Identification methodology and comparison of phenomenological ductile damage models via hybrid numerical–experimental analysis of fracture experiments conducted on a zirconium alloy

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1. Introduction

Understanding and modeling of ductile damage mechanisms remains a major issue for many industrial forming processes. The ability of numerical modeling to predict ductile fracture is indeed crucial. However, this modeling is limited because of the complexity to take into account the influence of complex loading paths (multi-axial and non-monotonic, non-proportional, shear effects, etc.) on material ductility. The ductility is understood as an intrinsic ability of materials to undergo a certain amount of plastic deformation without fracture (or without crack formation). The fracture of ductile material occurs after microvoids or shear bands develop in the metal matrix, around the inclusions or other discontinuities such as grain boundaries. The damage occurring under large plastic strain is called ductile damage (in comparison with brittle damage), and is frequently observed in metal forming failure. Microscopically, damage is associated with voids nucleation, growth and coalescence in high and moderate stress triaxiality or shear band formation in low stress triaxiality. Macroscopically, damage is represented as the progressive degradation of material, which exhibits a decrease in material stiffness and strength. The role of microvoids in ductile failure was firstly modeled by the study of McClintock (McClintock et al., 1966), which analyzed the evolution of an isolated cylindrical void in a ductile elastoplastic matrix. Rice and Tracey (Rice and Tracey, 1969) studied the evolution of spherical voids in an elastic-perfectly plastic matrix. In these studies, the interaction between microvoids, the coalescence process and the hardening effects were neglected and failure was assumed to occur when the cavity radius would reach a critical value specific for each material. These results showed that the voids growth is governed by the stress triaxiality. Gurson (Gurson, 1977), in an upper bound analysis of a finite sphere containing an isolated spherical void in a rigid perfectly plastic matrix, employed the void volume fraction f (or porosity) as an internal variable to represent damage and its softening effect on material strength. This model was then improved to account for different aspects: prediction accuracy (Tvergaard, 1981), void nucleation (Chu and Needleman, 1980), void coalescence (Needleman and Tvergaard, 1984; Tvergaard and Needleman, 1984), void shape effect (e.g. Gologanu et al., 1993; Pardoen and Hutchinson, 2000), void size effect (e.g. Wen et al., 2005), void/particle interaction (e.g. Sirugu et Leblond, 2002-7683/ - see front matter © 2013 Elsevier Ltd. All rights reserved.
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_1, D_2$</td>
<td>material constants in the Bai and Wierzbicki model</td>
</tr>
<tr>
<td>$E, \nu$</td>
<td>Young's modulus and Poisson's ratio</td>
</tr>
<tr>
<td>$E_M, \sigma_M$</td>
<td>Young's modulus and flow stress of undamaged material</td>
</tr>
<tr>
<td>$K, \epsilon_0, n$</td>
<td>material constants in the Swift hardening law</td>
</tr>
<tr>
<td>$N_f$</td>
<td>energy density release rate and weakening function (Lemaitre model)</td>
</tr>
<tr>
<td>$Y, W(D)$</td>
<td>equivalent plastic strain rate</td>
</tr>
<tr>
<td>$\alpha_1, \alpha_2$</td>
<td>additional material constants in the proposed enhanced Lemaitre model</td>
</tr>
<tr>
<td>$\bar{\sigma}$, $\bar{\tau}$</td>
<td>equivalent plastic strain rate</td>
</tr>
<tr>
<td>$\eta, \eta_{ini}, \eta_{av}$</td>
<td>stress triaxiality, initial and average stress triaxialities</td>
</tr>
<tr>
<td>$\mu, \mu_f$</td>
<td>Coulomb and Tresca friction coefficients</td>
</tr>
<tr>
<td>$\bar{\sigma}_p$, $\bar{\tau}_p$</td>
<td>equivalent plastic strain at fracture</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>von Mises equivalent stress</td>
</tr>
<tr>
<td>$\sigma_f$</td>
<td>von Mises equivalent stress at fracture</td>
</tr>
<tr>
<td>$\sigma_1, \sigma_2, \sigma_3$</td>
<td>3 principal stresses, $\sigma_1 \geq \sigma_2 \geq \sigma_3$</td>
</tr>
<tr>
<td>$\sigma_m$</td>
<td>mean or hydrostatic stress, $\sigma_m = (\sigma_1 + \sigma_2 + \sigma_3)/3$</td>
</tr>
<tr>
<td>$\sigma_n, \tau$</td>
<td>normal and shear stresses in Mohr–Coulomb failure criterion</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Lode angle, Lode parameter and average Lode parameter</td>
</tr>
<tr>
<td>$c_1, c_2$</td>
<td>material constants in the Modified Mohr–Coulomb model</td>
</tr>
<tr>
<td>$f, F_x, F_D$</td>
<td>plastic potential (yield function in associative flow), nonlinear kinematic hardening dissipative potential, damage dissipative potential</td>
</tr>
<tr>
<td>$p$</td>
<td>hydrostatic pressure</td>
</tr>
<tr>
<td>$s, S, D_1, h, \epsilon_D$</td>
<td>material constants in the Lemaitre model</td>
</tr>
</tbody>
</table>

2004), isotropic strain hardening (e.g. Leblond et al., 1995), kinematic hardening (e.g. Leblond et al., 1995; Muhllich and Brooks, 2003), plastic anisotropy (e.g. Benzerga and Besson, 2001; Benzerga et al., 2004), rate dependency (e.g. Tvergaard, 1989), shear effect (e.g. Nahshon and Hutchinson, 2008; Xue, 2008).

On the other hand, the Continuum Damage Mechanics (CDM) models have been developed within a consistent thermodynamic framework, in which the evolution of the phenomenological damage parameter is obtained through a thermodynamic dissipation potential. Starting from the early work of Kachanov (1958), this class of models has been continuously developed (Lemaitre, 1986; Lemaitre and Desmorat, 2005; Wang, 1992) and widely used (see Besson, 2010 for a complete review of continuum models of ductile fracture).

In addition to the phenomenological CDM models and micro-mechanical based damage models, uncoupled phenomenological models have been increasingly developed, especially for industrial applications. The uncoupled models employ an indicator variable to predict material failure when its critical value is reached. This variable is often taken as a weighted cumulative plastic strain, in which the weighting function accounts for the effect of stress state on the fracture initiation.

Another track to constitute a damage model can be based on the combination of different physically based criteria: a nucleation law (e.g. Gaussian function Chu and Needleman, 1980, exponential function Maire et al., 2008) combined with a void growth criterion (e.g. Rice and Tracey, 1969 or (Huang, 1991)) and a void coalescence criterion (e.g. (Thomason, 1990) or Tvergaard and Needleman, 1984). This approach is indeed interesting from a microstructural point of view, and has few parameters to be identified. However, since it is physically based, the identification of some of the parameters should be based on microstructure measurement.

The early ductile damage models used only the stress triaxiality in order to account for the influence of stress state, e.g. Gurson-type model, Lemaitre model, or several uncoupled models, e.g. Oyane et al. (1980). From their experimental results, Bao and Wierzbicki (2004) showed that the stress triaxiality is not enough to formulate ductile fracture models. Several recent studies demonstrated the importance of the third stress invariant in damage prediction (e.g. Barsoum and Faleskog, 2007, 2011), especially at low stress triaxiality; the Lode angle parameter is generally used to include it. Xue (2007) developed a damage-plasticity model, which accounts for the influence of hydrostatic pressure and the Lode angle. Bai and Wierzbicki (2008) constructed an asymmetric fracture locus using a weighting function of the stress triaxiality and the Lode parameter. More recently, the same authors transformed the stress-based Mohr–Coulomb failure criterion into the space of the stress triaxiality, the equivalent plastic strain and the Lode parameter (Bai and Wierzbicki, 2010). The common idea of these works is to account for the stress state in damage model formulation, which is defined by the stress triaxiality, the von Mises equivalent stress, and the Lode parameter. Regarding more physical models, Gurson based models have also been enhanced to better describe ductile damage for low stress triaxiality (e.g. Nahshon and Hutchinson, 2008 or (Xue, 2008)). Despite their interest from a microstructural point of view, it has been decided here to focus on phenomenological models.

