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Strain-rate effects on the texture evolution of low-symmetry metals: Modeling and validation using the Taylor cylinder impact test

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Abstract. In this paper, a model for describing the influence of evolving texture on the response of pre-textured metals for dynamic loading conditions is proposed. Yielding is described using a recently developed criterion which captures simultaneously anisotropy and compression-tension asymmetry associated with deformation twinning. The anisotropy coefficients as well as the size of the elastic domain are considered to be functions of the accumulated plastic strain. The specific expressions for the evolution laws are determined based on experimental data and numerical test results performed with a self-consistent viscoplastic model together with a macroscopic scale interpolation technique. An overstress approach is used to incorporate rate effects in the formulation. Application of the model to the description of the high-strain rate response of low-symmetry (clock-rolled hexagonal-closed-packed zirconium) is presented. The very good agreement between the simulated and experimental post-test geometries of the Taylor impact specimens in terms of major and minor side profiles and impact-interface footprints shows the ability of the model to describe the evolution of anisotropy as a function of the strain rate.

1. INTRODUCTION

Development of theoretical and simulation capabilities for modeling the high-strain rate stress strain response of pre-textured hexagonal closed-packed (hcp) is essential for a variety of applications ranging from analysis of crash-worthiness and foreign-object damage in aerospace systems, ballistic and armor applications, high-rate forming and high-rate machining, etc. Historically, in order to keep the analyses tractable, only a minimal description of the material behavior was included by simplifying the material characterization down to just a few parameters. However, systematic experimental studies have shown that structure evolution in these materials is significantly altered by changes in strain rate and temperature as well as alloy and interstitial content and texture (e.g. [1]). While under quasi-static and dynamic loading conditions hcp materials may deform by slip and twinning, as the strain rate increases or temperature decreases the propensity of twinning becomes higher. Recent efforts in development of computational models for describing temperature and strain-rate effects on the inelastic response of pretextured metals have given risen to robust predictive methods for simulating the anisotropic high-strain rate behavior of body-centered metals. Maudlin and co-workers employed an anisotropic representation of the yield surface obtained by tessellation from polycrystal calculations using Los Alamos polycrystal plasticity (Lapp) code for modeling a pre-textured rolled body-cubic-centered tantalum [2]. Anand and collaborators have developed finite-element polycrystal models for describing the high-strain rate and large deformation behavior of face-and body-centered-cubic polycrystals. The models describe qualitatively well the important geometry changes in Taylor-impact specimens of textured tantalum (see for example [3]).

In contrast, modeling the behavior of hcp materials is less advanced. This is due to the difficulties associated with description of twinning and its effects on the mechanical response. Indeed, since

twinning activity is accompanied by grain reorientation and highly directional grain interactions, the influence of the texture evolution on hardening of hcp materials cannot be neglected even for the simplest monotonic loading paths. To describe with accuracy the evolution of anisotropy and how it is affected by variations in temperature or strain rate it is imperative to account for the most important sources of anisotropy in the given material: slip and/or twinning activity, substructure evolution at grain level, and texture development during deformation. Since in crystal plasticity models, the distribution of crystal orientations in the given polycrystal, the available slip/twinning deformation systems and the stress levels necessary to activate them are taken into account explicitly, the evolution of anisotropy due to texture development can be characterized by measuring the initial texture and calculating the grain reorientation (i.e. updating the texture) using a suitable homogenization scheme (e.g. a Taylor model or a self-consistent model). Recently, the application of crystal plasticity models to hcp metals and the incorporation of crystal plasticity calculations directly into finite element (FE) analyses has received much attention. For example, a self-consistent visco-plastic model (VPSC) linked to the explicit FE code EPIC has been successfully used to describe the quasi-static deformation of pre-textured pure zirconium subjected to quasi-static monotonic loading at room and liquid nitrogen temperatures (see [4]). In this model, twinning contribution to texture development is incorporated through the Predominant Twin Reorientation (PTR) scheme, which essentially consists in determining the grains where twinning is most active and reorienting them completely into the orientation of their most active twinning system, accounting in this way for the volumetric effect of twinning reorientation on texture development and at the same time maintaining fixed the number of orientations that represent the polycrystal, (see for details the review paper by Tome and Lebensohn, [5]).

