A study of the influence of precipitate free zones on the strain localization and failure of the aluminium alloy AA7075-T651

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Age-hardened aluminium alloys have to various degrees precipitate-free zones (PFZs) along grain boundaries. The PFZs are weak zones and their existence promotes combined transgranular and intergranular fracture, thus reducing the ductility of the alloy. In this study, transmission electron microscopy (TEM) is used to display the geometrical properties and the chemical composition of the PFZs in the AA7075-T651 aluminium alloy. PFZs are found along grain and sub-grain boundaries and their widths are about 40 nm and 20 nm, respectively. The PFZs are depleted of alloying elements compared with the nominal composition due to grain boundary precipitation, but still they contain a certain amount of such elements in solid solution which will contribute to increase the yield strength and the work hardening compared to pure aluminium. Based on the results from the TEM study a micromechanical finite element model of an idealized microstructure including grains and soft zones along the grain boundaries is established. The Gurson model was used to represent the behaviour of the material in the grains and in the soft zones, using different initial void volume fractions to account for grain boundary precipitation. Several loading conditions were applied to the micromechanical model in order to evaluate the localization of strains inside the soft zones and thus to get a better understanding of the role of the PFZs in ductile fracture of age-hardened aluminium alloys. It was found that the global failure strain varies non-monotonically with the global stress triaxiality due to the heterogeneity of the idealized microstructure.

Keywords: age-hardening; precipitate free zones; transmission electron microscopy; micromechanics; localization; failure

1 Introduction

The AA7075 high strength aluminium alloy considered in this paper is widely used due to its competitive strength to weight ratio [1]. It belongs to the class of age-hardenable aluminium alloys, such as the 2xxx, 6xxx and 7xxx series, where the strength is gained from a final precipitation process during artificial ageing. The precipitates provide an appreciable impediment to plastic deformation by slip. A general review of these

microstructural evolutions for the cited alloys can be found in [2], based on a number of observations made through atom probe field-ion microscopy and transmission electronic microscopy (TEM).

The high-strength properties of the 7xxx series alloys are shadowed somewhat by loss of other properties. In the case of the AA7075 aluminium alloy, the most critical are the susceptibility to stress-corrosion [3] and the loss of ductility [4]. These weaknesses are to a large extent attributed to the existence of so-called precipitation free zones (PFZs) adjacent to the grain boundaries (GBs) where the material is softer. It has been recognized for a long time that during the isothermal ageing sequence when elaborating these materials, the precipitation-hardenable aluminium alloys exhibit a condition in which the interior of the grains is highly hardened while the grain boundaries and their surroundings are softer. Following the work of Geisler [5], a number of studies have been carried out in order to understand the mechanisms that are responsible for the formation of PFZs [6]–[8]. These softer zones are relatively free of precipitates and the above investigations indicate that this can be due to either an absence of a critical vacancy concentration in the vicinity of the GBs or to a depletion of solute atoms following a preferential precipitation at the GBs. In the latter case, the zones are narrow bands (smaller than 100 nm) and the PFZ is a solid solution with relatively low solute content. In the former case, when a slow quenching rate or an interrupted quench is applied, the PFZ width is of the order of a micron and the PFZ is a highly supersaturated solid solution. As a rule, the width and the properties of the PFZ depend on solution treatment temperature, quenching rate, ageing temperature and ageing time.

The above remarks lead to the fact that beside constituent particles, dispersoids and hardening precipitates, the AA7075 aluminium alloy in peak hardness condition

contains zones with different plastic flow. All these heterogeneities contribute in a way or another to the initiation of failure and its propagation, and to the localization of plastic flow leading to fracture. Complex competition between different failures modes is thus expected and indeed observed. Earlier investigations concluded that the dominant feature of fracture in high strength Al-Zn-Mg alloys is intergranular, though transgranular fracture also occurs partially [9]. Kawabata and Izumi [10][11] have reported predominant intergranular failure for an Al-Zn-Mg alloy. They observed that the intergranular fracture occurred at the GBs lying at 45° to the tensile axis and suggested that shearing along the GBs plays an important role. In an important paper, Ludtka and Laughlin [4] investigated in a very comprehensive manner the mechanisms responsible for failure in three high-strength 7075 alloys with different Mg and Zn contents but all produced and processed in an identical manner. The three materials only differed in the volume fractions of the fine matrix strengthening precipitates. While the material with the lowest contents of Mg and Zn showed predominantly transgranular failure, the two others (intermediate and high contents) showed predominantly intergranular fracture. However, partial intergranular and transgranular cracking was observed in the two cases respectively.

There are a number of investigations in the literature considering PFZs and their effects on the mechanical behaviour of high strength aluminium alloys. These studies suggest that the grain morphology and the PFZs located at the grain and sub-grain boundaries may play an important role in the failure process of such alloys. A series of approaches are used to describe the fracture toughness of aluminium alloys in the case where one fracture mode is dominant. In the general case where several fracture modes are simultaneously present, a number of authors have proposed some mixture rules between the fracture toughness predicted for each of the individual fracture modes

alone. These different approaches are reviewed by Dumont *et al.* [12] who also developed a simple analytical model for situations with competing fracture modes, both ductile, either intergranular or transgranular. In one of these models, Kawabata and Izumi [10][11] developed the idea that intergranular fracture of the alloy occurs due to the void formation at interfaces between the GB precipitates and the matrix followed by their growth and coalescence in the PFZ. Ludtka and Laughlin [4] suggested that the fracture toughness of the AA7xxx series alloys is dependent on two parameters, the coarseness of the matrix slip and the difference in strength between the matrix and the PFZ. They also argued that this difference in strength between the matrix and the PFZ can be considered a relative measure of the tendency towards intergranular failure, as the higher is this difference, the more likely void initiation will occur within the PFZ.

The competition between intergranular and transgranular failure was studied numerically by Pardoen *et al.* [13]. As the PFZ is soft and the first to deform plastically, the elastic grain imposes a strong constraint on the PFZ leading to large stress triaxiality allowing rapid growth and consequently rapid coalescence of the voids in this zone. However, if the stress in the grain reaches the yield limit of the matrix before coalescence in the PFZ, the stress triaxiality will drop in the PFZ and with higher hardening rate induce a higher constraint in the grain and the voids will grow more rapidly in these grains. Due to the low hardening rate of the grain, a state of softening can be reached and voids may coalesce in the grain. Low global stress triaxiality will favour the transgranular failure mechanism.