The present work aims at comparing the Lemaitre coupled damage model and the two uncoupled models proposed by Bai and Wierzbicki (2008, 2010) through their abilities of predicting fracture for different mechanical tests. These uncoupled models were implemented in the FE software Forge2000® by the present authors. The methodology of the identification process is detailed and discussed, using hybrid experimental–numerical analysis. In the first part, the experimental tests as well as the studied damage models are presented. In order to identify the damage models parameters, the hardening parameter have to be calibrated first, based on the compression test and the tensile test on smooth round bar specimens. For the identification with the compression test, the friction influence needs to be evaluated. These identifications (friction and hardening) are the subject of the second part. The next step differs between the above-mentioned damage models: the identification of uncoupled models is carried out through the experimental fracture strains for different loading paths, while the identification of Lemaitre's model is based on the softening effect of damage. The analyses of the proportionality of these loading paths are carried out. The study suggests that the compression test is not suitable for the identification of the uncoupled formulations proposed by Bai and Wierzbicki since the loading path of a critical point is far from being proportional. Discussions and analyses on the identification results of these above-mentioned damage models are then given. The result shows that the Lemaitre model gives most accurate results for the test with high stress triaxiality level but it fails to predict fracture in torsion test. A modification of this model is proposed to overcome this shortcoming. The proposed en-
enhanced Lemaitre model gives overall best result for all tests in terms of fracture prediction. Moreover, between the two uncoupled models, the B&W model gives better results while the MMC model, which has only two parameters, also gives relatively satisfactory result.

2. Material characterization and damage model reviews

2.1. Material

All specimens are prepared from the same batch of zirconium alloy (M5\textsuperscript{TM}) and from the same location and direction. The chemical properties as well as crystallographical properties of this material can be found in Gaillac\textsuperscript{(2007)} and Gaillac and Barberis\textsuperscript{(2007)}.

2.2. Experimental setup

The objective of the experimental campaign is to perform mechanical tests which can “cover” the whole range of Lode parameter (\(\bar{\theta}\) from \(-1\) to \(1\)) and a large range of stress triaxiality (\(\eta\) from \(-1/3\) to \(0.65\)) for damage study (see Fig. 1). The analytical formulation as well as the signification of these two parameters are presented in A. This range of stress triaxiality seems suitable since \(-1/3\) is the cut-off value of the stress triaxiality, below which damage does not occur, as shown in Bao and Wierzbicki\textsuperscript{(2005)}. Moreover, the final applications of the present study are the forming processes, in which the stress triaxiality is negative or slightly positive largely lower than 0.65. All the mechanical tests were conducted at Cezus Research Center, in Ugine, France. The configurations of all these tests were defined in order to have the same order of strain rate, about \(0.1-0.15\) \(\text{s}^{-1}\) (obtained from the preliminary analytical as well as finite elements analyses) and at room temperature. The load–displacement curves obtained from tension and compression tests as well as the [torque-number of rotation] curve from torsion test were used for the identification procedure: due to the heterogeneous deformations of these tests, the stress–strain curves are difficult to exploit correctly. All the tests performed are summarized in Table 1.

For the compression test, the cylinder was lubricated both on top and bottom faces before the test. Two specimens were used and the results in terms of load–displacement curves are superimposed. Significant variation in terms of maximum torque was observed in the three torsion tests performed (Fig. 2).

Table 1

<table>
<thead>
<tr>
<th>Tests/specimens</th>
<th>Velocity (mm/s)</th>
<th>(\bar{\theta})</th>
<th>(\eta)</th>
<th>Fracture strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tension on RB</td>
<td>3.68</td>
<td>1</td>
<td>1/3</td>
<td>0.717</td>
</tr>
<tr>
<td>Tension on NRB, R = 4 mm</td>
<td>0.24</td>
<td>1</td>
<td>0.652</td>
<td>0.441</td>
</tr>
<tr>
<td>Tension on NRB, R = 6 mm</td>
<td>0.316</td>
<td>1</td>
<td>0.557</td>
<td>0.482</td>
</tr>
<tr>
<td>Tension on NRB, R = 9 mm</td>
<td>0.44</td>
<td>1</td>
<td>0.488</td>
<td>0.513</td>
</tr>
<tr>
<td>Torsion on RB</td>
<td>0.5 (fps)</td>
<td>0</td>
<td>0</td>
<td>0.594</td>
</tr>
<tr>
<td>Compression on cylinders</td>
<td>0.32</td>
<td>-1</td>
<td>-1/3</td>
<td>No crack</td>
</tr>
</tbody>
</table>

The error might be due to both the error in machining of specimens’ diameters (\(4\) \(\text{mm} \pm 0.045\) \(\text{mm}\)) and experimental setup. It is worth mentioning that the torque is proportional to the cube of the diameter and this error in machining could lead to a maximum error of 7% of torque. Among three tests that we performed, two tests gave a same number of rotations to fracture (\(\approx 2.97\) rounds) and this value of number of rotation to fracture was retained as the “experimental number of rotations to fracture”. The torsion test was only used to validate damage models using the number or rotations to fracture.

For experimental tensile tests on notched round bars, extensometers were set up to measure the displacement on 15 \(\text{mm}\) length of specimen (25 \(\text{mm}\) for tensile test on round bar), while the tensile forces were measured at the driven crosshead. For each test, three specimens were used and the results were quite reproducible (\(< 1\%\) of maximum load variation and \(< 3\%\) displacement to fracture variation).

2.3. Finite element model

Implicit finite element simulations of all experiments are performed using Forge2009\textsuperscript{TM}, which is based on mixed finite element (FE) formulation of velocity and pressure. In this software, the updated Lagrangian formulation is adopted, which allows using the small strain approach. The local integration of constitutive equations is solved by backward Euler method (return mapping algorithm). Since the mesh gets distorted at large deformation, an automatic adaptive remesher (Coupez et al., 2000) allows Forge2009\textsuperscript{TM} to deal with large strain simulations (e.g. forming processes simulations). The present simulations are carried out with the 3D solver (Forge3), in which the so-called MINI element (\(P1^+ / P1\)) is used. This linear isoparametric tetrahedron element has a velocity node added at its center, which ensures the stability...
condition – the Brezzi/Babuska condition of existence and uniqueness of solution (Arnold et al., 1984). Exploiting the symmetry of the specimens geometries and loading conditions, only a fourth of compressed specimen and one eighth of tensile specimens are modeled.

2.4. Damage models reviews

2.4.1. The Lemaitre damage model

The Lemaitre model is derived from the thermodynamics framework of continuum damage mechanics, which consists in 3 steps: (1) state variable definitions (e.g. damage variable), which define the present state of corresponding physical mechanism (i.e. damage); (2) state potential definitions, from which one can derive the state laws, and definition of associated variables (i.e. the variables which are associated with the internal state variables); (3) dissipation potential definition: to derive the evolution law of state variables, which are associated with the dissipative mechanisms. The scalar \( D \) (0 ≤ \( D \) ≤ 1), which is an internal variable, is adopted to describe the isotropic damage \( (D \) represents the ratio of damaged area of \( S_0 \) to the total surface \( S : D = S_0 / S \).)

