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**Modeling Anisotropic Plasticity: Eulerian Hydrocode Applications
of High Strain-Rate Deformation Processes**

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Abstract: Previously developed constitutive models and solution algorithms for anisotropic elastoplastic material strength are implemented in the two-dimensional MESA hydrodynamics code. Quadratic yield functions fitted from polycrystal simulations for a metallic hexagonal-close-packed structure are utilized. An associative flow strength formulation incorporating these yield functions is solved using a geometric normal return method. A stretching rod problem is selected to investigate the effects of material anisotropy on a tensile plastic instability (necking). The rod necking rate and topology are compared for MESA simulations performed for both isotropic and anisotropic cases utilizing the Mechanical Threshold Stress flow stress model.

1. INTRODUCTION

Accurate constitutive descriptions are required for high-deformation processes involving metals whose strength response demonstrates a significant directional behavior. The viability of utilizing anisotropic elastoplastic constitutive modeling to predict the large rigid body rotation and plastic deformation is shown using the EPIC[1] code for a realistic high-rate explosive forming problem[2]. These calculations show strong sensitivity to the yield function shape for a hexagonal-close-packed (HCP) material having high yield anisotropy. Constitutive models and solution algorithms for anisotropic elastoplastic strength[2] developed for the Lagrangian (EPIC) continuum mechanics code are implemented in the two-dimensional MESA[3] Eulerian code. The ability to model an anisotropic elastoplastic response with MESA allows us to study the stability characteristics of selected stretching rod geometries using an Eulerian code that is well-suited for large deformation.

MESA is an explicit, Eulerian continuum mechanics code designed to predict large material deformation at elevated strain-rates. Some special features of MESA include a high-order advection algorithm, a material interface tracking scheme, and van Leer monotonic advection-limiting. The implemented anisotropic constitutive modeling is posed in an unrotated material frame using the theorem of polar decomposition to describe rigid body rotation[4]. Analytical quadratic yield functions fitted to polycrystal simulations for an metallic HCP structure is utilized. An associative flow strength formulation incorporating these yield functions is solved using a geometric normal return method[2].

The model is exercised on a "stretching rod" problem for the purpose of investigating the effects of material anisotropy on plastic localization phenomena at high strain-rates. MESA predictions of the rod necking rate and topology are compared for both isotropic and anisotropic cases utilizing the Mechanical Threshold Stress (MTS) flow stress model[5]. Also, the influence of material advection on the anisotropic constitutive variables is evaluated.

2. ANISOTROPIC PLASTICITY MODELING

The anisotropic constitutive modeling used in this effort is posed in an unrotated material frame as discussed in Refs. [4] and [2]. Constitutive modeling in this material frame is convenient in that it can be performed ignoring rigid body rotation. The modeling assumes that the material's elastic stress-strain response out to the anisotropic yield surface is isotropic. The quadratic yield surface is similar to the classical Hill function [6] written here in terms of deviatoric stress (s_{ij}) in indicial form:

$$f = \frac{1}{2} \alpha_{ijkl} s_{kl} s_{ij} - \sigma^2 = 0 \quad (2.1)$$

where the quantity σ is a flow stress that is assumed to be a function of strain, strain-rate and temperature invariants. The traditional isotropic strength formulation found in most explicit hydrocodes uses an objective Jaumann stress rate, a Von Mises yield function and the geometric method of radial return. Our approach uses polar decomposition of the deformation gradient to obtain the rigid body rotation, rotating the deviatoric strain rate tensor into the material frame, using a geometric normal return method analogous to the radial return method to find the new stress state and then rotating this stress back into the laboratory frame; the quadratic yield function given by Eq. (2.1) represents the surface that a trial stress is returned to as part of the normal return algorithm.

