Prediction of the torsional response of HCP metals

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Abstract. One of the greatest challenges that a researcher in the field of the theory of plasticity is facing is that it has to establish general mathematical relations between the stresses and strains that should be applicable to any loading, although the experimental information available is generally restricted to uniaxial tension and/or compression tests. In particular, it has been long recognized that classic yield criteria cannot accurately capture the torsional response of hcp metals. In this paper, it is shown that Cazacu et al. [1] orthotropic yield criterion, identified based on uniaxial tests, captures the unusual characteristics of the torsional response of hcp AZ31 Mg. Furthermore, for the first time, on the basis of the same criterion, it is predicted the shape of the yield surface of this material for combined tension-torsion and combined compression-torsion loadings. Most importantly, it is shown that from the analysis of the stress-strain responses in a few very simple mechanical tests, using this criterion one can predict whether axial strains develop in torsion.

1. Introduction
The basic assumption of the mathematical theory of plasticity is that there exists a continuous scalar yield function $f(\sigma', \zeta)$, where $\sigma'$ denotes the Cauchy stress deviator and $\zeta$ the set of internal variables that defines the onset of plastic deformation. However, in most cases the experimental information available to derive this 5-D yield surface $f(\sigma', \zeta) = 0$ is limited to simple uniaxial tests.

Another task of the researchers in this field is to recommend and design experiments or numerical tests to verify the mathematical formulations developed, and further demonstrate their validity for combined loadings. In particular, it has been long recognized that classic yield criteria such as von Mises or Hill cannot capture with accuracy the torsional response and combined tension-torsion or compression-torsion loadings of hexagonal closed packed (hcp) materials.

In this paper, it is shown that Cazacu et al. [1] criterion in conjunction with distortional hardening is able to capture the particularities of the plastic deformation of AZ31 Mg. Although the identification of the parameters is done on the basis of uniaxial tests, it is shown that this model captures the unusual features of the plastic response for loadings that were not used for calibration. Moreover, this model allows prediction of the evolution of the yield surfaces for combined tension-torsion loadings. Analysis of these surfaces enables the explanation of the very specific features of the torsional response of AZ31 Mg.
2. Constitutive modelling for hcp metals

We begin with a brief presentation of the elastic-plastic model with yielding according to Cazacu et al. [1] orthotropic criterion. The total rate of deformation \( \mathbf{d} \) is considered to be the sum of an elastic part and a plastic part \( \mathbf{d}^p \). The elastic stress-strain relationship is given by

\[
\dot{\mathbf{\sigma}} = \mathbf{C}^e \cdot (\mathbf{d} - \mathbf{d}^p)
\]

where \( \mathbf{\sigma} \) is an objective rate of the Cauchy stress tensor \( \mathbf{\sigma}^e \), \( \mathbf{C}^e \) is the fourth-order stiffness tensor while “;” denotes the doubled contracted product between the two tensors. In Eq. (1), \( \mathbf{C}^e \) is the fourth-order stiffness tensor. With respect to any Cartesian coordinate system, it is expressed as,

\[
\mathbf{C}_{ijkl} = 2G \delta_{ik} \delta_{jl} - \left( K - \frac{2}{3}G \right) \delta_{ij} \delta_{kl}
\]

with \( i, j, k, l = 1…3 \), \( \delta_{ij} \) being the Kronecker unit delta tensor while \( G \) and \( K \) are the shear and bulk moduli, respectively. The key features of Cazacu et al. [1] yield criterion is that it accounts for both orthotropy and strength differential effects that are observed in hcp metals. Indeed, the equivalent stress, \( \mathbf{\sigma}^e \), is:

\[
\mathbf{\sigma}^e = m \sqrt{ (|\Sigma_1|-k \cdot \Sigma_1)^2 + (|\Sigma_2|-k \cdot \Sigma_2)^2 + (|\Sigma_3|-k \cdot \Sigma_3)^2 } 
\]

where \( \Sigma_1, \Sigma_2, \Sigma_3 \) are the principal values of the transformed stress tensor \( \mathbf{\Sigma} \) defined as:

\[
\mathbf{\Sigma} = \mathbf{L} \cdot \mathbf{\sigma}'
\]

where \( \mathbf{\sigma}' \) is the deviator of the Cauchy stress tensor. In the above equation, \( \mathbf{L} \) is a fourth-order symmetric tensor that describes the plastic anisotropy of the material. Modelling plastic anisotropy by means of a 4th order symmetric and orthotropic tensor ensures that the material's response is invariant under any orthogonal transformation belonging to the symmetry group of the material. Furthermore, the minimum number of independent anisotropy parameters that is needed such as to satisfy these symmetry requirements is introduced here. For example, for an orthotropic material, in the coordinate system associated with the material symmetry axes (\( x, y, z \)) and in Voigt notations the tensor \( \mathbf{L} \) is represented by a 6x6 matrix given by:

\[
\mathbf{L} =
\begin{bmatrix}
L_{11} & L_{12} & L_{13} & 0 & 0 & 0 \\
L_{12} & L_{22} & L_{23} & 0 & 0 & 0 \\
L_{13} & L_{23} & L_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & L_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & L_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & L_{66}
\end{bmatrix}
\]