The energy density release rate \( Y \), the variable associated with \( D \), is derived from the state potential (see Lemaitre and Desmorat, 2005 for more details):

\[
Y = \frac{\sigma^2}{2E(1 - D)^2} \left[ 2 \left( 1 + v \right) + 3(1 - 2v) \left( \frac{\sigma^2}{\sigma} \right)^2 \right] 
\]

where \( \sigma \) is the von Mises equivalent stress, \( E \) is the Young’s modulus, \( v \) is the Poisson ratio, \( p \) is the hydrostatic pressure. Lemaitre (Lemaitre, 1986) defined the dissipation potential, which is a convex function of associated variables:

\[
F = f + F_x + F_D
\]

with \( f, F_x, F_D \) are respectively the plastic potential (also the yield function in associative flow), the nonlinear kinematic hardening dissipative potential (which is not considered in the present study), and the damage dissipative potential. The latter is defined as:

\[
F_D = \frac{S}{(s + 1)(1 - D)} \left( \frac{Y}{5} \right)^{s+1}
\]

where \( s \) (MPa) and \( s \) are two material parameters (which might depend on temperature). Finally, the damage evolution is given by:

\[
\dot{D} = \lambda \frac{\partial F_D}{\partial Y} = \frac{\lambda}{1 - D} \left( \frac{Y}{5} \right)^s \equiv \bar{F} \left( \frac{Y}{5} \right)^s
\]

where \( \lambda \) is the plastic multiplier, which can be deduced from the equivalent plastic strain rate as: \( \dot{\lambda} = \bar{F} (1 - D) \), with \( \bar{F} = \sqrt{2} \varepsilon^p : \tilde{\varepsilon}^p \) (\( \tilde{\varepsilon}^p \) denotes plastic strain rate tensor). Lemaitre has proved that there exists a limit of equivalent strain \( \varepsilon_p \) below which the damage accumulation does not occur. Moreover, based on the observations of the experimental results of Bridgman, 1952 and Bao and Wierzbicki (2005) showed that there exists a limit of the stress triaxiality \( (\tilde{\varepsilon}^p) \) below which, there is no damage. This observation has been applied to the Lemaitre model by Bouchard and co-workers (Bouchard et al., 2011a). The damage evolution is therefore modified as:

\[
\dot{D} = \begin{cases} \frac{\tilde{\varepsilon}^p (\tilde{\varepsilon}^p)}{K} & \text{if } \tilde{\varepsilon}^p > \varepsilon_p \text{ and } -\frac{p}{E} > -\frac{1}{3} \\ 0 & \text{otherwise} \end{cases}
\]

In order to account for the softening by damage accumulation, the weakening function \( w(D) \) has been adopted:

\[
\begin{cases} \sigma = w(D)\sigma_m & \text{with } w(D) = \begin{cases} 1 - D & \text{in tension} \\ 1 - hD & \text{in compression} \end{cases} \end{cases}
\]

where \( \sigma_m \) and \( E_m \) are the flow stress and Young’s modulus of undamaged material, \( h \) is a material parameter (0 < \( h \) < 1), which accounts for the “micro-crack closure effect”, i.e. the distinction between “compressive” and “tensile” damages (Lemaitre and Desmorat, 2005). By measuring the variation of Young’s modulus in compression and tension, Lemaitre proposed the parameter \( h \) equals to 0.2, which is assumed to be valid for most materials.

2.4.2. Bai and Wierzbicki’s model

Bai and Wierzbicki (2008) constructed the 3D fracture locus in the space \( (\tilde{F}_f, \eta, \tilde{\varepsilon}) \) which defines the strain to fracture as a function of the stress triaxiality \( (\eta) \) and the Lode parameter \( (\tilde{\varepsilon}) \). This function is based on three limiting cases: \( \tilde{F}_f \) (corresponding to \( \eta = -1 \)), \( \tilde{F}_f^0 \) (corresponding to \( \eta = 0 \)) and \( \tilde{F}_f^1 \) (corresponding to \( \eta = 1 \)). By adopting a parabolic function to represent the effect of the Lode parameter on fracture locus, the fracture envelope \( \tilde{F}_f = f(\eta, \tilde{\varepsilon}) \) is thus defined as:

\[
\tilde{F}_f(\eta, \tilde{\varepsilon}) = \left[ \frac{1}{2} (\tilde{F}_f^{1-} + \tilde{F}_f^{1+}) - \tilde{F}_f^{1+} \right] \tilde{\varepsilon}^2 + \frac{1}{2} (\tilde{F}_f^{0-} - \tilde{F}_f^{0+}) \tilde{\eta} + \tilde{F}_f^{0+}
\]

From the early studies of McClintock et al. (1966) and Rice and Tracey (1969), for each limiting bound, the influence of stress triaxiality on material ductility can be introduced through an exponential function, hence:

\[
\tilde{F}_f^0 = D_1 e^{-D_2 \eta}, \quad \tilde{F}_f^1 = D_3 e^{-D_4 \eta}, \quad \tilde{F}_f^{1-} = D_5 e^{-D_6 \eta}, \quad \tilde{F}_f^{1+} = D_7 e^{-D_8 \eta},
\]

Eq. (7) can be rewritten as:

\[
\tilde{F}_f(\eta, \tilde{\varepsilon}) = \left[ \frac{1}{2} (D_1 e^{-D_2 \eta} + D_7 e^{-D_8 \eta}) - D_3 e^{-D_4 \eta} \right] \tilde{\varepsilon}^2 
+ \frac{1}{2} (D_5 e^{-D_6 \eta} - D_7 e^{-D_8 \eta}) \tilde{\eta} + D_5 e^{-D_6 \eta}
\]

where \( D_1, D_2, D_3, D_4, D_5, D_6 \) are 6 material parameters which need to be identified. A linear incremental relationship is assumed between the damage variable \( D \) and the equivalent plastic strain \( \tilde{\varepsilon}^p \):
where the triaxiality \( (\eta = \eta(\bar{\tau}_p)) \) and the Lode parameter \( (\bar{\psi} = \bar{\psi}(\bar{\tau}_p)) \) are functions of the equivalent plastic strain. For the proportional loadings (also called radial loadings), these two stress state parameters are constant during loading. If not, their average values are defined as:

\[
\eta_{av} = \frac{1}{T} \int_0^T \eta(\bar{\tau}_p) \, d\bar{\tau}_p, \quad \bar{\psi}_{av} = \frac{1}{T} \int_0^T \bar{\psi}(\bar{\tau}_p) \, d\bar{\tau}_p
\]

In the present study, average values of the stress triaxiality and the Lode parameter are employed to construct the fracture locus based on different “nearly proportional” mechanical tests. The advantage of this method is that fracture is obtained when the damage variable \( D \) reaches unity. This is not that case if one uses the current values of the stress triaxiality and the Lode parameter. In the latter case, the critical value of damage is a parameter to be identified. However, in order to use the average values of the stress triaxiality and the Lode parameter, the proportionality of loading paths must be studied (see 4.3). Throughout the present study, this model is referred as Bai and Wierzbicki (B&W) model.

### 2.4.3. Modified Mohr–Coulomb model (MMC)

The Mohr–Coulomb failure criterion (Coulomb, 1776; Mohr and Beyer, 1928) has been widely used in rock and soil mechanics (Palchik, 2006) as well as brittle materials communities (Lund and Schuh, 2004). This criterion, an extension of the maximum shear stress failure criterion, is a good candidate to predict shear fracture, which is nowadays still a challenge for the ductile damage and fracture community. Recently, Bai and Wierzbicki (2010) transformed the Mohr–Coulomb (M–C) model into stress triaxiality and Lode parameter dependent formulation. This modified model was then successfully used to predict fracture of different proportional loadings in several recent studies, e.g. Dunand and Mohr (2011) and Luo et al. (2012), and was implemented in different FE software (e.g. LS Dyna, Abaqus).

