MICROMECHANICS OF DUCTILE FRACTURE IN MULTIPHASE ALLOYS – APPLICATION TO CAST ALUMINIUM ALLOY WITH PENNY SHAPE VOIDS

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ABSTRACT
The use of many multiphase metal alloys reaching superior strength is impeded by a poor resistance to damage and fracture. In order to relate the fracture properties to the elastic and plastic behaviour and distribution of phases, it is essential to develop micromechanical models that properly capture the elementary damage mechanisms occurring in the different phases at the various length scales as well as the stress and strain partitioning among the phases. For the sake of illustrating the importance of modelling the stress transfer and accounting for the initial crack-like shape of voids, the ductility of a quasi cast aluminium alloy has been investigated experimentally and modelled. In contrast with classical void growth based analysis of ductile fracture, three key aspects of the particular mechanisms of fracture in cast Al alloys have received special attention: (i) a void nucleation condition that takes into account the stress partitioning among the elastic inclusions and the plastically deforming matrix, (ii) a proper description of the initial penny shape of the crack, (iii) a coalescence criterion incorporating the effect of the current void shape and void spacing.

1 INTRODUCTION
Nowadays, most advanced metal alloys used in structural applications exhibit a multiphase microstructure (the most notable exception is provided by high strength Al alloys). By “multiphase”, it is meant that the second phases amount for typically more than 5-10% contributing significantly to the global strength of the material, and that their scale is of the order of the micrometer or larger so that they can be considered more as inclusions leading to stress partitioning than as obstacles to dislocation motion by contrast with the precipitates in precipitation hardened materials. The microstructures are usually optimized such as to increase the strength (per unit mass), the resistance to plastic localization or both, following the logic of the composite materials science. The idea is to play with the volume fraction, topology and mechanical properties of the phases to create synergetic effects resulting from the mismatch of elastic and plastic properties. Good examples are provided by multiphase steels, $\alpha/\beta$ Ti alloys or $\gamma/\gamma'$ Ni based superalloys. The resistance to damage and fracture is often not a primary concern, which might lead to deceiving results when performing, after long materials engineering developments, a structural integrity assessment analysis. For instance, alloys involving brittle second phases (e.g. dual phase steels or aluminium alloys with Si particles) frequently involve premature damaging, low ductility and poor fracture toughness. There is thus an obvious need for developing microstructure-based damage models for multiphase alloys, e.g. [1,2].

Although most elementary plasticity and damage phenomena taking place in multiphase alloys have already received attention in the frame of ductile single phase alloys, many progresses are still required in order to properly address (i) multiple length scales as involved in complex microstructure arrangements (e.g. $\alpha/\beta$ Ti alloys); (ii) size effects related to the small dimension of one of the phase (e.g. in advanced $\gamma/\gamma'$ Ni based superalloys); (iii) the competition between different damage kinetics in the different phase which might lead to various mode of fracture depending on the applied stress state (e.g. Al alloys with precipitate free regions along grain
boundaries); (iv) heterogeneities in the distribution of the phases and complex topology such as bipercolated phases (e.g. duplex steels); (v) large volume fraction of second phases (>10%); (vi) the growth of penny shape voids (i.e. very flat voids) initiated by partial decohesion at interphases or by cleavage fracture of brittle second phases (e.g. dual phase steels).

Only the two last issues are discussed in this paper. More exactly, the objective is to present and discuss a model of ductility which can be used in general situations where a ductile matrix contains elastic brittle inclusions in relatively large volume fraction (between 10% to 50%) initiating a penny shape crack which progressively opens with plastic deformation and finally coalesce in a stable manner to reach final fracture. The usual approach assumes an effective porosity with effective spherical voids (see a discussion in [1]). This approach requires parameter adjustment and does not allow relating the ductility to the true particle content.