An alternative approach is to develop anisotropic formulations at the macroscopic level. The major difficulty in developing analytic expressions for the plastic potential of hcp materials is related to the description of the tension/compression asymmetry associated to twinning. Recently, three-dimensional yield functions which capture both anisotropy and strength differential effects have been proposed (e.g. [6]-[7]). In particular, it was shown that Cazacu et al. [7] yield criterion (further denoted as CPB05) can describe with accuracy the shape of the yield loci corresponding to individual fixed levels of accumulated plastic strain.

In this paper, we propose a macroscopic anisotropic elastic/viscoplastic model for describing the high-strain rate mechanical response of hcp textured metals. Yielding is described using the CPB05 yield criterion. The evolution laws for the anisotropy coefficients involved in the expression of this criterion and for the strength differential parameter are obtained using numerical test results performed with the VPSC model. Since this polycrystalline model incorporates explicitly the evolution of texture, we can thus obtain information concerning the deformation-induced anisotropy. An overstress approach is used to incorporate strain rate effects in the formulation. We then apply the model to the description of the high-strain rate behavior of high-purity pre-textured zirconium. The very good agreement between the simulated and experimental post-test geometries in terms of major and minor side profiles and impact-interface footprints shows the ability of the model to describe the influence of twinning on texture evolution.

2. CONSTITUTIVE MODEL

The objective is to develop a macroscopic anisotropic elastic/viscoplastic model that describes simultaneously the influence of strain rate and evolving texture on the inelastic response of textured metals. The basic assumption is that the viscous properties of materials become manifest only after the passage to the plastic state. Thus, the strain rate $\dot{\epsilon}$ can be decomposed additively into an elastic $\dot{\epsilon}_{\rm E}$ and a viscoplastic part, $\dot{\epsilon}_{\rm vp}$, i.e.

$$\dot{\varepsilon} = \dot{\varepsilon}_E + \dot{\varepsilon}_{vp} \tag{1}$$

EURODYMAT 2006

The evolution of the viscoplastic strain rate is considered to be given by an overstress type law of the form:

$$\dot{\varepsilon}_{vp} = \gamma \langle \phi(f) \rangle \frac{\partial g}{\partial \sigma},$$

$$\langle \phi(f) \rangle = \begin{cases} 0 & \text{for } f \leq 0, \\ f^m & \text{for } f > 0. \end{cases}$$
(2)

In Eq. (2) f is the quasi-static yield function, g is the quasi-static plastic potential, γ a viscosity parameter while *m* is a strain rate sensitivity constant. The quasi-static yield function is the CPB05 yield function (see [7]):

$$f(\sigma, \bar{\varepsilon}_{\rm vp}) = \frac{\bar{\sigma}(\sigma, \bar{\varepsilon}_{\rm vp})}{Y(\bar{\varepsilon}_{\rm vp})} - 1$$
(3)

where $Y = Y(\bar{\varepsilon}_{vp}, T)$ is the hardening function which is considered to be a function of the accumulated viscoplastic strain $\bar{\varepsilon}_{vp}$ and possibly of temperature, T, while $\bar{\sigma}$ is the equivalent stress associated to the CPB05 yield criterion (see [7]). Specifically,

$$\bar{\sigma} = \mathbf{B}[(|\Sigma_1| - k \cdot \Sigma_1)^a + (|\Sigma_2| - k \cdot \Sigma_2)^a + (|\Sigma_3| - k \cdot \Sigma_3)^a]^{\frac{1}{a}}$$
(4)

where B is a constant defined such that $\bar{\sigma}$ reduces to the tensile yield stress in the rolling direction, i.e.

$$B = \left[\frac{1}{\left(|\Phi_1| - k\Phi_1\right)^a + \left(|\Phi_2| - k\Phi_2\right)^a + \left(|\Phi_3| - k\Phi_3\right)^a}\right]^{\frac{1}{a}}$$
(5)

and

$$\Phi_1 = \left(\frac{2}{3}L_{11} - \frac{1}{3}L_{12} - \frac{1}{3}L_{13}\right), \qquad \Phi_2 = \left(\frac{2}{3}L_{12} - \frac{1}{3}L_{22} - \frac{1}{3}L_{23}\right), \qquad \Phi_3 = \left(\frac{2}{3}L_{13} - \frac{1}{3}L_{23} - \frac{1}{3}L_{33}\right).$$