The analytical formulation of this model is revisited in Bai and Wierzbicki (2010). For the case of proportional loadings (constant stress triaxiality and Lode parameter), the equivalent stress at fracture \( \bar{\tau}_f \) can be expressed as:

\[
\bar{\tau}_f = 2c_2 \left[ \frac{1 + c_1^2}{3} \cos \left( \frac{\pi}{6} \right) + c_1 \left( \eta + \frac{1}{3} \sin \left( \frac{\pi}{6} \right) \right) \right]^{-1}
\]

with the introduction of Lode parameter: \( \bar{\psi}_f = \bar{\psi} - \theta \). In the present study, the Swift hardening law is employed (Eq. (15)) and \( J_2 \) plasticity is assumed, Eq. (11) then becomes:

\[
D(\bar{\tau}_p) = \frac{\int_0^{\tau_f} \frac{d\bar{\tau}_p}{\bar{\tau}_f(\eta, \bar{\psi})}}{\eta_{av}}
\]

The strain to fracture for proportional loading is then defined as:

\[
\frac{\bar{\tau}_f}{c_2} = \left[ \frac{1 + c_1^2}{3} \cos \left( \frac{\pi}{6} \right) + c_1 \left( \eta + \frac{1}{3} \sin \left( \frac{\pi}{6} \right) \right) \right]^{-1}
\]

The strain to fracture for proportional loading is then defined as:

\[
\frac{\bar{\tau}_f}{c_2} = \left[ \frac{1 + c_1^2}{3} \cos \left( \frac{\pi}{6} \right) + c_1 \left( \eta + \frac{1}{3} \sin \left( \frac{\pi}{6} \right) \right) \right]^{-1/\eta} - \epsilon_0
\]

Since \( \epsilon_0 \) is very small in our study (\( \epsilon_0 = 0.0038 \), see Table 3 in the following section), this term can be omitted in Eq. (13). This equation represents an asymmetric fracture envelope with respect to
Lode parameter, which becomes symmetric when $c_1 = 0$ (maximum shear stress criterion). There are two parameters $c_1$ and $c_2$ which need to be identified. In Bai and Wierzbicki (2010), the authors carried out a parametric study, which showed that when $c_1$ increases, the fracture strain becomes more stress-triaxiality dependent. Moreover, the fracture strain was proved to increase with $c_2$.

The damage indicator evolution is defined similarly to Eq. (9). This modified model is called the Modified Mohr–Coulomb model (MMC) hereinafter.

### 3. Isotropic hardening law identification

The matrix material is considered to be isotropic and the plastic deformation is isochoric, obeying the $J_2$ plasticity theory: isotropic yield surface, associated flow rule and isotropic hardening law. Examples of fractured surfaces of tensile test on NRB-R4 and torsion test are presented in Fig. 3, which shows that the specimens kept their circular forms. It suggests that the behavior of this material is isotropic on the cross section.

#### 3.1. Friction identification for compression

Generally, the load–displacement curve of compression test is often employed to identify the isotropic strain hardening law because: (1) the influence of damage process is less significant in upsetting test, (2) the fracture strain in this type of test is remarkably higher than that in the tensile test, which enables a more accurate curve fitting and the applicability of the hardening model in large deformation. However, during the compression test, the influence of friction on the load–displacement curves due to the loss of lubricant is remarkable. In order to obtain the correct parameters of hardening law, the average friction coefficient needs to be identified first, based on the variation of specimen geometry (Fig. 5). The friction law involves two coefficients: the Coulomb’s friction coefficient $\mu$ and the limiting friction parameter $m$ (Eq. (14)). They are supposed constant all along the numerical simulation:

$$\tau = \min\left(m \sigma / \sqrt{3}, \mu \sigma_n\right)$$

where $\sigma_n$ and $\tau$ are the normal and shear contact stresses respectively.

Only half a specimen was modeled, with a virtual marking grid attached to the cutting section in order to follow the variation of specimen geometry (Fig. 4(a)). Moreover, two numerical sensors were set up to follow the materials point initially located at upper surface corner and middle–height external surface (Fig. 4(b)). Based on the three characteristic dimensions (Fig. 5), the values of $m = 0.85$ and $\mu = 0.5$ are identified. Note that the results of friction coefficients obtained by the present methods do not depend on the hardening law used.

#### 3.2. Strain hardening law identification

The hardening law identified is expected to be valid for different loading cases. For this reason, the hardening law is thus identified from both the whole compression load–displacement curve and the plastic part before necking of the load–displacement curve in the tensile test on round bar (to avoid post-necking instabilities). After testing several isotropic hardening laws (e.g. Ludwik, Voce), the Swift law (Swift, 1952) is retained since it gave better result (Eq. (15)):

$$\sigma_0 = \sqrt{3}K(\epsilon_0 + \epsilon_p)^n$$

where $\sigma_0$ is the flow stress of material; $\epsilon_p$ is the equivalent plastic strain; $K$(MPa). $\epsilon_0$ and $n$ are material parameters. An automatic optimization process by inverse analysis was carried out to identify these 3 material parameters by minimizing the differences between numerical load–displacement curves and the experimental ones (Bouchard et al., 2011b).

#### 3.2.1. Mesh size sensitivity

In order to study the influence of mesh size on the numerical results, the comparisons of 3 different meshes were carried out on the tensile test on smooth round bar (Fig. 6). The characteristics of meshes used as well as the simulations performed are reported.
in Table 2. Note that all the simulations were carried out with the maximum time increment equal to 0.05 s.

As one can observe in Fig. 6(b) and Table 2, the coarse mesh gives incorrect results for both global quantity (load) and local quantity (strain). Furthermore, the load–displacement curve is nearly insensitive when changing from medium mesh to fine mesh, while CPU time sharply increases (Table 2). In addition, the predicted local strain at specimen center is noticeably influenced by the mesh size (Table 2), but the variation is still acceptable (3.48%). In the following, all the simulations of tensile tests are carried out using the local mesh size of 0.12 mm (mesh 2) for a compromise between CPU time and precision.

3.2.2. Identification result

Fig. 7(a) and (b) show the comparison between the experimental and the numerical load–displacement curves for the compression and the tensile tests. The identified parameters are reported in Table 3.

3.3. Discussions on the hardening law

Since the identified parameters of Swift’s law give relatively good results both in compression and tensile test on round bar, they have been then used for the simulation of tensile tests on notched round bars with different notch radii. The comparative results were presented in Fig. 8, which also shows the validity of this identified Swift’s law to describe the hardening of the studied material for different states of stress.

Regarding the tensile tests on NRB specimens, we observe a mismatch in the elastic region, which might be due to an error in extensometer setup. However, the maximum error of displacement is about 20–30 μm, which does not influence the displacement to fracture. This error could be corrected based on the Young’s modulus of this material.

In Table 4, the comparisons between numerical and experimental necking radii and fracture strains are reported. In terms of geometry (necking radii), the errors between the simulation results and the experimental results are very small (< 1%). Although the simulations can capture accurately the geometry variation of notched round bar specimens, the differences of local fracture strains are relatively high except for the tensile test on NRB-R4 (but still < 10%). These differences are due to the assumption of constant strain over cross section when calculating the experimental logarithmic fracture strains based on the cross section of neck. Fig. 9 shows the strain map of half specimens at the end of simulations. As one can observe, for the NRB-R4 specimen, the equivalent plastic strain is nearly constant in the cross section; the error between numerical and “experimental” strains is thus small. However, for other cases, the strain localization can be observed in the center of specimens. Fig. 9(b) shows the variation of the equivalent plastic strain as the function of relative position in the minimum cross section (a denotes radial position, i.e. a = 0 is the center and a = R is the border). The variation in the case of RB, NRB-R6 and NRB-R9 is noticeable while for NRB-R4, the equivalent plastic strain varies slightly. Therefore, the local values of numerical simulations for the three former cases are different from the “experimental” average values across the cross section.