The MTS flow stress model[5] is used to isotropically harden the yield surface shape given by Eq. (2.1). The MTS relationship can be expressed in general form as a superposition of $n+1$ threshold-stress contributions to σ , where each contribution represents a dislocation interaction with some barrier i :

$$\sigma = \sigma_a + \frac{\mu}{\mu_0} \left(\sum_i s_{th,i} \hat{\sigma}_i \right) \quad (2.2)$$

The summed product shown in the above equation separates the contribution from interaction i into a structure evolution term ($\hat{\sigma}_i$) modified with a constant-structure thermal activation term (s_i) that is primarily a function of temperature and strain rate. The athermal threshold stress (σ_a) represents dislocation interactions with grain boundaries, and typically is a constant that depends upon the material grain size. The MTS model is described in detail by Kocks and Follansbee[5]. In the simulations discussed below the MTS model, as characterized for Ti-6Al-4V[7], is used.

3. ANISOTROPIC PLASTICITY IMPLEMENTATION IN MESA2D

The MESA2D numerical approach consists of two phases, Lagrangian and remap (or advection). It uses an explicit, predictor-corrector method for the Lagrangian phase. The method is essentially an Euler predictor step, which is first order accurate, plus a Leapfrog corrector step, which is second order accurate. Overall, the method in the Lagrangian phase is second order accurate despite being first order accurate in the predictor step. In the advection phase of the code, it uses a third order accurate van Leer limited remap. At the beginning of a time cycle, the following quantities are assumed known:

$$\rho^n, \epsilon^n, P^n, v^n, S_{ij,L}^n, \text{ and } S_{ij,M}^n$$

where,

ρ	cell-centered mass density
ϵ	cell-centered specific internal energy
P	cell-centered pressure
v	vertex-centered velocity
S_{ij}	cell-centered deviator stress tensor

The unrotated (material) stress field is just $S_{ij,M}^n = R_{ij}^T S_{kl,L}^n R_{ik}$ where R is the rotation tensor computed from polar decomposition of the deformation gradient into a left-hand stretch tensor and R using a rate form algorithm [4]. The superscript implies time level n , and subscripts L and M correspond to laboratory and

material frames, respectively. Also, the rotation angle θ^n is calculated from the rotation tensor. The purpose of the predictor step is to update velocity field v^n to full time step v^{n+1} . In doing so, the cell-centered quantities must be temporarily updated to half time step values (e.g. $\rho^{n+1/2}$, $\epsilon^{n+1/2}$, etc.) before updating the velocity field to time level $n+1$ (corrector step). After the predictor step, the velocity field and the cell-centered quantities can be updated to full time step values using the temporarily updated half time step quantities. Updating the cell-centered quantities to the full time step values is accomplished during the corrector step. After the Lagrangian corrector step, all cell and vertex quantities are advected from the Lagrangian grid to the Eulerian mesh. MESA recycles the normal return correction via Murphy's algorithm[8] to adjust the stress field $S_{ij,M}^{n+1}$. The reason for doing this is that the deviatoric stress state at the yield surface may have drifted off the yield surface during the advection step. The stress tensor in material frame $S_{ij,M}^{n+1}$, the rotation angle θ^{n+1} , and the stretch tensor V_{ij}^{n+1} are also advected back to Eulerian grid, but the rotation tensor R_{ij}^{n+1} is not because it is recalculated from the rotation angle. Finally, the stress field in the material frame is rotated back to the laboratory frame (e.g. $S_{ij,L}^{n+1} = R_{ij}^{n+1} S_{kl,M}^{n+1} R_{ik}^{T,n+1}$). Table I shows the sequence of calculations performed during the MESA2D Lagrangian phase corrector step, where Δt is the time step and μ is the shear modulus.