The prediction of the influence of the PFZs on the macroscopic behaviour is challenging for several reasons. Firstly, the mechanical behaviour of the PFZs, different from the bulk since depleted of hardening precipitates, remains difficult to evaluate due to the nanometre scale of the zones. The evaluation of these properties can be done by

using macroscopic specimens of temper conditions that are believed to be similar to the PFZ material, even though the microstructure of such macro-specimens (grains, inclusions, etc.) will inherently influence their behaviour. If it is assumed that the PFZ is a highly supersaturated solid solution, the behaviour of the W temper should be representative for the PFZs. Secondly, the stress states that PFZs are subjected to may significantly differ from the macroscopic loading conditions due to geometrical constraints. This can be evaluated by numerical simulations but again, due to the nanometre size of the PFZs, several length scales need to be modelled in order to reproduce the failure modes observed at a macroscopic scale on physical specimens. Finally, and as strongly underlined in the literature, even in the most idealized description of the microstructure, the number of parameters potentially influencing the macroscopic behaviour is rather large: the width of the PFZ, the size and spacing of grain boundary precipitates, the size and spacing of dispersoids inside the grain, and the yield stress and work hardening behaviour of both the grain interior and the vicinity of the grain boundaries [14]–[17]. For all these reasons, we strongly emphasize the qualitative character of the numerical investigation presented in this study. In addition to the microstructural characteristics of the material, the stress state, usually represented by the stress triaxiality and the Lode parameter, is known to be important for ductile fracture of macroscopically homogeneous materials [18]–[26].

The objective of this paper is twofold: to experimentally characterize the microstructure and the PFZs of the studied high-strength AA7075-T651 aluminium alloy through transmission electronic microscopy (TEM) and energy X-ray dispersive spectroscopy (EDS), and to present a qualitative numerical model based on these observations to capture changes of the macroscopic failure modes. This will help later to analyse the results obtained in recent extensive experimental investigations carried

out on this material including ballistic impact tests [19][28] and quasi-static material tests under various stress states [29][30].

Section 2 describes the high strength AA7075-T651 aluminium alloy used in this investigation. It also provides the microscopic and mechanical features obtained in former studies, and the characterization of the mechanical behaviour of the AA7075 alloy in W temper used to model the PFZ's mechanical behaviour. Section 3 presents in detail the characterization of the material using TEM and EDS allowing the determination of the different constituents and their geometrical features, in particular those of the PFZ, and the chemical composition of the microstructural elements of the material. Based on the qualitative features of the microscopy investigation, Section 4 displays the micromechanical model of an idealized microstructure and its finite element implementation, designed to evaluate the influence of loading on the local states of stress and the localization process along the grain boundaries. Also the boundary conditions used to span a range of stress triaxialities and Lode angles and the material modelling of grains and soft zones are described. Section 5 provides the obtained numerical results in the form of stress-strain behaviour depicting strain localization, failure limit diagrams and failure loci. Finally, Section 6 contains the discussion and the conclusions of the study.

2 Material

2.1 Microstructure

The AA7075 aluminium alloy was delivered as 20 mm thick plates obtained by a combined cold and hot rolling process. The nominal chemical composition is presented in Table 1. The material was provided in the T651 temper, which implies that the material is artificially aged to peak hardness condition and subsequently stress-relieved by slight stretching [1]. The artificial ageing results in a high density of nano-sized

hardening precipitates which increases the strength of the alloy. In addition, the AA7075-T651 material contains constituent particles and dispersoids (see [31] for details).

In the rolling direction, the plate has nominal yield and tensile strengths of 505 and 570 MPa, respectively. Due to the rolling operations, the non-recrystallized grains are pancake-shaped and the constituent particles are broken-up and aligned along the rolling direction in the plane of the plate [19]. The rolling process implies crystallographic texture and leads to anisotropic strength, plastic flow and ductility [19]–[30]. The crystallographic texture of the plates of AA7075-T651 was determined using the electron back-scatter diffraction (EBSD) technique in a scanning electron microscope (SEM). The grain map presented in Figure 1 shows the grain structure and orientations in the plane normal to the rolling direction (RD). It is seen that the alloy has a non-recrystallized structure with flat, elongated grains due to the rolling process. Using grain maps in the three principal directions of the plate, the average grain size and its standard deviation were determined as: $l_{RD}^{G} = 91 \pm 31$ μm along the RD, $l_{TD}^{G} = 41 \pm 15$ μm along the transverse direction (TD) and $l_{ND}^{G} = 13 \pm 5$ μm along the normal direction (ND). In average, the grains are seven times longer than they are thick, so the grain boundaries (GBs) are seven times more densely distributed in the ND than along the RD of the plate. As will be demonstrated below, the grains consist of sub-grains separated by low-angle grain boundaries (LAGBs), defined by a misorientation between the two adjacent grains less than about 10 degrees. High-angle grain boundaries (HAGBs) are those with misorientation greater than about 15 degrees. The orientation distribution function (ODF) of the AA7075-T651 alloy presented in Figure 2 shows that the crystallographic texture is strong (maximum intensity about 30) and

typical for rolled plates [32], and thus explains that marked plastic anisotropy found in previous studies [29].

2.2 Brief summary of previous experimental results

Previous experimental studies by some of the authors [19]–[30] have included quasi-static material tests exploring a wide range of stress triaxiality and different material directions, dynamic tensile tests in a split-Hopkinson tension bar and plate impact tests using a compressed gas-gun. Optical and scanning electron microscopy was used to examine the failure modes. In uniaxial tension tests on cylindrical specimens taken in the plane of the plate, the crack growth was found to be partly intergranular along the GBs or PFZs and partly transgranular by void formation around fine and coarse intermetallic particles. Tensile tests in the ND exhibited largely intergranular fracture due to the large and elongated grains in the rolling plane. Using notched cylindrical specimens to increase the stress triaxiality, delamination occurred along the GBs in the rolling plane and at right angle to the primary crack path. In the impact tests, delamination along the GBs in the rolling plane and fragmentation of the plates occurred due to the tensile stresses set up during the perforation process.

