$ s$^{-1}$) and high strain-rate Taylor testing ($>10^4$ s$^{-1}$), all predict nearly the same yield surface shape. Therefore, for Ta, and possibly for other BCC materials where two modes of slip deformation are a good assumption, the use in FE calculations of a rate-independent yield surface shape is well justified.
In like manner, Fig. 14 illustrates the Table II zirconium quadratic coefficients as \( \pi \)-plane ellipses. It is again interesting to note that the low strain-rate compression testing and rate-independent polycrystal simulations both produce very similar ellipses in the \( \pi \)-plane, predicting practically identical anisotropic deformation. However, the high strain-rate Taylor testing (>10^4 s\(^{-1}\)) predicts yield topography that approaches isotropy, demonstrating a very dramatic shape rate effect. Obviously, the rather limited deformation mechanisms (prismatic and pyramidal slip) present in the
lower-symmetry Zr at quasistatic rates must transition somehow at higher rates. This high rate behavior must introduce additional deformation mechanisms (other competing slip and twinning modes) in such a way that the Taylor loading is accommodated with near-isotropic deformation. Initial metallographic examination of Zr deformed at high rate reveals evidence of substantial twin activation which is consistent with this postulate. High-rate FE code constitutive modeling involving a lower-symmetry material like Zr needs to be cognizant of this behavior.

Figure 14: A π-plane subspace comparison of quadratic zirconium yield functions as interpolated from VPSC simulations and experimentally extracted in terms of r-values from the quasistatic compression tests and Taylor cylinder impact test.
The effect of evolution on yield surface shape can be judged for the Ta and Zr after review of both the low-rate and high-rate converted experimental data sets. In the proceeding discussion it is difficult to unfold from the experiment information whether the evidence of shape coefficient evolution with respect to strain is related to grain reorientation or some transition of the deformation mechanism. For Ta, the low-rate results of Fig. 4 show virtually constant shape coefficients (ignoring the unload/reload transients) out to the rather modest strain of 12%. It would be interesting to extend the experimental loading for these compression blocks to larger strain. The high-rate Taylor results of Fig. 11, which extend to 80% strain, show moderate shape coefficient evolution: The coefficient $\alpha_{1122}$ jumps from 1.4 to 2.5 and then decreases slowly back to approximately 1.25 during the course of the Taylor impact event. This high-rate evolution in yield topography implies concurrent texture evolution and possibly some slip mode competition. However, the practical side of the importance of this topography evolution is that the strain-averaged shape is very close to the initial shape, and thus the importance of evolution for Ta is seen to be vanishing for the more integrated Taylor test.

For Zr, the low-rate Fig. 8 results show strong yield topography evolution and thus strong implied deformation mechanism transition and texture evolution; the coefficient $\alpha_{1122}$ evolves from 18 to 8.6 as the compression specimen realizes 30% strain. Further analysis of the Zr Taylor
test specimens in terms of r-value versus strain profiles and metallurgical structure evolution basis are in progress.

References