For the sake of illustration and validation, the model is applied to predict the ductility of a quasi eutectic cast aluminium alloy (see [3] for more details). The material has been investigated experimentally at the macro-level by performing tests under different states of stress triaxiality and at a micro-level by performing in situ tests in the SEM and fractographic observations. Such a system presents from the fundamental viewpoint the following advantages: (i) it is a sort of natural "in situ" composite with perfectly elastic particles (eutectic silicon) which are, for the quasi eutectic composition, relatively evenly distributed; (ii) the plastic properties of the matrix in this composite can be varied independently from the reinforcing particles features with a heat treatment – the annealed state noted A (low yield stress and large hardening capacity) and the T6 state (high yield stress and low hardening exponent) have been chosen.

2 EXPERIMENTAL RESULTS ABOUT DAMAGE IN CAST AL ALLOYS

The sequence of events in the damage accumulation process in both A and T6 materials observed during in situ tensile testing are gathered in Figure 1. The two materials, A and T6, involving 15% volume fraction of Si particles, present qualitatively a similar behaviour: the first step is cracking of the silicon particles, giving birth to a penny-shaped crack. Increasing deformation, leads to further particle cracking and crack opening. Progressively the cavities nucleated from the initial cracks grow and coalesce. This damage accumulation leads to final fracture. The only obvious difference between the two materials is in the nucleation step: in the T6 sample, particle cracking occurs right from the plastic yielding, whereas it occurs much later in the softer material A.
Figure 1: The schematics outline the damage events sequence. The micrographs has been taken from an in situ tensile test during the final stage of deformation.

Tensile tests on smooth and notched round bars were performed on both A and T6 material samples in order to quantify the ductility and the variation of the ductility as a function of the stress triaxiality.

3 MICROMECHANICAL MODEL FOR DUCTILE FRACTURE SPECIALIZED TO CAST ALUMINIUM ALLOYS

Several assumptions or approximations are made in order to develop a model for the damage and fracture process described in Fig. 1:

1. The initial void configuration consists of flat, penny-shape microcracks resulting from the fracture of the Si particles. The initial microstructure can be idealised by regularly distributed particles with initial spacing \( L_{px} \) and \( L_{pz} \) and radii \( R_{px} \) and \( R_{pz} \) (see Fig. 1). The dimensionless geometrical parameters are \( \chi_p = L_{px}/R_{px} \), \( W_p = R_{pz}/R_{px} \), and \( \lambda_p = L_{pz}/L_{px} \). As no orientation effects are present in the material, the distribution parameter \( \lambda_p \) is taken equal to 1. The particle volume fraction \( f_p \) can be expressed in terms of these last three variables. Penny-shape voids with a very small aspect ratio \( W_0 \) nucleate when the stress state in the particle is large enough for the inducing particle fracture. The particle is assumed to fail instantaneously when fracture initiates. The initial void shape \( W_0 \) is of course extremely small as the critical crack opening in Si is on the order of a few nanometers and particle diameter is several micrometers. The initial void volume fraction \( f_0 \) can be related to the particle void volume fraction \( f_p \) by

\[
f_0 = W_0 f_p.
\]

2. A critical stress based nucleation criterion is motivated by the fact that silicon is a brittle material. A critical maximum principal stress corresponds physically to the critical overall stress on the particle required to reach the critical stress intensity factor for the propagation of the sub-micron defects present within the particles [4].

3. The fracture process is also controlled by a stable void growth stage as can be deduced from the observed significant opening of the microcracks that become more or less ellipsoidal voids (Fig. 1) in the course of plastic deformation.

4. The void coalescence process (or void linking process) leading to small cracks is stable and also controlled by the plastic strain.

These aspects are incorporated into a constitutive model the response of the material before void nucleation, and for the nucleation, growth and coalescence of voids:

**Before void nucleation.** The material is assumed to be initially perfectly dense and homogeneous, i.e. the differences between the flow properties of the dendritic and interdendritic phase are neglected. The isotropic J2 flow theory is used to approximate the response of the material before voids start to nucleate. This is a reasonable assumption considering that no crystallographic or morphological texture is expected in these cast alloys.