It was further concluded that the ductile fracture of the AA7075-T651 is influenced by a number of features, such as the plastic anisotropy, the elongated grain structure, the stringers of constituent particles aligned along the rolling direction, and the PFZs along the GBs. In [31], the damage resulting from large particles (constituents) and small particles (dispersoids) is studied in great detail.

2.3 Work-hardening curves in W and T651 tempers

As already mentioned, the aim of the current study is to investigate in more detail the geometrical and chemical features of the PFZs and their potential influence on strain

localization and eventually ductile failure. It will be shown below that even if the PFZs are free of hardening precipitates and depleted of solute atoms due to GB precipitation, they still contain a significant amount of alloying elements in solid solution, even close to the nominal concentration for some elements. These elements in solid solution will increase the strength and work hardening of the material inside the PFZs compared with pure aluminium.

In an attempt to estimate the strength and work-hardening behaviour of the PFZs, uniaxial tensile tests were performed on the AA7075 aluminium alloy in W temper. This temper is obtained by solid solution heat treatment followed by water quenching. The alloying elements are then in super-saturated solid solution. Since this is an unstable condition, the cylindrical specimens were kept in liquid nitrogen until testing and the tests were completed within 15 min at room temperature.

Figure 3 presents representative work-hardening curves for tempers W and T651 based on three parallel tests along the RD in terms of the Cauchy stress, $\sigma = F / A$, and the logarithmic strain, $\varepsilon = \ln\left(A_0 / A\right)$, where A_0 and A are the initial and current areas of the minimum cross section of the test sample. The sample geometry and the test set-up and procedures are as described in [29]. The average yield stress is significantly lower for W temper ($\sigma_y = 170$ MPa) than for T651 temper ($\sigma_y = 540$ MPa), but the material work hardens more in W temper. The failure strain is slightly lower for temper W ($\varepsilon_f = 0.137$) than for temper T651 ($\varepsilon_f = 0.169$), while the failure modes are similar, i.e., localization of strains along a 45° band.

The work-hardening curve for W temper exhibits oscillations after 2% strain. These oscillations are assumed to be caused by the Portevin-Le Chatelier (PLC) effect, which is due to dynamic strain ageing, i.e., pinning of dislocations by solute Mg atoms, resulting in negative steady-state strain-rate sensitivity. Experimental evidence on Al-

Mg alloys suggests that the PLC effect may promote premature strain localization along shear bands [33]. The PLC effect is not observed for the T651 temper, since the Mg atoms are tied up in the hardening precipitates. Thus, the somewhat lower failure strain observed for the W temper could well be a consequence of the PLC effect.

It is important to recall that the behaviour of the W temper is considered as representative of the PFZ only in a qualitative manner. However, it is believed that by assuming the PFZs to behave as the W temper and the grain as the T651 temper, some insight into the role of the PFZs in the strain localization and the ductile failure process of the AA7075-T651 material may be achieved from micromechanical simulations of idealized microstructures.

3 Characterization of precipitate-free zones

As already mentioned, the 7xxx series of aluminium alloys are characterized by the presence of PFZs at nanometre scale, located around the GBs. They are created as a consequence of quenching after the solution heat treatment and subsequent ageing. These zones are generally softer than the matrix hardened by precipitates. Experiments indicate that plastic strain can be highly localized inside these zones and can therefore lead to premature failure of such materials [12]. The PFZs are engendered by two closely related phenomena:

- the local depletion of vacancies which inhibits the formation of fine dispersion of hardening precipitates
- the local solute depletion initiated by heterogeneous precipitation of phases at the GBs

These two phenomena require atom mobility and occur therefore during the thermal treatment of the alloy. The cooling rate of the quenching operation influences the width

of the PFZs [34]; i.e., fast cooling inhibits the migration of vacancy and solute toward the GBs and therefore reduces the size of the PFZs.

3.1 TEM analysis

A transmission electron microscope (TEM) study was performed on the AA7075-T651 alloy to reveal some of the features of the microstructure. Two TEMs have been used: a Philips CM30 operated at 150 KV which provided bright field images such as those presented in Figure 4, and a Jeol 2010F operated at 200 kV used for X-ray energy dispersive spectroscopy (EDS) elemental mapping (see Figures 5 and 6). In the latter case, the TEM was operated in Scanning Transmission mode (STEM) with 1.0 nm probe size. The EDS was performed with an INCA system from Oxford Instruments.

Figure 4 (a) is taken in the RD-TD plane and shows that grains are elongated and dispersoids are aligned in the rolling direction (RD). Figure 4 (b)–(d) show the hardening precipitates inside the grains and the presence of PFZs along the GBs. In average, the total width of the PFZs are larger in the case of HAGB ($l_H^{PFZ} \approx 40$ nm) than for LAGB ($l_L^{PFZ} \approx 20$ nm). The GBs are defined as LAGB (HAGB) when the misorientation between the two neighbouring grains is $\leq 10^{\circ}$ ($\geq 15^{\circ}$) (see [35]). A fortiori, sub-grains within the same grain are separated by a LAGB since they have nearly the same orientation (within a few degrees). The misfit in the orientation of two grains is accommodated by perturbations in the atomic packing at the GB. In the case of HAGBs, these perturbations become severely disordered and promote the vacancy and solute migration more than the LAGBs. The PFZ formation is then facilitated around the HAGBs. It is also observed that the LAGBs contain a higher amount of smaller GB precipitates, while lower amounts of larger GB precipitates form along HAGBs. In the case of 7xxx alloys, the precipitates at the GBs need a certain degree of coherency with

the matrix in order to form and grow. This cannot be achieved if the adjacent grains have large misorientations. The orientations <110>Al and <112>Al stipulated on the TEM pictures correspond to the zone axis (orientation) of the respective grains along the viewing direction.