In addition, since the identification of hardening law was based on the pre-necking part of the load–displacement curve of tensile test on smooth round bar, the post-necking behavior was not well captured (Fig. 7(b)). Before necking, the bar is subjected to uniaxial tension, then the necking formation introduces triaxial loading. The identified hardening law overestimates the force level (the red curve in Fig. 7(b)). The difference between the experimental and numerical curves in Fig. 7(b) can be explained by the coupling between damage and necking: ductile damage (voids) increases rapidly after necking, which has not been taken into account in this section. Another explanation might be the questionable validity of the Swift law after necking, which needs a special treatment. In Xue et al. (2010), the authors varied the hardening coefficient n in order to reproduce the experimental stress–strain curve in post-necking area. However, since these authors used only the tensile test on round bar for identification and validation, the influence of this modification on other strain levels (e.g. tensile tests on notched round bars) was not studied. In Dunand and Mohr (2010), an extrapolation technique was adopted to modify the Swift hardening law after necking occurs. In order to obtain a better extrapolation of the measured stress–strain curve, the authors defined two segments of constant slope H1 and H2; where H1 corresponds to the range of intermediate plastic strains (from 0.2 to 0.35), H2 to the range of high plastic strains (higher than 0.35) (note that in Dunand and Mohr (2010), the strain level of 0.2 cor-

In the present study, the term “experimental strain” must be understood as the logarithmic strain calculated from the experimental measurement of specimen diameter: \( \varepsilon = \ln(R_0/R_f) \), where \( R_0 \) and \( R_f \) are the initial and the fracture radii. For the torsion test \( \varepsilon = 2\theta /R \), where \( \theta \) is the number of rotations to fracture; \( L \) is specimen length.
responds to the onset of necking. These two parameters $H_1$ and $H_2$ were then identified to reproduce the experimental load–displacement curves. In the present authors’ point of view, with this method, one could introduce not only two parameters $H_1$ and $H_2$, but also a set of parameter $H_i$ (i.e. successively constant slopes), which would be calibrated with experimental results. The flow curve is thus reduced to point-to-point type (i.e. the table of one to one mapping of equivalent plastic strain and yield stress). Furthermore, since these approaches (Xue et al., 2010; Dunand and Mohr, 2010) neglect the influence of damage on material strength, their physical origins were not well established. A systematic methodology to obtain hardening law valid up to large strain was presented in Tar-dif and Kyriakides (2012), in which the authors used the force–elongation curves combined with an accurate measurement of the deformation in the necked region. In the present study, the hardening law is also identified from compression test, in which the nominal strain at the end of test reaches a high value ($\tau \approx \ln(\frac{a_0}{a}) = 1.53$). The hardening law is thus valid for a relative large range of strain.

In the present study, applying such modifications proposed by Dunand and Mohr (2010) or Xue et al. (2010) may give better result in the tensile test on round bar, but at the same time modifies the results of the tensile test on notched round bars and the compression test: the load levels in these tests are underestimated. For this reason, the identified Swift law (Table 3), which gives relatively accurate results for different tests, is used hereafter to describe the hardening law of the studied material. The difference at the end of the two curves can be considered as the influence of damage at this strain level. Identification of this influence and accounting for it is the purpose of the next section.

### 4. Damage models identifications

The Lemaitre model has been implemented in Forge2009 by Bouchard and co-workers (Bouchard et al., 2011a) through a user subroutine, with a “weak coupling” of damage and elastoplastic behavior: the damage variable at time step $n-1$ is used to solve the mechanical equations at time step $n$. The two uncoupled models B&W and MMC were introduced into this software by the present authors.

#### 4.1. Damage observation

The fractured specimens were observed under SEM and revealed dimpled surface (see Fig. 10) which was the result of ductile damage.

Table 4

<table>
<thead>
<tr>
<th>Specimen</th>
<th>NRB-R4</th>
<th>NRB-R6</th>
<th>NRB-R9</th>
<th>RB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical necking radius (mm)</td>
<td>2.389</td>
<td>2.331</td>
<td>2.302</td>
<td>2.111</td>
</tr>
<tr>
<td>Experimental necking radius (mm)</td>
<td>2.405</td>
<td>2.355</td>
<td>2.320</td>
<td>2.096</td>
</tr>
<tr>
<td>Numerical local fracture strain</td>
<td>0.442</td>
<td>0.515</td>
<td>0.558</td>
<td>0.768</td>
</tr>
<tr>
<td>Experimental local fracture strain</td>
<td>0.44</td>
<td>0.48</td>
<td>0.51</td>
<td>0.72</td>
</tr>
<tr>
<td>Error % (radius)</td>
<td>0.66</td>
<td>1.0</td>
<td>0.797</td>
<td>0.701</td>
</tr>
<tr>
<td>Strain discrepancy (%)</td>
<td>0.4</td>
<td>7.26</td>
<td>9.43</td>
<td>7.02</td>
</tr>
</tbody>
</table>

Fig. 8. Comparisons between the experimental and numerical load–displacement curves of tensile tests on notched round bars.

Fig. 9. (a) The strain map on the cross section of specimens at the end of different tensile tests. For the NRB-R4 specimen, the equivalent plastic strain is nearly constant in the cross section. However, for other cases, the strains are localized in the centers of specimens. (b) Variation of numerical equivalent plastic strain with relative position in the cross section.
4.2. The onset of fracture

Before carrying out the identification of the damage models, it is important to define the onset of fracture. In this present study, the fracture is defined by the instant at which one can observe the sharp drop of load–displacement curves (or torque-number of rotation curve). The corresponding displacement (or rotation) at that instant is defined as the displacement to fracture (or the rotation to fracture for the torsion test).

4.3. Loading paths to fracture

The loading paths to fracture of the tensile tests and the torsion test are presented in Fig. 11, where the equivalent plastic strains are plotted as function of the stress triaxiality and the Lode parameter (the last point of these curves correspond to the fractures in these tests). The values were extracted from critical point, which is positioned in the center axis for the tensile specimens and on the specimen surface for the torsion experiment.

For the tensile tests, the Lode parameter is nearly constant and equal to unity, except the tensile test on NRB-R4 (Fig. 11). The variations of the stress triaxialities during loading can be observed in Fig. 11, which shows the non-proportionality of these loading paths. For the tensile test on round bar (blue curve in Fig. 11), the stress triaxiality changes sharply when necking develops: the stress state is no longer uniaxial ($\eta = 1/3$) but rather triaxial. Moreover, one can also observe in this figure, when the notch radius decreases from 9 mm to 4 mm, the lower variation of stress triaxiality during loading is obtained.

For the present torsion test, a strictly pure shear state ($\eta = 0$, $\bar{\theta} = 0$) was not obtained but the values of the stress triaxiality and the Lode parameter are nearly constant during the experiment. This loading can be considered as proportional.

In our study, there was no crack observed on the external surface of the compressed specimen. The crack observed in the compression test is mainly due to the presence of friction, which then causes barreling: a high positive stress triaxiality region (Fig. 12(a)). A material point located at the middle of the external surface of specimen is firstly subjected to compressive stress, then tensile stress when barreling develops. The definition of fracture strain based on the average stress triaxiality and Lode parameter required a priori knowledge of fracture location. The value of average stress triaxiality and Lode parameter are then obtained from a material point located at this critical zone, via Eq. (10), as it was done in the literature, e.g. Bai and Wierzbicki (2010), Dunand and Mohr (2010) and Luo et al. (2012). For the compression test,
the loading history of a material point located at external surface middle position is presented in Fig. 12. As one can easily observe, the loading experienced by this material point is far from proportional.

4.4. Calibration of the Lemaitre model

For the Lemaitre coupled damage model, the identification was based on the softening behavior due to damage accumulation. This softening, however, depends on the mesh size as stated in previous studies (e.g. Peerlings et al., 1996; Jirásek, 1998 among others): a finer mesh leads to a faster damage accumulation. Several methods were proposed in the literature in order to overcome this limitation (Peerlings et al., 1996, 2001; Engelen et al., 2003). In the present study, no particular technique was employed, the mesh size was thus kept constant for all the simulations. The tensile test on smooth round bar was chosen for the curve fitting procedure by inverse analysis. The comparison of experimental and numerical load–displacement curves are presented in Fig. 13, while identified parameters are reported in Table 5.