**Nucleation.** The nucleation of voids by cleavage of Si particles is assumed to occur when the maximum principal stress in the particle reaches a critical value noted \( \sigma_c \). Following the Eshelby theory [5] and the “secant modulus” extension to plastically deforming matrix by Berveiller and Zaoui [6], it was proposed by the Beremin group [7] that the maximum principal stress in an elastic inclusion \( \sigma_{max}^{proc} \) can be related to the overall stress state \( \Sigma \) by the following expression:
\[
\sigma_{\text{princ}}^{\text{max}} = \Sigma_{\text{princ}}^{\text{max}} + k(\Sigma_{\varepsilon} - \sigma_0)
\]  

(2)

where \(\Sigma_{\text{princ}}^{\text{max}}\) is the maximum overall principal stress, \(\Sigma_{\varepsilon}\) is the overall effective von Mises stress and \(k\) is a parameter of order unity which is a function of the inclusion shape and loading direction. For the fracture of spherical inclusions, reasonable values for \(k\) lie between 1 and 2 (Beremin [7] proposes \(k = 1.6\) based on experimental measurements in A508 steel).

**Growth and coalescence.** The extension of the Gurson model used in this paper to account for the effect of the growth and coalescence of voids on the behaviour of the material has been presented in details in refs. [8,9]. It is based on the works by Gologanu et al. [10] for the account of the void aspect ratio and by Thomason [11] for the onset of coalescence with extensions to strain hardening and for the modelling of the coalescence process. Only the structure of the model will be recalled here. The model is based on two different solutions for the expansion of a void in an elastoplastic material: one solution is called "void growth" corresponding to diffuse plasticity around the void, and the other is called "void coalescence" corresponding to localized plasticity in the intervoid ligament. These two solutions can be presented in the form of two distinct plastic yield surfaces \(\Phi_{\text{growth}}\) and \(\Phi_{\text{coalescence}}\) supplemented by evolution laws for the internal variables of the model (the porosity \(f\), the void aspect ratio \(W\), the relative void spacing, \(\chi\) and the mean yield stress of the matrix material \(\sigma_y\) is the mean effective plastic strain of the matrix material) and the normality rule for the plastic strain increment. The first yield surface to be reached is \(\Phi_{\text{growth}}\). With increasing deformation \(\Phi_{\text{growth}}\) first tends to expand due to hardening and then to contract due to void growth softening. Void growth and ligament reduction also induces a contraction of \(\Phi_{\text{coalescence}}\). When the two yield surfaces intersect at the current loading point, the transition to coalescence occurs. With increasing deformation the coalescence yield surface tends to contract very rapidly towards the zero stress state.

When criterion (2) is fulfilled, with the corresponding strain noted \(\varepsilon^p = \varepsilon^p\), the nucleation is assumed to start and to take place during a range of strain \(\Delta\varepsilon^p\). The evolution laws for the porosity is given by

\[
\dot{f} = (1 - f)\dot{\varepsilon}^{pl} + g(\varepsilon^p)\dot{\varepsilon}^{pl}
\]

where the function \(g\) accounts for the increase in porosity due to the nucleation of the penny shaped cracks.

The constitutive model has been implemented in the general purpose finite element code "ABAQUS Standard" through a User defined MATerial subroutine (UMAT) with a fully implicit integration scheme for the J2 flow theory before nucleation, for the extended Gurson model and for the coalescence response. Note that the uniaxial response \(\sigma_y = h(\varepsilon^p)\) is introduced in the model point by point to allow an exact match with the experimental curve. The fracture strain is taken when full coalescence has been completed in the most loaded element, i.e. when a mesocrack has been formed. This strain is very close to the strain obtained experimentally on the uniaxial tension specimens when measuring the reduction of section on the broken parts of the specimens. Very refined meshes are used for all the simulation with typically 50 fully integrated four-noded axisymmetric elements on half the cross-section.