3.2 Energy dispersive X-ray spectroscopy

An energy dispersive X-ray spectroscopy (EDS) analysis was performed in parallel to the TEM analysis and gave information about the chemical composition of the microstructural features. Figure 5 shows the maps of several alloying elements on a given scanned area. The upper-left picture in Figure 5 presents the scanned area and depicts a PFZ along a GB, fine precipitates in the adjacent grains, two large precipitates formed at the GB (3-4) and a large precipitate in the grain (1) that was formed on a dispersoid (2). The five maps given in Figure 5 are the spatial distribution of different alloying elements (Zn, Mg, Cu, Cr, Fe) within the area. The following observations can be drawn from the maps:

- The fine precipitates contain Zn and Mg, as expected. Based on [36], Cu may enter the composition of the fine precipitates as well, but if so, it must be to a level below the detection limit of the EDS used in this work.
- The large precipitates (1), (3) and (4) have a Zn-Mg-Cu composition.
- Cr is present in the dispersoid (2) on which particle (1) is nucleated, and in another dispersoid on which particle (3) is nucleated, but Cr does not enter the composition of the Zn-Mg-Cu precipitates.
- Mg, Cu and to a lower extent Zn are present along the GB as thin continuous films. Solute depletion in the PFZ is also observed.

- Fe has no preferential location, indicating that this element is not associated with precipitation and mostly left in solid solution. This is also the case for the elements Mn, Ti and Si, the maps of which are not presented here.

Figure 6 gives a more accurate description of the alloying content across the whole scanned area (i.e. the whole picture), inside the grain (area 5) and inside the PFZ (area 6). These data confirm the observations made from Figure 5 and give the following additional information:

- Zn and Mg have slightly lower values in the grain than in the alloy composition. This confirms the presence of a low volume fraction of large Zn-Mg-Cu precipitates nucleated on dispersoids (like (1) and (3) in Figure 5) and along GBs (like (3) and (4) in Figure 5), in addition to a much higher volume fraction of small Zn-Mg-Cu hardening precipitates.
- Zn, Mg and possibly Cu are depleted in the PFZ area, most probably due to the formation of Zn-Mg-Cu GB precipitates that use this solute. Compared with the grain (area 5), the Zn content in the PFZ (area 6) is lower by a factor of 4, whereas the Mg and Cu content is only lower by a factor of 2 or less.
- Even though it is depleted, the PFZ still contains a low amount of alloying elements in solid solution.
- Cr is strongly depleted in the grain (area 5) and PFZ (area 6), indicating that most of it is absorbed into dispersoids. However, its (low) value is similar in grain and PFZ.
- Fe, Mn, Ti and Si have similar values in all areas and close to their respective nominal compositions, indicating that these elements do not have a strong association with precipitation and therefore most of them are left in solid

solution. This observation indicates that the formation of PFZs is a vacancy driven process. Consequently, the composition of a certain element in the PFZs should be similar to its composition in the nearby grain. The exceptions are Zn, Mg and perhaps Cu, as mentioned above, because GB precipitates contain these elements and therefore they become depleted in the neighbouring PFZ.

- Cu has unrealistically high values in all areas. This may be an artefact due to the presence of an oxide layer on the sample's surface as a consequence of the sample preparation.

This analysis suggests that the PFZs, although often considered as pure aluminium zones inside a harder matrix, contain non-negligible amounts of alloying elements in solid solution. The behaviour of the PFZs could then differ from pure aluminium, in terms of plastic hardening for instance. These observations are both important and helpful for the modelling of the microstructure.

4 Micromechanical model

4.1 Finite element discretization

A finite element model of an idealized microstructure representing several grains and soft zones located at the GBs was developed in an attempt to simulate the above observed microstructure in a qualitative manner, and used to evaluate the influence of the applied loading on the local stress states and the strain localization along the GBs. The numerical simulations were performed using the explicit solver of the finite element code LS-DYNA [37]. Quasi-static simulations were carried out using mass-scaling to reduce the computation time. It was checked that the kinetic energy remained a small percentage of the internal energy.

The idealized microstructure is modelled with hexagonal grains using one layer of hexahedral solid elements, see Figure 7. Thus, the microstructure is modelled as two-dimensional, assuming uniform conditions through the thickness. The use of hexagonal-shaped grains was motivated from the TEM images of the PFZs where three-branch intersections between grains and sub-grains are mainly observed (see also Figure 19 in [4]). These soft zones are represented by narrow layers of elements between the neighbouring grains. The number of elements over the width of the soft zone was found to have limited influence on the results and was fixed to four in the rest of the study.

A close-up of a three-branch intersection between neighbouring grains is provided in Figure 8, where L^G and L^{SZ} are the characteristic grain size and the width of the soft zones, respectively. The aspect ratio $A = L^G / L^{SZ}$ then defines the relative size of the soft zones with respect to the grain size. In the TEM study, the size of the sub-grains l^G was found to be about 10 μm, while the width l^{PFZ} of the PFZ was in the range 20-40 nm. Thus, the experimental aspect ratio, defined as $a = l^G / l^{PFZ}$, is between 250 and 500. These values are very large and challenging to reproduce numerically with reasonable computation times. Consequently, numerical simulations were performed with $A = 20$, and a limited parametric study was conducted to evaluate the sensitivity of the results to the aspect ratio.

Eight-node solid elements with selective reduced integration were used. The layer thickness, i.e., the thickness of the solid elements, was chosen of the same order as the in-plane dimensions of the elements. Since the element size is governed by the discretization of the soft zones, which are very narrow compared with the size of the grains, the number of elements inside the grains is necessarily large. With the adopted mesh size, i.e., with four elements across the width of the soft zones, each grain

contains 882 elements. As a result, only 16 grains were modelled to keep the computation time within reasonable limits.

4.2 Boundary conditions

Several boundary conditions (BCs) were applied to cover a range of stress triaxialities and Lode angles. The node sets and coordinate system used to define the BCs are shown in Figure 9.

Biaxial straining is achieved by specifying the following displacements: $u_1 = U$ for node set (1) and $u_1 = 0$ for node set (3); $u_2 = \xi U$ for node set (2) and $u_2 = 0$ for node set (4); node sets (5) and (6) are constrained to remain plane-parallel but otherwise free. The scalar ξ is set to values between -0.5 and 1 to obtain different degrees of biaxial straining. Note that even if the displacements u_1 and u_2 are prescribed here to be proportional, the resulting strain path will be slightly non-proportional, i.e., the strain-rate ratio $\beta = \dot{E}_2 / \dot{E}_1$ will vary somewhat with straining, where E_1 and E_2 are the major and minor principal global logarithmic strains. Uniaxial tension is obtained by removing the BC for node set (2) and instead requiring this node set to be plane-parallel to node-set (4) but otherwise free. To investigate the influence of the orientation of the microstructure, two cases were considered: $x = x_1, y = x_2, z = x_3$ and $x = x_2, y = -x_1, z = x_3$; i.e., the local coordinate system used to describe the BCs is rotated 90º in the latter case.