In Eq. (3), \( k \) is a material parameter describing strength-differential effects while \( m \) is a constant defined such that the equivalent stress, \( \mathbf{\sigma}^e \), reduces to the tensile flow stress along \( x \) (or RD) direction. Thus, \( m \) is expressed in terms of the anisotropy coefficients \( L_{ij} \), with \( i, j = 1…3 \) and the material parameter \( k \) as follows:

\[
m = 1/ \sqrt{ (|\Phi_1|-k \Phi_1)^2 + (|\Phi_2|-k \Phi_2)^2 + (|\Phi_3|-k \Phi_3)^2 } 
\]

where \( \Phi_1 = (2L_{11} - L_{12} - L_{13})/3 \), \( \Phi_2 = (2L_{12} - L_{22} - L_{23})/3 \), \( \Phi_3 = (2L_{13} - L_{23} - L_{33})/3 \). Note that for isotropic materials ( i.e. \( \mathbf{L} = \mathbf{I} \), the 4th order symmetric identity tensor ) for which the material parameter \( k = 0 \) (i.e. no tension-compression asymmetry), \( m = \sqrt{3}/2 \), so the equivalent stress \( \mathbf{\sigma}^e \) according to Cazacu et al. [1] criterion reduces to the Von Mises equivalent stress.
The evolution of the plastic strain is given by an associated flow rule. Hardening is considered to be isotropic, with the plastic potential, $F$, of the form:

$$F(\sigma, \bar{\varepsilon}^p) = \bar{\sigma}(\sigma, \bar{\varepsilon}^p) - Y(\bar{\varepsilon}^p),$$

(7)

where $\bar{\varepsilon}^p$ is the equivalent plastic strain, associated to $\bar{\sigma}$ given by Eq. (3) using the work-equivalence principle, and

$$Y(\bar{\varepsilon}^p) = A_0 - A_1 \exp\left(-A_2 \bar{\varepsilon}^p\right),$$

(8)

where $A_0$, $A_1$, $A_2$ are constants. For AZ31 Mg the detailed procedure for identification of the parameters of the model given by Eqs.(1)-(8) from data in uniaxial tests is given in ref. [2]. To make this paper self-consistent, the calibration procedure and comparison with uniaxial tests data is presented very briefly in the following. Next, the predictions of the cross-sections of the Cazacu et al. [1] yield surface for combined tension-torsion and compression-torsion loadings are presented, along with the analysis and interpretation of the model predictions for free-end torsion. Irrespective of loadings, the respective boundary-value problem is solved numerically using an user material routine (UMAT) routine that was developed for the anisotropic elastic-plastic model given by Eqs. (1)-(8) and implemented in the F.E. code Abaqus. A fully implicit integration algorithm was used for solving the governing equations (for more details, see [2]). The usual definitions of the axial and shear strains will be used in the present paper, namely:

$$\varepsilon = \ln\left(1 + \frac{u}{L_0}\right)$$

and

$$\gamma = \frac{\Phi r}{L_0},$$

(9)

where $r$ is the current radius, $L_0$ is the initial length, $u$ is the axial displacement, and $\Phi$ is the twist angle.

3. Model calibration for AZ31-Mg alloy using uniaxial tests

Data concerning the mechanical behavior of a strongly textured AZ31 Mg alloy sheet in quasi-static tension and compression were reported by Khan et al. [3]. Results of the tests on specimens cut along several in-plane directions, namely in the rolling direction (RD) and at 45° and 90° from the rolling direction (i.e. in the transverse (TD) direction) and in the through-thickness direction of the sheet have shown that the material is orthotropic. Irrespective of the in-plane orientation the material displays very pronounced differences between uniaxial tension and uniaxial compression both in yielding and strain-hardening behavior. The compression stress-strain curves exhibit a concave-up shape and steadily increasing hardening rate while the tensile curves have the standard concave-down appearance. In the through-thickness direction (ND), only results in uniaxial compression were reported. Based on the experimental data in uniaxial tension and compression, the anisotropy coefficients and the parameter $k$ involved in the orthotropic form of the Cazacu et al. [1] yield criterion (see Eq.(3)-(6)) and their evolution with $\bar{\varepsilon}^p$ were determined. The numerical values of these parameters corresponding to five individual levels of equivalent plastic strain are listed in [2]. The parameters involved in the Voce-type isotropic hardening law (Eq. (8)) were estimated from the axial stress vs. true strain curve in uniaxial tension in the rolling (RD or $x$ direction): $A_0 = 315.4$ MPa, $A_1 = 140.6$ MPa, $A_2 = 16.3$. The values for the Young modulus and Poisson coefficient were taken as: $E=45$ GPa and $\nu=0.3$, respectively. Comparison between experimental and predicted stress-strain response is shown in Fig. 1 (a)-(c). It is worth noting that the model describes remarkably well the particularities of the plastic behaviour of Mg AZ31 alloy, specifically the S-shape of the experimental stress-strain curve in uniaxial compression along RD and TD directions. Note also that the model predicts that in uniaxial tension in the ND direction, the stress-strain curve should have a S-shape. In Fig. 1(d) is represented in the plane $(\sigma_{xx}, \sigma_{yy})$ ($x$ being the rolling direction (RD) while $y$ the transverse direction (TD)) the theoretical yield surfaces for the orthotropic Mg AZ31 alloy according to the criterion (Eq.
3) for different strain levels of $\varepsilon_p$, (up to 10%). It is worth noting that at initial yielding, and under 8% strain, the tension-compression asymmetry is very pronounced (compare the tension-tension and compression-compression quadrants) and the surfaces have triangular shape, at 8% strain and beyond the surfaces have an elliptical shape, and the difference in response between tension and compression becomes small.