### 4 RESULTS OF THE MODELLING AND DISCUSSION

As shown in Fig. 2, a preliminary set of calculations for pure uniaxial tension conditions (i.e. without necking) with various initial void aspect ratio \(W_0\) at constant volume fraction of particles \(f_0\) have demonstrated that, to a very good approximation, the ductility can be considered as independent of the initial void aspect ratio \(W_0\) when \(W_0\) is typically lower than 0.02. Hence, in
order to avoid numerical problems appearing at very low $W_0$, the initial shape $W_0$ has been taken equal to 0.01 and thus $f_0$ equal to 0.01 $f_p$ for all the calculations performed in this study.

![Figure 2](image1.png)

Figure 2: The ductility $\epsilon_f$ is independent of $W_0$ for low $W_0$ at constant particle volume fraction $f_p$. The example is given here for flow properties typical of the studied aluminium alloys (i.e. $n = 0.1$ and $\sigma_0/E = 0.002$)

![Figure 3](image2.png)

Figure 3: Variation of the ductility as a function of the mean stress triaxiality in the most damaged region, comparison of experiments and modelling for (i) for the A heat treatment using $f_p=15\%$, $W_0=0.01$, $\sigma_c/\sigma_0=6.15$; (ii) For the T6 heat treatment using $f_p=14\%$, $W_0=0.01$, $\sigma_c/\sigma_0=6.15$

In order to simulate the tensile tests on notched and smooth cylindrical bars, the only “free” parameter to be calibrated is the critical stress $\sigma_c$ for void nucleation. The parameter $\Delta\sigma^*$ was
kept constant equal to 2\% in every calculation (which is reasonably small compared to the overall ductility). In other words, we consider here that cavities nucleate at a critical stress which is representative of the average distribution of brittleness. The real behaviour is of course a dispersion in particle sizes (and also local environment), and an intrinsic dispersion of the stress for which the particle will fracture due to the intrinsic brittleness and defect sensitivity of Si. The critical stress $\sigma_c$ had been tuned on material A for uniaxial tension, i.e. by finding the value that leads to the experimental ductility. The experimental particle volume fraction is equal to 15\%. The initial void shape is imposed to be 0.01. The calibration provides a value of $\sigma_c$ equal to 550 MPa. The effect of the factor $k$ in the range 1 to 2 has been tested for the problem at hand and no major effect has been observed: $\sigma_c$ changes by no more than 100 MPa when increasing $k$ from 1 to 2. The value $k = 2$ was chosen for this study. The response of material T6 has been simulated using exactly the same values $\sigma_c=550$MPa and $W_0=0.01$, and the proper flow properties.

Fig. 3 presents the comparison between the experimental and predicted ductility (from the simulations of the tensile tests on uniaxial and notched specimens) as a function of the mean stress triaxiality in the most damaged region for the A and T6 materials. The decrease of the ductility with decreasing notch radius has been recognized from a long time in the literature (e.g. [12]). Good agreement is observed between the prediction and the experiments, considering the experimental dispersion and the approximation made by taking the response of the full material as flow properties for the matrix in the model. For the case of the T6 treatment, $\sigma_c = 550$MPa leads to very early nucleation as also observed experimentally. On the other hand, modelling the A alloy without accounting for delayed void nucleation, i.e. using $\sigma_c = 0$, leads to underestimate the ductility by more than a factor of two. In other words, depending on the state of hardening in the matrix the ductility of these materials can be controlled by both the nucleation and growth. None of these two stages can be neglected.

Accounting for the initial penny shape of the freshly nucleated voids allows to directly link the initial void volume fraction to the particle volume fraction, avoiding the introduction an effective porosity parameter not directly related to a microstructural quantity. Many other materials involving brittle second phases will present a similar mechanisms of particle fracture leading to initial flat voids, e.g. dual phase steels, WC-Co alloys, AlSiC composites. Note that the approach remains valid for partial interface decohesion as observed in AlSiC composites for instance.

Acknowledgements. The authors wish to thank Dr J.C.Ehrstrom and Dr G. Laslaz for enlightening discussions. This project was partly supported by PECHINEY and a Franco Belgian Tournesol collaborative Program and the German Academic Exchange Service, DAAD.

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