In Eq. (4), $\Sigma_1, \Sigma_2, \Sigma_3$ are the principal values of the tensor $\Sigma = \mathbf{L} : \mathbf{S}$, where \mathbf{L} is a fourth-order orthotropic tensor which reflects the plastic anisotropy of the material and \mathbf{S} is the deviator of the Cauchy stress tensor; k is a strength differential parameter, and a is a homogeneity constant. Note that for the case of a = 2, k = 0, and \mathbf{L} the fourth-order identity tensor, CPB05 reduces to the Von Mises criterion while B reduces to $\sqrt{3/2}$ which is the constant associated with the von Mises effective stress. The evolution of anisotropy due to evolving texture is accounted for by means of a multi-scale procedure, which essentially consists in using polycrystalline calculations and macroscopic scale interpolation techniques. Specifically, using the VPSC code, the polycrystal is prestrained up to a given deformation level $\bar{\epsilon}_{vp}^j$ along a given deformation path. Then, to quantify the deformation induced anisotropy, it is further used to determine the coefficients $\mathbf{L}(\bar{\epsilon}_{vp}^j), k(\bar{\epsilon}_{vp}^j), a(\bar{\epsilon}_{vp}^j)$ involved in the macroscopic CPB05 yield criterion and thus determine the macroscopic yield surface corresponding to the texture for the given level of prestrain by calculating $\bar{\sigma}^j$ according to Eq.(4) as well as $\mathbf{Y}^j = \mathbf{Y}(\bar{\epsilon}_{vp}^j)$. This procedure is repeated for a finite set of prestrain levels, say $\bar{\epsilon}_{vp}^1 < \bar{\epsilon}_{vp}^2 < \ldots < \bar{\epsilon}_{vp}^n$, $j = 1 \ldots n$. Further, an interpolation procedure is used to obtain the macroscopic yield surfaces corresponding to any prestrain level (see [8]), i.e.:

$$\bar{\sigma}(\boldsymbol{\sigma}, \bar{\epsilon}_{\rm vp}) = \zeta(\bar{\epsilon}_{\rm vp})\bar{\sigma}^{\rm j} + \left[1 - \zeta(\bar{\epsilon}_{\rm vp})\right]\bar{\sigma}^{\rm j+1} \tag{6}$$

$$Y(\bar{\varepsilon}_{vp}, T) = \xi(\bar{\varepsilon}_{vp}) \cdot Y^{j} + (1 - \xi(\bar{\varepsilon}_{vp})) \cdot Y^{j+1}$$
(7)

for any $\bar{\varepsilon}_{vp}^{j} \leq \bar{\varepsilon}_{vp} \leq \bar{\varepsilon}_{vp}^{j+1}$, $j = 1 \dots$ m-1. For linear interpolation, the weighting parameter $\zeta(\bar{\varepsilon}_{vp})$ appearing in Eqs. (6) is defined as

$$\xi(\bar{\epsilon}_{\rm vp}) = \frac{\bar{\epsilon}_{\rm vp}^{\rm j+1} - \bar{\epsilon}_{\rm vp}}{\bar{\epsilon}_{\rm vp}^{\rm j+1} - \bar{\epsilon}_{\rm vp}^{\rm j}} \tag{8}$$

3. APPLICATION TO MODELING THE DYNAMIC BEHAVIOR OF ZIRCONIUM

Results of uniaxial compression tests on a high-purity zirconium plate were reported in [1], [4] and [8]. This hcp material is highly anisotropic both at the single crystal and polycrystal level. It was processed through a series of clock-rolling and annealing cycles to produce a plate with strong basal texture (<c> -axes of the hcp crystals predominantly oriented along the plate normal direction). The process of multiple rolling passes with rotation was used in order to obtain a nearly isotropic in-plane texture. In order to characterize the anisotropy induced by texture evolution, a material should be subjected to loading in a given direction up to a predetermined level of accumulated deformation. Then, tests specimens should be cut from the pre-strained sheet and further tension and compression tests performed to quantify the anisotropy induced by the deformation. However, this will require a large number of mechanical tests which are very difficult to carry out because at large compressive pre-straining levels buckling of the sheets is very likely. Alternatively, for a given strain path, the evolution of the yield surface can be studied by performing numerical tests using the VPSC model. For the clock-rolled plate of zirconium described previously, the VPSC code was first used to characterize the evolution of the yield surface during IPC (uniaxial compression along the in-plane x direction). For this purpose, the polycrystal was prestrained up to a given deformation level. Then, to quantify the deformation induced anisotropy, it was further probed along various testing directions to describe the yield surface corresponding to the texture for the given level of prestrain. Next, for each individual prestraining level, say $\bar{\varepsilon}_p^l$, using the VPSC yield stresses, we determined the coefficients $L(\bar{\varepsilon}_{vp}^l), k(\bar{\varepsilon}_{vp}^l), a(\bar{\varepsilon}_{vp}^l)$ involved in the CPB05 by calculating $\bar{\sigma}^j$ according to Eq.(4) as well as $Y^j = Y(\bar{\varepsilon}^j_{vp})$. Further, a linear interpolation procedure was used to obtain the macroscopic yield surfaces corresponding to any prestrain level (see Eq. (6-7)). In addition to the yield surface evolution due to plastic deformation, the viscosity coefficient γ and the strain rate sensitivity parameter m (see Eq. (2)) need to be determined. Results of dynamic tests at strain rates from 1000/s to 3500/s conducted using a Split-Hopkinson Pressure Bar (SHPB) were reported [1]. Based on these test results, we determined that: $\gamma = 2500s^{-1}$ and m = 7.0 (see Fig. 1). The constitutive behavior for the in-plane compression corresponding to strains beyond the range of the experimental data was estimated based on polycrystalline calculations.