Table I

Event Sequence for Computational Anisotropy Calculations Performed during the MESA2D Lagrangian Phase Corrector Step

Quantities to be Updated / Procedure Description	Updated/Modified Quantities	Basis
ρ^n, ϵ^n, P^n	$\rho^{n+1}, \epsilon^{n+1}, P^{n+1}, \dot{\epsilon}_{ij}^{n+1/2}, \omega_{ij}^{n+1/2}, L_{ij}^{n+1/2}, \text{ and } D_{ij}^{n+1/2}$	$v^{n+1/2} = \frac{1}{2}(v^n + v^{n+1})$
$R_{ij}^n, \theta^n, V_{ij}^n$	$R_{ij}^{n+1}, \theta^{n+1}, \text{ and } V_{ij}^{n+1}$	polar decomposition theorem
deviatoric strain rate tensor in laboratory frame rotated to material frame	$d_{ij}^{n+1/2} = R_{ij}^{T,n+1} D_{kl}^{n+1/2} R_{ik}^{n+1}$	
elastic trial deviatoric stress calculation in material frame	$S_{ij}^* = S_{ij,M}^n + 2\mu\Delta t d_{ij}^{n+1/2}$	
$S_{ij,M}^n$	$S_{ij,M}^{n+1}$	plastic normal return correction via Murphy's algorithm
plastic strain-rate and strain invariant calculations	$d_{ij}^p = d_{ij}^{n+1/2} - (S_{ij,M}^{n+1} - S_{ij,M}^n) / 2\mu\Delta t$, and $e^{p,n+1} = e^{p,n} + \Delta t \left(\frac{4}{3} d_{ij}^p d_{ij}^p \right)^{1/2}$	
plastic work joint invariant calculation	$w^{p,n+1} = w^{p,n} + \Delta t (S_{ij,M}^{n+1} d_{ij}^p) / \rho^n$	
stress tensor in material frame rotated to laboratory frame	$S_{ij,L}^{n+1} = R_{ij}^{n+1} S_{kl,M}^{n+1} R_{ik}^{T,n+1}$	

4. A STRETCHING ROD PROBLEM

Plastic tensile instability (necking) is an important consideration for a variety of stretching rod deformation processes. A potential stabilization mechanism for the rod necking problem is yield anisotropy. The stability of a stretching metal rod has dependencies that include the material flow stress (σ), density (ρ), axial strain rate ($\dot{\epsilon}(t)$), rod radius ($a(t)$), and the initial distribution of geometric perturbations[9,10]. Romero[10] defines the following isotropic dimensionless stability parameter $\Gamma(t)$ based upon these parameters :

$$\Gamma(t) = \sqrt{3} \rho \dot{\epsilon}^2(t) a^2(t) / \sigma(t) \quad (4.1)$$

Perturbations are stable (no necks should develop on the rod surface) for $\Gamma(t) > 1$. As the rod is stretched, $\Gamma(t)$ decreases. For $\Gamma(t) < 1$, perturbations on the rod surface can become unstable. Note that Eq. (4.1) predicts a softer flow stress to produce a more stable rod geometry.

Our numerical investigation of rod stability consists of a comparison of isotropic and anisotropic cases for an initial geometric set of random perturbations using the quadratic yield function and MTS model indicated above. Equation (2.1) is characterized based upon the properties of a cross-rolled (transversely isotropic) HCP sheet:

$$\begin{pmatrix} \alpha_{1111} \\ \alpha_{2222} \\ \alpha_{3333} \\ \alpha_{1122} \\ \alpha_{1133} \\ \alpha_{2233} \\ \alpha_{1212} \\ \alpha_{1313} \\ \alpha_{2323} \end{pmatrix} = \begin{pmatrix} 4.782 \\ 4.757 \\ 1.999 \\ -3.770 \\ -1.012 \\ -0.987 \\ 4.402 \\ 1.840 \\ 1.966 \end{pmatrix} \quad (4.2)$$

This sheet has a maximum R value[6] (defined as the ratio of transverse plastic strain rates in a metal rod of rectangular cross-section loaded in a state of uniaxial tensile stress) of 3.82, which corresponds to a yield stress anisotropy ratio (Z/X) of 1.55, where Z is the through-thickness direction and X is in the plane of the sheet. Crystallographic texture (the preferred orientation of single-crystal grains in a polycrystalline solid) is the major source of the yield anisotropy. If the grain orientations are not random, the material tends to be anisotropic because single crystals are normally anisotropic.