These identified parameters are then used to verify the prediction of fracture on other tensile tests on notched round bars and the torsion test. The relative errors between experimental and predicted displacements to fracture are presented in Fig. 13(b); they are relatively small (< 2.1%) except the torsion test. For numerical simulations, the fracture is supposed to occur when the damage parameter reaches its critical value (e.g. \( D = D_c \approx 0.21 \) for Lemaitre's model). The numerical results are in good agreement with experimental observations for the tensile tests. However, the identified Lemaitre model is unable to predict fracture in the torsion test. This model thus needs to be enhanced to predict the fracture in shear-dominated loading.

4.5. Enhanced Lemaitre model for shear loading

4.5.1. Modified dissipative potential and damage evolution

In this section, the Lemaitre model is improved by incorporating the influence of the third stress invariant represented by the Lode parameter in its formulation. The present authors propose to modify the damage dissipative potential (Eq. (3)) as:

\[
F_D = \frac{S}{(s + 1)(1 - D)} \left(\frac{Y}{S}\right)^{s+1} \left(\frac{1}{\alpha_1 + \alpha_2 s^2}\right)
\]

where

\[
\alpha_1 = \frac{D - D_c}{S}, \quad \alpha_2 = \frac{\eta}{s(1 - D)S}
\]

and

\[
\eta = -\frac{1}{3}, \quad D_c = \frac{1}{1 - \frac{1}{3}}
\]

The loading history of a material point located at external surface middle position is presented in Fig. 12. As one can easily observe, the loading experienced by this material point is far from proportional.

### Table 5

<table>
<thead>
<tr>
<th></th>
<th>Lemaître</th>
<th>Modified Lemaître</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S ) (MPa)</td>
<td>( s )</td>
<td>( \epsilon_D )</td>
</tr>
<tr>
<td>6</td>
<td>3.2</td>
<td>0.202</td>
</tr>
<tr>
<td></td>
<td>3.8</td>
<td>0.208</td>
</tr>
<tr>
<td></td>
<td>0.27</td>
<td></td>
</tr>
</tbody>
</table>

The loading path to fracture of a material point in barreling region (a) and the iso-value of stress triaxiality at the end of simulation.

Fig. 12.

(a) The loading path of a material point located in the barreling region, showing its non-proportionality. The calculated average stress triaxiality and Lode parameter are respectively equal to 0.11 and 0.156, which are far from the corresponding values of a uniaxial compression stress state \( (\eta = -1/3, \tilde{\theta} = -1) \).

(b) Stress triaxiality map on cutting surface at the end of test, showing the high triaxiality region in the barreled area.

Fig. 13.

(a) Numerical and experimental load-displacement curves of tensile test on round bar.

(b) Error of displacement to fracture for all the tests predicted by the identified model.

Fig. 13. Comparison between the experimental and numerical result with Lemaitre model: (a) load–displacement curve of tensile test on round bar; (b) errors of displacement to fracture predicted by identified model.
where $\alpha_1$ and $\alpha_2$ are two new positive parameters. Note that with a simple choice: $\alpha_2 = 1 - \alpha_1$, for $\bar{\sigma} = 1$, the original Lemaitre model is obtained, which means the modified model coincides with the original model in uniaxial tension (which has often been used to identify the Lemaitre model). In this case, the parameters identified of the Lemaitre model can be used for the modified Lemaitre model and there is only one additional parameter to be identified (since $\alpha_2 = 1 - \alpha_1$).

With this modified potential, the damage evolution can be deduced:

$$
\bar{D} = \lambda \frac{\partial f_D}{\partial \sigma} = \frac{\sigma}{Y} \left( \frac{1}{\alpha_1 + \alpha_2 \bar{\sigma}^2} \right)
$$

(17)

where $Y$ is defined in Eq. (1).\(^5\)

4.5.2. Coupling function

For the Lemaitre model, the coupling function was defined as in Eq. (6). Lemaitre proposed such a coupling function based on his uniaxial compression ($\eta_{\text{un}} = -1/3$) and tension ($\eta_{\text{un}} = 1/3$) tests. The coupling function thus may be valid for these two limits of stress triaxiality but nothing proves its validity for the intermediate values of the stress triaxiality. The present authors propose a phenomenological coupling function as:

$$
\mathbf{w}(D) = \begin{cases} 
1 - D, & \text{if } \eta \geq \eta_1 \\
1 - \left( \frac{1-h}{\eta_1-\eta_2} \right)^{\eta_1-\eta_2} D, & \text{if } \eta_1 > \eta > \eta_2 \\
1 - hD, & \text{if } \eta < \eta_2
\end{cases}
$$

(18)

where $\eta_1$ and $\eta_2$ are two parameters to be identified, which can be chosen as $\eta_1 = 1/3$ and $\eta_2 = -1/3$ in the first approximation; $h$ can also be chosen equal to 0.2 as proposed by Lemaitre.

4.5.3. Identification

For the modified model, $\alpha_2 = 1 - \alpha_1$ was chosen and $\eta_1 = 1/3$, $\eta_2 = -1/3$, $h = 0.2$ as discussed above. The parameters of the original model were identified above. In principle, these parameters can be kept for the modified model. However, in the inverse analysis procedure, we allow slight variations of these parameters for a better result. The complete set of parameters for the modified Lemaitre model is presented in Table 5 while the comparison of the load–displacement curves for tensile test on RB and relative error of displacements to fracture for all tests are shown in Fig. 14.

5 Since the term added is a positive multiplicative term ($\frac{1-h}{\eta_1-\eta_2}$), the product $\mathbf{YD}$ does not change sign and the positive damage dissipation is maintained.

4.6. Calibration of the uncoupled models: B&W and MMC

The two uncoupled models B&W and MMC were calibrated via the strain to fracture of different tests. Fracture is assumed to occur when the damage variable reaches unity.

4.6.1. B&W model

There are 6 parameters that need to be identified (Eq. (8)), in which the two parameters $D_1$ and $D_2$ define the function $\mathbf{F}_{\nu_0} = D_1 e^{-D_2 \nu_0}$, which correspond to the fracture strain at $\bar{\sigma} = 1$. These two parameters were thus estimated a priori via the experimental fracture strains of tensile tests.

The fracture locus was then assumed to be symmetric with respect to $\bar{\sigma} = 0$, i.e. $D_1 = D_3$ and $D_2 = D_6$. All the parameters estimated define a set of input parameters for an automatic optimization process by inverse analysis, which aims at minimizing the difference between the numerical and experimental displacements to fracture of the tensile tests and the torsion test (for the torsion test, the “displacement to fracture” corresponds to the “number of rotations to fracture”).

4.6.2. MMC model

For this model, there are just 2 parameters $c_1, c_2$ which need to be calibrated. An identification process by inverse analysis was also carried out to identify these two parameters.

4.6.3. Results and discussions

The identified parameters of B&W and MMC models are reported in Table 6. Fig. 15 shows the relative errors between the experimental and the numerical displacements to fracture predicted by these two models. Globally, the errors are small (< 5%) except the result of MMC model with torsion test (error of 6.79%). This difference, however, could be expected since the
The discrepancy between the “experimental” and the numerical local plastic strains to fracture are also presented (Fig. 15(b)). We can observe the same tendency as for the displacement to fracture: the B&W model is better than the MMC model since it has more calibrated parameters. For all cases, the local strain maximum error is still smaller than 10%. These results show that, if one uses either the error of displacement to fracture or the discrepancy of local strain to fracture, same tendency is observed, the B&W is still globally better.

From the identified parameters, the fracture loci obtained with these two models can be constructed. They correspond to the plots of strains to fracture as the function of the stress triaxiality and the Lode parameter (Fig. 16 and Fig. 16(b)). The triangle symbols represent the experimental fracture strains of the tests, with their corresponding average stress triaxiality and Lode parameter. Since the loading paths of our tensile experiments are non-proportional, these points are not expected to lie exactly on the identified fracture envelopes. However, the difference is small and these loci help estimating the strain to fracture for a given proportional loading.