![Stress-strain response](image)

Figure 1: Stress-strain response in uniaxial tension and compression for an Mg AZ31 alloy in RD (a), TD (b), and ND (c) directions; (d) Theoretical yield surfaces in the $(\sigma_{xx}, \sigma_{yy})$ plane. The symbols represent the experimental data from [3] and the dashed lines the predictions based on the orthotropic yield criterion of Cazacu et al. [1] and isotropic hardening law (after Ref. [2]).

4. Model predictions for combined shear-normal stress loadings and free-end torsion

Although data are not available, it is worth examining the projection of the yield surface in the shear-normal stress planes, i.e. $(\sigma_{xx}, \sigma_{xy})$, $(\sigma_{xx}, \sigma_{xz})$, $(\sigma_{zz}, \sigma_{xz})$, and $(\sigma_{zz}, \sigma_{yz})$ plane (see Fig. 2).
Figure 2 Projection of the yield surfaces according to the orthotropic yield criterion of Cazacu et al. [1] for AZ31 Mg alloy for different levels of accumulated plastic strain: (a) \((\sigma_{xx}, \sigma_{xy})\) plane; (b) \((\sigma_{xx}, \sigma_{xz})\) plane, (c) \((\sigma_{zz}, \sigma_{xz})\), (d) \((\sigma_{zz}, \sigma_{yz})\).

It can be seen that due to the tension-compression asymmetry of the material along RD (uniaxial yield in tension greater than that in compression), the normal to the \((\sigma_{xx}, \sigma_{xy})\) and \((\sigma_{xx}, \sigma_{xz})\) surfaces for states corresponding to pure shear loading (i.e. \(\sigma_{xx} = 0\)) is pointed such that the axial strain is negative. Therefore, according to the criterion for torsion of a specimen with the long axis along RD shortening (negative axial strain) of a specimen will occur. On the other hand, because in the ND direction the material has the uniaxial yield in tension smaller than that in compression, the predicted shape of the yield locus in the \((\sigma_{zz}, \sigma_{xz})\) and \((\sigma_{zz}, \sigma_{yz})\) are such that for pure shear loading (i.e. \(\sigma_{zz} = 0\)) the respective normal is pointed such that the axial strain is positive. This means that under torsion along ND, lengthening of the specimen will occur.

F.E. simulations of free-end torsion for this AZ31 Mg using the model (Fig. 3) show these unusual features of the torsion response, namely that axial strains occur (see also [2]). On the same figure are also plotted the data obtained by Guo et al [4]. Note also that irrespective of the twist direction, the model predictions are in excellent agreement with the experimental observations. In particular, the calculated initial slopes of the two predicted curves, which is a physical parameter that depends on texture evolution, are almost in perfect agreement with the experimental slopes.
Figure 3  Variation of the axial strain with the shear strain during free-end torsion along RD and ND directions for a AZ31 Mg alloy according to Cazacu et al. [1] criterion and data [4] (after Ref.[2]).

The model correctly reproduces the switch of the sign of the axial strain with the change in the loading direction of the torsion specimen (results consistent with the shape of the yield loci in Fig. 2). Furthermore, the sign of the axial strains (also called Swift phenomenon ([5])) is correlated to the tension-compression asymmetry of the material in the direction about which the specimen is twisted. Indeed, in the RD direction, for which the flow stress is higher in uniaxial tension than in compression, shortening of the specimen is observed. On the other hand, in the ND direction, for which the model predicts that the flow stress is higher in compression than in tension (see Fig. 1(d)), lengthening of the specimen occurs, in agreement with the experimental results in torsion reported in [4]. Thus, the sign of the axial strain that develops (elongation or contraction) under free-end torsion of AZ31-Mg depends on the ratio between uniaxial tension and compression in the given orientation.

5. Conclusions
In this paper, it was shown that Cazacu et al. [1] orthotropic yield criterion, identified based on uniaxial tests, captures the unusual characteristics of the torsional response of AZ31 Mg. Furthermore, for the first time, on the basis of the same criterion, it was predicted the shape of the yield surface of this material for combined tension-torsion and combined compression-torsion loadings; the occurrence of axial strains under free-end torsion was correlated with the direction of the normal to the respective yield surfaces for pure shear. Therefore, it can be concluded that by analysing stress-strain responses in a few very simple mechanical tests, using this criterion one can predict whether axial strains develop in torsion.

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