With the adopted BCs, plane stress conditions are insured in the grains, while the soft zones are subjected to highly triaxial stress states. Since yielding occurs first in the soft zones, the elastic grains constrain the behaviour of the soft zones and increases the stress triaxiality. However, these stress states are believed to be somehow

representative of the physical processes, provided the soft zones actually yield sooner than the grains.

4.3 Material modelling

A hypoelastic formulation of the Gurson model [38] is applied in the simulations, using the Jaumann objective stress rate and assuming isotropic elastic and plastic behaviour. The Gurson yield function is defined by

$$\Phi = \frac{\bar{\sigma}^2}{\sigma_M^2} + 2fq_1 \cosh\left(\frac{q_2}{2}\frac{\sigma_{kk}}{\sigma_M}\right) - \left(1 + q_3 f^2\right) = 0 \tag{1}$$

where $\bar{\sigma} = \sqrt{\frac{3}{2} s_{ij} s_{ij}}$ is the von Mises equivalent stress, $s_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$ is the stress deviator, σ_{ij} is the Cauchy stress tensor, and σ_M is the flow stress of the matrix material. The coefficients q_1, q_2, q_3 were introduced in [39] and the values suggested there are adopted: $q_1 = 1.5$, $q_2 = 1$ and $q_3 = q_1^2$. The void volume fraction f is defined by the evolution equation

$$\dot{f} = (1 - f) D_{kk}^p \tag{2}$$

where the plastic rate-of-deformation tensor D_{ij}^p is defined by the associated flow rule. The initial void volume fraction is denoted f_0 and in this study void nucleation is neglected. The flow stress σ_M is defined as a function of the plastic strain of the matrix material, i.e., $\sigma_M = \sigma_M\left(\varepsilon_M\right)$, where ε_M is defined from the plastic power as

$$\dot{\varepsilon}_M = \frac{\sigma_{ij} D_{ij}^p}{(1 - f)\sigma_M} \tag{3}$$

The relation $\sigma_M = \sigma_M\left(\varepsilon_M\right)$ is given in the form of tabulated data in this study.

The elastic behaviour was assumed the same for the grains and the soft zones and defined by Young's modulus $E = 70000\ \mathrm{MPa}$ and Poisson's ratio $\nu = 0.3$. The work-hardening curves of the grains and the soft zones were determined from the true

stress-strain curves up to necking of AA7075 in temper T651 and W, respectively, see Figure 3. The work-hardening curves were assumed to follow a Voce relation, i.e., $\sigma_M = \sigma_0 + Q\left(1-\exp\left(-C\varepsilon_M\right)\right)$, where the parameters σ_0, Q and C were fitted to the experimental data using the least squares method. The Voce relation was used to extrapolate the work-hardening curve to larger strains than those obtained experimentally in uniaxial tension. The porosity was neglected in the calibration of the work-hardening curve, since the void growth in uniaxial tension is small owing to the low stress triaxiality [40][41]. The initial porosity f_0 was taken as 10^{-3} within the grains and as 10^{-2} within the soft zones. These values are qualitative, but motivated from the observation in the TEM study of GB precipitation which is anticipated to promote void nucleation during straining. Failure is assumed to occur at a critical porosity f_C, and in the simulations $f_C = 0.2$ was adopted. A parametric study in which f_C was varied between 0.2 and 0.9 showed that the value of the critical porosity had no noticeable influence on the global failure strain due to the strong localization in the soft zones. As the critical porosity was attained in an integration point, the element was eroded.

4.4 Global stress and strain measures

The global principal Cauchy stresses of the micromechanical FE model are obtained as

$$\Sigma_1 = \frac{F_1}{A_1}, \quad \Sigma_2 = \frac{F_2}{A_2}, \quad \Sigma_3 = \frac{F_3}{A_3} \tag{4}$$

where F_i are the resultant forces in the x_i directions with $i = \{1,2,3\}$, and A_i are the current areas of the side faces with unit normal vectors along these directions. The corresponding principal strains are defined as

$$E_1 = \ln\frac{L}{L_0}, \quad E_2 = \ln\frac{H}{H_0}, \quad E_3 = \ln\frac{T}{T_0} \tag{5}$$

where L, H and T are the current dimensions of the micromechanical FE model in the x_1, x_2 and x_3 directions, respectively; L_0, H_0 and T_0 being the corresponding initial values. The global equivalent stress and strain are defined according to von Mises plasticity, viz.

$$\overline{\Sigma} = \sqrt{\Sigma_1^2 + \Sigma_2^2 + \Sigma_3^2 - \Sigma_1\Sigma_2 - \Sigma_2\Sigma_3 - \Sigma_3\Sigma_1} \tag{6}$$

$$\overline{E} = \int \sqrt{\frac{4}{3}\left(dE_1^2 + dE_2^2 + dE_3^2 + dE_1dE_2 + dE_2dE_3 + dE_3dE_1\right)} \tag{7}$$

where elastic strains are neglected and the associated flow rule is assumed in the derivations. Note that the equivalent strain is obtained by integration along the strain path as the logarithmic strains are not entirely proportional. The global stress triaxiality Σ^* and the Lode parameter μ_Σ are defined as

$$\Sigma^* = \frac{\Sigma_I + \Sigma_{II} + \Sigma_{III}}{3\overline{\Sigma}}, \quad \mu_\Sigma = \frac{2\Sigma_{II} - (\Sigma_I + \Sigma_{III})}{\Sigma_I - \Sigma_{III}} \tag{8}$$

where $\Sigma_I \geq \Sigma_{II} \geq \Sigma_{III}$ are the ordered global principal stresses. The local equivalent stress and strain, $\overline{\sigma}$ and $\overline{\varepsilon}$, as well as the local values of the stress triaxiality and Lode parameter, σ^* and μ_σ, are obtained by substituting the global principal stresses $\Sigma_I, \Sigma_{II}, \Sigma_{III}$ by the local principal stresses $\sigma_I, \sigma_{II}, \sigma_{III}$ in the above expressions. The global failure strain $\overline{E}_f$ is herein defined as the global equivalent strain at the last time step before the critical porosity $f_C = 0.2$ was obtained locally.