MMC model has just only two parameters to be calibrated from five different tests. The discrepancy between the “experimental” and the numerical local plastic strains to fracture are also presented (Fig. 15(b)). We can observe the same tendency as for the displacement to fracture: the B&W model is better than the MMC model since it has more calibrated parameters. For all cases, the local strain maximum error is still smaller than 10%. These results show that, if one uses either the error of displacement to fracture or the discrepancy of local strain to fracture, same tendency is observed, the B&W is still globally better.

From the identified parameters, the fracture loci obtained with these two models can be constructed. They correspond to the plots of strains to fracture as the function of the stress triaxiality and the Lode parameter (Fig. 16 and Fig. 16(b)). The triangle symbols represent the experimental fracture strains of the tests, with their corresponding average stress triaxiality and Lode parameter. Since the loading paths of our tensile experiments are non-proportional, these points are not expected to lie exactly on the identified fracture envelopes. However, the difference is small and these loci help estimating the strain to fracture for a given proportional loading.

Fig. 15. The relative errors between experimental and numerical displacements to fracture (a) and strain to fracture (b) of different tests, with the two uncoupled damage models B&W and MMC. Note that for the torsion test, the “displacement to fracture” corresponds to the “number of rotations to fracture”.

5. Discussions and recommendations

5.1. On the experimental validation of fracture prediction ability: what is the reliable measurement?

In this section, different measurements used to characterize the validation of fracture predictions are discussed to choose, if possible, the most relevant one.

Considering the displacement to fracture, which can be seen as a “global variable”, a given damage model is said to be valid, if its counter indicates that fracture occurs at the applied displacement level, which is equal to the experimental displacement to fracture. If it is not the case, a measurement of the displacement at which fracture numerically occurs (i.e. when the damage variable reaches its critical value $D = D_c$) is performed. This displacement is then compared with the real “experimental displacement to fracture” to deduce the relative error of displacement to fracture. These measurements of displacement (numerical or experimental) can be extracted directly from experimental test and numerical simulation. Apparently, the relative error depends on the gauge length and cannot characterize the local event.

Another measurement, the local strain to fracture, can be deduced experimentally by measuring the local section and using the logarithmic formula. It is often called “experimental local fracture strain”, although it is not really an experimental measurement. The experimental measurement in this case is none other than the specimen section (or its diameter). Then, an analytical formula, which is also an approximation, is used to calculate the
so-called local strain. It is the first source of error. For numerical simulation, e.g. tensile tests simulations, fracture often occurs after a diffuse then a localized necking. In this softening zone, the value of “numerical local plastic strain” depends strongly on the mesh size used (even without damage coupling). In order to overcome such an influence, non-local plastic strain must be used, using non-local formulation (evidently, coupled damage variable also depends strongly on the mesh size but here the authors just focus on the plastic strain). This topic was addressed by several authors (e.g. Peerslings et al., 1996; Jirasek, 1998). In order to have a mesh-independent plastic strain using non-local formulation, the mesh size must be smaller than certain characteristic length, which is often small. To summarize, even based on this local measurement, numerical and experimental sources of error may still occur. The numerical local plastic strain cannot be considered as a strict reliable measurement if non-local formulation is not employed when softening is involved.

In the present study, both measurements are used to validate the ability of fracture prediction for uncoupled models as shown in Fig. 15(a). Same tendency is obtained basing on these two measurements: the B&W model is better than the MMC model in terms of fracture prediction. For coupled damage models, since mesh size sensitivity is higher, only the displacement to fracture is used.

5.2. Application of damage models to non-proportional loading cases, a limitation of uncoupled approach?

In this section, the application of damage models for non-proportional loadings is discussed, even if several approaches are not used in the present study. For the micro-mechanical based models (e.g. Gurson) or coupled phenomenological models such as Lemaitre (CDM approach) or other uncoupled formulation (e.g. Rice and Tracey), their applications to non-proportional loading configurations are not an issue since the derivation of these models is not based on the assumption of proportional loadings. The present authors also carried out the identification and application of micromechanical type model in forming process and it gives relative good results both in terms of damage localization and fracture prediction (to appear).

As mentioned above, uncoupled damage models used in the present study were initially based on an assumption of proportional or radial loadings to define the so-called strain to fracture function. For a non-proportional loading, the use of average measurements to construct a fracture locus does not make sense since these measurements cannot account for the whole loading history (e.g. a cyclic tension–compression test on axisymmetric specimen). In the study of Bai and Wierzbicki, the authors constructed the fracture loci based on their “proportional” experiments. Moreover, they transformed the stress-based M–C criterion (see Section 2.4.3 or Bai and Wierzbicki (2010)), to a mixed strain/stress-based formulation to predict fracture. This transformation is valid only if the loading is proportional. Recently, Benzerga and co-workers (Benzerga et al., 2012) examined the influence of strain history on fracture behavior by using cell model calculation. In their simulations, the authors considered two cases: radial loading and non-radial loading. For the latter case, loading was composed of two steps. In each step, the stress triaxiality was kept constant (i.e. a piecewise constant function) and the strain-averaged value of the stress triaxiality was equivalent to the case of radial loading. By varying the stress triaxiality, these authors showed that for each value of average stress triaxiality, the value of "fracture strain" was not unique. For these reasons, in the present authors opinion, the application of these criteria for non-proportional loading needs further consideration about the meaning of the function $r_f$. In this case, $r_f$ is no longer the strain to fracture function, but rather a weighting function, which accounts for the stress state.

Uncoupled damage models (or fracture criteria) can be based on physical assumptions (e.g. Rice and Tracey criterion) or pure phenomenological assumptions, in which damage parameter is defined as an integration of a stress-based function along the strain path: $D = \int_0^1 f(\sigma) \, d\varepsilon_p$. If the stress-based function $f(\sigma)$ is chosen as: $f(\sigma) = 1/\tau_f$, with $\tau_f$ defined as in Eq. (8) (B&W model) or in Eq. (13) (MMC model), the damage variable of B&W and MMC models can be obtained respectively. If proportional (or nearly proportional) tests are used to calibrate these models, this function coincides with the fracture strain. To summarize, $r_f$ must not be considered as a fracture strain function in a strict sense. It is only a phenomenological weighting function, which coincides with the fracture strain for radial loadings. The fracture prediction in numerical simulation is based on the damage variable $D$.

5.3. Cut-off value of fracture

From the famous series of tests under pressure of Bridgman (1952), Bao proposed a cut-off value of stress triaxiality of $-1/3$, below which fracture does not occur. As presented in Section 2.4.1, this cut-off value was introduced into the Lemaitre model in Forge2009 by Bouchard et al. (2011a). For the MMC model, the cut-off region is defined by a combination of the Lode parameter and the stress triaxiality. Starting from Eq. (13), the cut-off region is obtained by setting the denominator to be zero:

$$\sqrt{1 + \frac{c_1^2}{3}} \cos \left(\frac{7\pi}{6}\right) + c_1 \left(\eta + \frac{1}{3} \sin \left(\frac{7\pi}{6}\right)\right) \leq 0 \quad (19)$$

This equation can be expressed in terms of stress triaxiality condition:

$$\eta \leq -\frac{1}{c_1} \sqrt{1 + \frac{c_1^2}{3}} \cos \left(\frac{7\pi}{6}\right) - \frac{1}{3} \sin \left(\frac{7\pi}{6}\right) \quad (20)$$

Fig. 17(b) represents the cut-off regions in 2D space of $(\eta, \eta)$ obtained with the Lemaitre model and the identified MMC model. As one can easily observe, the cut-off value of stress triaxiality obtained with the identified MMC model is significantly smaller than that obtained by the study of Bao and Wierzbicki (2005), which was introduced into the Lemaitre model.