To measure high-rate mechanical response of materials, controlled impact tests are carried out. Such tests provide data in the 10^4 - 10^5 /s strain rate regime directly above that accessible via Hopkinson Bar techniques and below shock experimentation. One standard approach used is the impact of a right circular cylinder on either a massive anvil (rigid plate) or a receptor rod of identical material. This experiment is commonly called a Taylor impact test after G.I. Taylor, who designed it. Due to the impact, the rod plastically deforms and shortens causing the material at the impact surface to flow radially outward relative to the rod axis.

Maudlin et al. [8] reported results of Taylor cylinder impact tests using IP specimens cut from the same zirconium plate described in the previous section (i.e. cylindrical axes were coincident with inplane directions (either x or y)). The specimens were 50.8 mm in length and have a length over diameter ratio of 6.67. The anvil was AF1410 steel, heat treated to a surface hardness of Rc 58 and lapped to a mirror finish. The cylinders were fired using a gas-driven gun at various velocities: 50, 101, 170, and 243 m/s. Only post-test data for the 243 m/s impact velocity were reported. As discussed in Maudlin et al. [9], the data set consists of high-resolution scans of the photographed footprint i.e. the cross-sectional area at the impact interface (i.e the y-z plane) and of the photographed side profiles for the

EURODYMAT 2006



Figure 1. In-plane compression simulation results using the proposed elastic/viscoplastic model (solid lines) for various strain rates in comparison with experimental data (symbols). Data after [1].

major and minor dimensions. From the analysis of the digitized side profiles, axial strain profiles (log strain) as a function of axial position *z*, measured relative to the impact interface, were obtained.

In order to simulate Taylor impact testing of zirconium, the proposed elastic/viscoplastic model was implemented into the explicit finite element code EPIC [10] as a user material subroutine. The zirconium cylinder was modeled using 8208 single integration point tetrahedral elements with free boundary conditions. The anvil target was modeled as an analytical rigid surface. Simulations were done for the impact velocity of 243 m/s. Calculations were performed for 90 μ s, at which time the specimen had rebound off of the target, and all plastic deformation had ceased. Figure 2 depicts a visual comparison between the simulated and experimental major and minor profiles and footprint of the post-test specimen.



Figure 2. Comparison of the simulated and experimental cross-sections of the post-test zirconium Taylor impact experiment for (a) the major profile, (b) the footprint, and (c) the minor profile. Data after [8].

JOURNAL DE PHYSIQUE IV

4. CONCLUSIONS

A macroscopic anisotropic elastic/viscoplastic model that captures the influence of evolving texture on the mechanical response of pretextured- metals was proposed. Initial yielding was described using a recently developed anisotropic yield function proposed by Cazacu et al. [7]. This yield function can capture simultaneously both anisotropy and tension/compression asymmetry. The anisotropy coefficients as well as the size of the elastic domain were considered to be functions of the accumulated plastic strain. The specific expressions for the evolution laws were determined using a multi-scale methodology i.e. experimental measurements of the crystallographic texture, polycrystalline calculations, and macroscopic scale interpolation techniques. An overstress approach was used to incorporate rate effects in the formulation. The proposed model was applied to the description of the high-strain rate response of low-symmetry (clock-rolled hexagonal-closed-packed zirconium) pretextured metals. The very good agreement between the simulated and experimental post-test geometries of the Taylor impact zirconium specimens in terms of major and minor side profiles and impact-interface footprints shows the ability of the model to describe the evolution of anisotropy in the zirconium specimen.

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