The stretching rod specimen is assumed to have an initial radius and length of 2.13 mm and 8.52 mm, respectively. The Ti-6Al-4V density is 4.5 g/cm^3 . The stretching rate (strain-rate) is held constant throughout the calculation at $6.1 \times 10^4 \text{ s}^{-1}$ by imposing the appropriate accelerating velocity boundary conditions to the ends of the rod. The rod begins to produce necks as a result of the initial perturbations prescribed to the surface. A random number generator is used to create geometric perturbations along the rod surface. The amplitude of the perturbations were approximately 1/3 of the cell size dimension. The lower right insert of Fig. 1 shows the actual size and a partial magnified view of the random perturbations (length magnified by 4X and the amplitude by 20X).

The rate at which the perturbations developed into major necks along the rod's surface is evaluated by monitoring the neck growth rate as a function of time in terms of rod radii:

$$[r_{\max}(t) - r_{\min}(t)] / r_{\text{avg}}(t) \quad (4.3)$$

Both isotropic and anisotropic calculations are performed using the same set of perturbations allowing the yield surface to harden or soften according to the MTS model. In the direction of rod stretching, so-called "strong" and "weak" orientations of the yield function are used in the calculations corresponding to

assumptions of rolling and extrusion material textures, respectively. The calculated rod shapes and growth rates given by Eq. (4.3) are provided in Fig. 1. Under our set of assumptions, MESA predicts that the necks began to grow earlier and at a much faster rate for the strong anisotropic case. The weak anisotropic case shows a very stable response. The isotropic case neck growth rates are found to be bracketed by the two anisotropic cases.

Figure 1: MESA predictions of rod shapes and growth rates as a function of time for an isotropic and two anisotropic cases using the MTS material strength model and a set of random geometric perturbations.

4.1 Material Advection

Finally, we calculate the difference in the second invariant of the stress deviators predicted by MESA before and after the advection phase during each cycle for several locations within the rod. This allows us to assess the magnitude of advection adjustments on the stress state computed by the strength model within the Eulerian formulation. Fig. 2 shows the magnitude of the instantaneous (per cycle) change for a initial axial location of 0.25 cm within the rod. An axial location of 0.0 cm corresponds to the rod middle while, a location of 0.8 cm corresponds to the rod end. The initial radial position is 0.1 cm above the symmetry axis. This location is selected because a neck forms in this region as the rod stretches. Advection adjustments are more prominent in regions of larger material deformation. Fig. 2 shows that the adjustment associated with advection begins to grow at $\sim 16 \mu\text{s}$ as the neck begins to form (material compressing radially and stretching axially). The neck breaks at $\sim 28 \mu\text{s}$. Also, the calculated instantaneous adjustments are typically two orders of magnitude smaller than the material flow stress. These small advection adjustments should not have a significant impact on the calculated deformation shapes and growth rates predicted by MESA.

5. SUMMARY

Constitutive models and solution algorithms for anisotropic elastoplastic material strength have been implemented in the two-dimensional MESA Eulerian hydrodynamics code. The anisotropic constitutive modeling is posed in an unrotated material frame using the theorem of polar decomposition to describe rigid body rotation. A stretching rod problem shows the viability of applying the anisotropic elastoplastic constitutive modeling, quadratic yield function, and numerical algorithms for problems involving rigid body rotation and large plastic deformation. The MESA2D predicted rod neck growth rates and rod topologies show a strong sensitivity to the yield surface coefficients α_{ijkl} . The adjustments associated with material advection have a minimal effect on the predicted stress invariant.

Figure 2: Second invariant stress deviator difference (before and after advection) for material location $r=0.1$ cm; $z=0.25$ cm. This calculation assumes the "strong" direction along the rod axis.

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