5 Numerical results

5.1 Stress-strain behaviour and FLDs

The work-hardening curves obtained with the micromechanical FE model in terms of the global equivalent stress and strain are shown in Figure 10 for the case of uniaxial

tension along the x axis with two widths of the soft zones ($A = 20$ and $A = 40$). By decreasing the width of the soft zones, the stress level increases somewhat while the failure strain decreases markedly. The reason for this is that the soft zones become more constrained by the grains when the aspect ratio A increases, thus increasing the stress triaxiality within the soft zone and decreasing the ductility. In the rest of the parametric study, the larger size of the soft zones, i.e., $A = 20$, is chosen to limit the computation time, since we are looking for the qualitative influence of the heterogeneity induced by the soft zones on failure. One simulation was performed with $f_0 = 0$ for the grains and the soft zones. This leads to a slight increase of the stress level compared with the baseline simulation (defined by loading direction, $x = x_1, y = x_2, z = x_3$; aspect ratio, $A = 20$; initial porosity in soft zone, $f_0 = 0.01$; initial porosity in grain, $f_0 = 0.001$), and supports the choice of calibrating the work-hardening without taking the porosity into account. Another simulation was performed with $f_0 = 0.01$ in both the grains and the soft zones. The effect is a slightly lower stress level and a higher failure strain. The reason for the improved ductility is that the strains are less localized in the soft zones and thereby the grains dissipate more energy when the porosity is uniform. It is emphasized here that the initial porosities for the grains and the soft zones in the baseline model were chosen rather arbitrarily and that this choice has a marked influence on the predicted failure strains.

The global equivalent stress-strain curves for $0 \le \xi \le 1$ and maximum global principal strain E_1 along the x axis are shown in Figure 11, where $\xi = 0$ corresponds to plane strain and $\xi = 1$ implies equi-biaxial tension. The figure also includes uniaxial tension (UT) along the x axis. It is seen that the global equivalent stress-strain curves in biaxial stretching are practically indistinguishable in the plastic domain, but that the

failure strain is markedly depending on the ξ ratio. To illustrate the dependence of the failure strain on the ξ ratio, a failure limit diagram (FLD) is constructed, Figure 12 (a), in which the strain path to failure is plotted in terms of the global principal strains E_1 and E_2. It is seen that in biaxial stretching the value of E_1 at failure increases with increasing degree of biaxiality—and thus with increasing stress triaxiality, while the lowest value of E_1 at failure is found in plane-strain tension. It should be noted that the global Lode parameter changes from $\mu_\Sigma = +1$ to $\mu_\Sigma = 0$ (i.e., from an axisymmetric stress state to a shear stress state) as the loading changes from equi-biaxial tension to plane-strain tension. The apparent Lode dependence observed here does not stem from the microscopic constitutive relation, but from the microstructure of the micromechanical FE model and should be taken into account in a macroscopic constitutive relation designed to represent the failure process of this material.

The influence of the orientation of the hexagonal-shaped GBs was evaluated by rotating the microstructure so that the maximum global principal strain is along the y axis. The corresponding FLD is shown in Figure 12 (b). It is clearly seen that the FLD depends on the orientation of the microstructure and, in particular, for values of ξ between -0.25 and 0.25, the values of E_1 at failure are considerably higher when the major principal axis is directed along the y axis. The reason for this anisotropy in ductility is the non-symmetry of the micromechanical model. The major global principal stress Σ_I acts perpendicularly to the soft zones along the y axis when the x_1 axis is parallel to the x axis, thus building up higher stress triaxiality than what is the case when the x_1 axis is parallel to the y axis (see Figure 7).

The FLDs obtained in various simulations are compared in Figure 13 (a), displaying more clearly the influence of the loading direction, initial porosity and

superimposed normal stress in the thickness direction. The FLD denoted “same porosity” was obtained by setting the initial porosity equal to $f_0 = 0.01$ in the grains and the soft zones. It is seen that the ductility increases when the initial porosity of the grains is set equal to the initial porosity in the soft zones. As already mentioned above, the reason for this somewhat “counter-intuitive” result seems to be that the plastic deformation becomes more spread into the grains, thus increasing the global strain to failure, when the grains and soft zones have the same initial porosity. The FLDs denoted “positive z stress” and “negative z stress” are obtained by superimposing in the z direction of the micromechanical model a constant normal stress Σ_3 equal to ±25% of the yield stress in the soft zone. This leads to higher/lower levels of global stress triaxiality and three-dimensional stress states. The influence of the uniform stress in the thickness direction—and thus the increased/reduced stress triaxiality and change of the Lode parameter—is a rather uniform reduction/increase in the FLD compared with the baseline case.

The global failure loci in terms of global equivalent strain to failure against global stress triaxiality are plotted for the same series of simulations in Figure 13 (b). It is seen that in biaxial stretching ($0 \le \xi \le 1$) the global failure strain increases with increasing global stress triaxiality. Under such circumstances, the global failure strain is also observed to increase with the global Lode parameter. On the contrary, for negative ξ ratios, the failure strain increases with decreasing global triaxiality and Lode parameter. The failure locus obtained with the rotated microstructure stands out among the failure loci due to its different shape, namely that there is a range with almost no influence of global stress triaxiality. In addition, the rotated microstructure gives mostly considerably larger global failure strain than the baseline case. The combinations of global stress triaxiality and Lode parameter obtained in the baseline series of

simulations and the simulations series with superimposed normal stress in the z direction are depicted in Figure 14 together with the trajectory of plane stress states. It is recalled that there is a relation between the stress triaxiality and the Lode parameter for plane stress states. It is seen that while the whole range of the Lode parameter is covered in the simulations, only a limited range of stress triaxialities is explored.