Bai and Wierzbicki (2010) showed that the cut-off region of the MMC model can be linked with the “friction–cone” concept, which is an interesting physical interpretation (Fig. 17(a)). When the stress triaxiality is smaller than a given value, the combination of shear and normal stresses will be contained within a cone similar to the “friction–cone”. The value of cut-off stress triaxiality of $-1/3$ found by Bao and Wierzbicki (2005) was deduced from empirical observations, which was based on the work of Bridgman (1952) and confirmed by the work of Teng on dynamic impact fracture (Teng, 2005). Although the cut-off region obtained with the MMC model is more physical sound, its predicted value of cut-off stress triaxiality is too low compared with experimental evidence (about $-4.3$ to $-5.18$ in our study – Fig. 17(b)). The reason might be link with the fact that the Mohr–Coulomb model was first used for brittle and granular materials, whose “cut-off” value of stress triaxiality might be small compare to that of ductile material.

Another shortcoming of the MMC model is its derivation from a stress-based MC criterion to a mixed strain/stress-based criterion. This transformation is only valid for proportional loading. The use of the MMC criterion for a non radial loading loses its initial meaning and this criterion in this case must be considered as a general uncoupled formulation (see Section 5.2).

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7 Here, the authors only mention the ability of application, not the ability of prediction.
5.4. Lode dependent function

The B&W model assumed the parabolic form of Lode dependent function. Bai and Wierzbicki (2010) also showed that at a given value of the stress triaxiality, the Lode dependent function of the MMC model can also be approximated by a parabolic curve. In Xue (2007), the author proposed a linear function of absolute value of Lode angle, the form of Lode dependent function is thus linear and symmetric with respect to $\bar{\tau} = 0$. In order to accurately identify the form of this function, one needs to carry out different mechanical tests at a fixed value of the stress triaxiality and different Lode parameter. This configuration is still a challenge and to the best of our knowledge, this problem has not been addressed yet.

5.5. Synthesis on studied damage models

The Lemaitre model gives the best results for high stress triaxiality region (tensile tests on round bar and notched round bars), which also shows the importance of the coupling between damage and elastoplasticity (not taken into account in the uncoupled models). Nevertheless, it fails to predict the ductile fracture in the present torsion test.

Among the studied damage models, the proposed enhanced Lemaitre model gives the overall best result for all the studied tests in terms of fracture prediction (via the displacement to fracture). This proposed model is also user-friendly since one can use the parameters of the original model (which are often identified from uniaxial tensile test) for this modified model with the choice: $x_2 = 1 - x_1$, only one additional parameter needs to be identified. Moreover, the proposed modified coupling function enables a more flexible interaction between damage and material strength.

Regarding the two uncoupled models, the B&W model gives a better result for all the studied tests in terms of fracture prediction (via the displacement to fracture). This model, which is based on the three limiting curves, is also easy to identify and friendly to use and implement. However, the identification of this model (as well as the MMC model) is based on the strong assumption of proportional loadings. In our experiments, the stress triaxiality and the Lode parameter vary moderately, the error is thus small. For a non-proportional loading (e.g. upsetting test), using the average values of the stress triaxiality and the Lode parameters may lead to unrealistic results. On the other hand, the fracture envelope is supposed to be symmetric in the present study since we do not have sufficient data in negative Lode parameter region. This assumption must be justified in future studies.

The MMC model itself predicts relatively exact fracture displacements for different tests, except for the torsion test (error of 6.79%). Since this model consists of two parameters, which are calibrated from 5 different tests, this shortcoming is expectable. Using another form of hardening law to account for the influence of Lode parameter and hydrostatic pressure (as in Bai and Wierzbicki (2008)) may introduce more parameters in the left hand side of Eq. (12) to be calibrated. It might give better results, but it is more expensive in terms of identification work.

5.6. Hardening law and plasticity

In the present study, the hardening law was assumed isotropic and the $J_2$ plasticity theory was adopted. The identified strain hardening law gave relatively good results in terms of global behavior of material for different tests (load–displacement curves). However, for the studied material with hexagonal compact form of crystal structure, the texture has demonstrated to have a strong influence on material mechanical properties (Gaillac, 2007). A more physical model, which accounts for the evolution of microstructure and/or an anisotropic plasticity criterion, might be used in future studies.

6. Concluding remarks

This paper presents the comparison between coupled and uncoupled damage models via a hybrid numerical-experimental analysis of some ductile fracture experiments for bulk metal (zirconium alloy). The uncoupled models were implemented in the FE software Forge2009® by the present authors. The Lemaitre model is enhanced by accounting for the influence of the Lode parameter (or the influence of the third deviatoric stress invariant). The procedures to obtain the isotropic strain hardening as well as the damage models parameters are described and discussed in details. The main conclusions can be summarized as:
1. The identification of hardening law based on compression test needs a good estimation of friction influence. The non-linear friction law parameters are identified by the geometry variation of specimen. The identified friction coefficients allows reproducing accurately the dimensional variation during the test and obtaining good hardening parameters.

2. In terms of fracture prediction, the Lemaitre coupled damage model gives best results for high triaxiality tests (i.e. tensile tests) in comparison with the two studied uncoupled models. This fact shows the importance of coupling damage and elastoplasticity in fracture prediction of high triaxiality tests, in which significant void growth can be observed. Therefore, the Lemaitre model, with few parameters to be calibrated, can be used for the fracture prediction in high triaxiality forming processes. However, this model fails to predict ductile fracture for torsion test.

3. The proposed enhanced Lemaitre model gives overall best results in terms of fracture prediction for all tests (based on the displacement to fracture). This model is also friendly to identify with a flexible coupling function. Fracture in shear-dominated loading can be accurately predicted by the proposed model. In terms of formulation, this enhanced model also ensures a positive dissipation of damage process.

4. Among the two uncoupled models, the B&W model gives better result. These two models are friendly to implement and identify and is interesting for engineering applications. Nevertheless, the proportionality of calibration tests must be verified to avoid unrealistic identification result. Moreover, the application of these models in non-proportional loading needs a special attention in interpreting the signification of function $r_i$: it is no longer the strain to fracture but rather a stress-dependent function used to defined the damage variable.

5. The identified cut-off region of the MMC model in terms of stress triaxiality, although it has an interesting physical interpretation, is too low compared with experiments from the literature. The reason may be link with the fact that the M–C model was first used for brittle material, whose cut-off value of the stress triaxiality might be small compare to that of ductile material. Moreover, since the M–C is a stress-based model, the transformation into a strain-based model is only valid in proportional loading. Again, the meaning of the function $r_i$ has to be re-interpreted.

6. The loading path of a critical point of quasi-static compression test is proven to be strongly non-proportional. This test thus cannot be used in the identification process of the models which are based on the fracture envelop using the average stress triaxiality and Lode parameter.

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**Appendix A. Characterization of stress states**

For an isotropic material, the stress state is characterized by the symmetric stress tensor ($6$ components) or its eigenvalues ($3$ principal stresses: $\sigma_1$, $\sigma_2$, $\sigma_3$). Material models can also be formulated in terms of the first stress together with the second and the third deviatoric stress invariants, which are defined as:

$$ p = -\sigma_m = -\frac{1}{3} \text{tr}(\sigma) = -\frac{1}{3} (\sigma_1 + \sigma_2 + \sigma_3) = -\frac{I_1}{3} $$

$$ q = \sqrt{\frac{2}{3}} : S = \sqrt{\frac{1}{2} \left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right] = \sqrt{3} J_2 } $$

$$ r = \left( \frac{27}{2} \det(S) \right)^{1/3} $$

The stress triaxiality is linked with the ratio between the first stress and the second deviatoric stress invariants:

$$ \eta = \frac{\sigma_m}{q} $$

The Lode angle $\theta$ ($0 \leq \theta \leq \pi/3$) is defined through the normalized third stress invariant:

$$ \xi = \left( \frac{r}{q} \right)^3 = \cos(3\theta) $$

The normalized Lode angle or the Lode parameter $\overline{\theta}$ is defined as:

$$ \overline{\theta} = 1 - \frac{6\xi}{\pi} = 1 - \frac{2}{\pi} \arccos \left( \frac{r}{q} \right)^3, \quad -1 \leq \overline{\theta} \leq 1 $$

**Appendix B. SEM observation of fractured torsion specimen**

See Fig. B.18.

**References**