5.2 Local states

Figure 15 presents the location of the maximum value of the predicted porosity inside the soft zones for selected loading conditions. Only the case with maximum global principal strain along the x axis is shown for biaxial stretching ($0 \le \xi \le 1$), while for uniaxial tension both cases are shown, i.e., the tension is either along the x axis or the y axis. The cases with negative ξ are not shown. In the cases of uniaxial tension along the x axis and biaxial stretching with small biaxiality ratio, $0 \le \xi \le 0.25$, the maximum porosity is found in the middle of the GBs orthogonal to the maximum global principal stress direction. In biaxial stretching with $\xi = 0.5$ and $\xi = 0.75$, the critical location is at the middle of the inclined GBs, whereas in equi-biaxial tension ($\xi = 1$) and uniaxial tension along the y axis the critical point has moved to the intersection of GB branches.

Figure 16 (a) presents the local porosity at the critical points as a function of the global equivalent strain $\overline{E}$ for the different loading conditions, while Figure 16 (b) presents the porosity inside the grains. As expected, $\overline{E}$ is comparable to the local equivalent strain $\bar{\varepsilon}$ computed inside the grains, but, owing to strain localization, it may differ dramatically from the values of $\bar{\varepsilon}$ computed within the soft zones. It is observed that the porosity inside the grains increases almost linearly with $\overline{E}$ and more rapidly when the biaxiality ratio ξ —and thus the stress triaxiality ratio Σ^*—increases. The

evolution of the porosity at the critical points inside the soft zones is highly nonlinear and the void growth rate is not increasing with increasing ξ. The highest void growth rate is obtained in plane-strain tension ($\xi = 0$), which is consistent with the low failure strain in this case.

To further illustrate this aspect, Figure 17 and Figure 18 display the local equivalent strain $\bar{\varepsilon}$ versus the local stress triaxiality σ^* at the critical location presented in Figure 15 and inside the grains. Only the case with maximum global principal strain along the x axis is shown. The stress triaxiality inside the grains is roughly constant and similar to the theoretical values calculated with von Mises plasticity for plane stress states. The stress triaxiality evolution at the critical locations inside the soft zones can be split in three to four regions.

The first very rapid increase from the theoretical value of the stress triaxiality towards much larger values ($\sigma^* \approx 2-3$) corresponds to yielding inside the soft zones under the constraints imposed by the elastic grains. Then, the triaxiality decreases abruptly when the grains start to yield, thus making plastic flow inside the soft zones less constrained. After reaching a local minimum, the triaxiality inside the soft zones again starts to increase because of the higher rate of void growth and associated strain localization in these zones. Recall that the initial porosity was ten times larger inside the soft zones compared with inside the grains. Finally, for uniaxial tension and biaxial loading with $\xi = 0$, the stress triaxiality slightly decreases just before failure. Due to a rapid increase in porosity at high triaxiality and large strain, the Gurson yield surface experiences a rapid shrinkage along the hydrostatic axis. The equivalent von Mises stress remains nearly constant due to the hardening rule, so this shrinkage imposes a quick decrease in hydrostatic stress—and consequently stress triaxiality.

As observed earlier in Figure 3 for uniaxial tension, the failure strain also depends on the orientation of the GBs with respect to the direction of loading. Under uniaxial tension, the void growth is promoted when GBs are oriented orthogonal to the loading direction. Figure 18 shows that the stress triaxiality under uniaxial tension with no grain boundaries oriented orthogonal to the loading direction is lower, i.e., when the tensile axis is along the y axis in Figure 7, and results in a larger failure strain. This figure also shows that the critical element for loading along the x axis is not critical anymore when loading in the y axis (see also Figure 15). This explains the anisotropy engendered by the grain morphology.

6 Discussion and conclusions

The TEM study shows that PFZs are found along both LAGBs and HAGBs. The width of the PFZs is about 20 nm for LAGBs and about 40 nm for HAGBs. GB precipitates are observed in both cases. The LAGBs have higher amounts of smaller GB precipitates, while HAGBs have lower amounts of larger GB precipitates. In addition, Cr-containing dispersoids were observed. According to the experimental study of Ludtka and Laughlin [4], both the transgranular and the intergranular fracture modes observed for the AA7075 alloys in peak hardness condition occurred by nucleation of voids at these dispersoids. The GB precipitates facilitated the void coalescence in the case of intergranular fracture.

The PFZs are depleted of Zn, Mg and Cu compared with the bulk material but still contains a certain amount of alloying elements in solid solution. These results indicate that the material in the PFZ is somewhere in-between pure aluminium and W temper, where the bulk concentration of alloying elements is in supersaturated solid solution. It is thus expected that the flow stress of the W temper overestimates the flow

stress of the PFZs but it should be kept in mind that the PFZs are very narrow and gradient effects might strengthen the PFZ material considerably [42].

The micromechanical finite element study was performed on an idealized, two-dimensional microstructure with hexagonal grains and soft zones along the grain boundaries. To keep the computation time reasonable, these soft zones were about about ten times wider than the PFZs in the real microstructure when compared with the characteristic grain size. This simplification would probably imply that our simulations are valid for soft zones that are not too narrow. As already mentioned, strain gradients effects, arising from geometrically necessary dislocations, may induce extra hardening in the PFZ. A numerical study performed with a strain gradient plasticity model by Pardoen and Massart [43] showed a non-negligible influence of the width of the PFZ. However this effect, which can be accounted for by taking the yield stress in the Gurson model as the gradient enhanced strength, was not included in the simulations presented here. The grains were assigned the stress-strain behaviour of AA7075-T651 while the soft zones were assumed to behave as the same alloy in temper W. The Gurson model with different initial porosity in the soft zones and the grains was used in the baseline simulations. The porosity was higher in the soft zones due to the extensive GB precipitation. In most simulations, global plane stress conditions were assumed, but some simulations were also conducted with superimposed tension or compression in the thickness direction. According to all these approximations, the simulations are only qualitative and were used to study the influence of the idealized microstructure on the global ductility. Other parametric studies and numerical simulations are needed to complete the understanding of the role of PFZs on localization and failure.

The numerical results give a non-monotonic variation of the global failure strain with the global stress triaxiality. Since the Gurson model predicts increased void growth

with increased stress triaxiality, independently of the Lode parameter, the non-monotonic global fracture locus stems from the heterogeneity of the local stress states engendered by the idealized microstructure. This leads to different critical locations for failure initiation, as defined by $f = f_C$, within the soft zones dependent on the global stress state. The numerical simulations show that the global equivalent strain to failure increases exponentially with increasing stress triaxiality in biaxial stretching. The increase in global triaxiality with increased biaxiality ratio ξ is associated with an increase in the global Lode parameter from 0 in plane strain to +1 in equi-biaxial tension. It is further observed that the failure strain depends markedly on the direction of the maximum principal stress (or, equivalently, on the orientation of the microstructure with respect to the applied loading). The global failure strain is mostly lower when this direction is perpendicular to the soft zones. Thus, the non-symmetric microstructure leads to anisotropic failure strains, in accordance with the experimental observations in [30].

In all simulations performed here the fracture extended along the soft zones and never propagated into the grains. It is believed that this is due to the two-dimensional microstructure and predominant plane stress states used in the simulations. Ludtka and Laughlin [4] observed combined transgranular and intergranular fracture in high solute AA7075 alloy in temper T6, where the opening-up of intergranular cracks engenders necking down and final fracture of the neighbouring grains. Combined fracture modes were also observed by Pedersen *et al.* [28] for the actual alloy. Pardoen *et al.* [13] used a bilayer damage model to investigate numerically the competition between transgranular and intergranular fracture, including effects of the stress-strain behaviour of the zones, the relative width of the PFZ, and particle spacing and volume fraction within the PFZ. Repeating the simulations performed in the present study on a three-

dimensional microstructure would allow studying the competition between the two failure modes, but such simulations would be very computation time intensive because of the small relative width of the PFZs.

The stress-strain responses of the grains and soft zones were not varied in the simulations. Based on their experiments, Ludtka and Laughlin [4] conclude that the two major factors governing fracture toughness of these alloys are the coarseness of the matrix slip, which is linked to the density of the hardening precipitates, and the difference between the flow stress curves in the matrix and PFZs, which is a relative measure of the propensity for intergranular fracture. It was observed in the simulations in this study that if the initial porosity was equal in the grains and PFZs, plasticity spreads more into the grains and the ductility increases. This is coherent with the observation in [4] that the ductility depends on the difference in behaviour between the grains and PFZs.

Acknowledgements

The financial support of this work from the Structural Impact Laboratory (SIMLab), Centre for Research-based Innovation (CRI) at the Norwegian University of Science and Technology (NTNU), is gratefully acknowledged. The authors would also like to aknowledge Dr. Torodd Berstad for help with the numerical simulations.

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Table 1. Chemical composition (weight %) of aluminium alloy AA7075.

Figure 1. SEM image showing grains and their orientations in the ND-TD plane of the AA7075-T651 plate (ND is horizontal and TD vertical in the grain map).

Figure 2. Orientation distribution function (ODF) for the AA7075-T651 plates.

Figure 3. Cauchy stress versus logarithmic strain curve in the RD of the AA7075 plate in tempers W and T651.

Figure 4. Bright field TEM pictures of the AA7075-T651 alloy showing grains, precipitates and PFZs. Approximate orientations of different grains are indicated, together with the PFZ widths.

Figure 5. STEM image and EDS maps for five different elements (Zn, Mg, Cu, Cr, Fe) of an area including two grains separated by a GB and its associated PFZ. A fine distribution of Zn-Mg-Cu hardening precipitates is observed in the bulk. The large Zn-Mg-Cu precipitates 1 and 3 are nucleated on Cr-containing dispersoids (like the number 2). Precipitates 3 and 4 are nucleated along the GB.

Figure 6. STEM image and alloying content (in wt%) in different areas for the picture. Alloying content inside whole area (picture), the grain (area 5) and inside the PFZ (area 6) is given in comparison with the nominal alloy composition.

Figure 7. Micromechanical finite element model with periodic microstructure containing 16 grains with associated soft zones along the GBs. One layer of hexahedral solid elements is used to simulate plane stress conditions on the global level.

Figure 8. Detail of three-branch intersection between neighbouring grains defining the characteristic grain size L^G and the width L^{SZ} of the soft zones. In the figure, the aspect ratio $A = L^G / L^{SZ} = 20$.

Figure 9. Definition of coordinate system and node sets used to define BCs for the micromechanical model in Figure 7.

Figure 10. Equivalent stress-strain curve in uniaxial tension as a function of initial porosity f_0 and aspect ratio $A = L^G / L^{SZ}$.

Figure 11. Equivalent stress-strain curves for different states of biaxial tension defined by the ratio $\xi = u_2 / u_1$ and uniaxial tension for x axis aligned with x_1 axis.

Figure 12. Failure limit diagrams obtained from numerical simulations with (a) x axis aligned with x_1 axis and (b) x axis aligned with x_2 axis. The ratio ξ equals -0.5, -0.25, 0, 0.25, 0.5, 0.75 and 1.0 in both series of simulations.

Figure 13. Comparison of (a) failure limit diagrams and (b) global failure loci showing the effect on the global strains to failure of loading direction, initial porosity, and superimposed positive or negative normal stress in the z direction. The ratio ξ equals -0.5, -0.25, 0, 0.25, 0.5, 0.75 and 1.0 in all series of simulations.

Figure 14. Global stress triaxiality versus global Lode parameter in the baseline (or reference) simulation and the simulations with positive and negative superimposed normal stress in the z direction. The ratio ξ equals -0.5, -0.25, 0, 0.25, 0.5, 0.75 and 1.0 in all series of simulations.

Figure 15. Location of critical elements within the PFZ for selected loading conditions.

Figure 16. Evolution of porosity with macroscopic equivalent strain for selected loading conditions (a) inside the critical element in the soft zones depicted in Figure 15 and (b) inside the grains.

Figure 17. Local equivalent strain versus local stress triaxiality inside the grains and at the critical GB elements for uniaxial tension (UT) and biaxial tension (BT) with different values of ratio ξ. Only the case with major global principal strain along the x axis is shown.

Figure 18. Local equivalent strain versus local stress triaxiality inside the grains and critical soft zone elements for uniaxial tensile loading conditions (UT) in the two orthogonal directions (x in black and y in magenta). The state of the element that was critical for loading along the x axis is shown as the grey line in the case of loading along the y axis.