Finite Element Simulations of Crack Propagation in Al₂O₃/6061Al Composites

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Received: 8 April 2014 / Revised: 25 June 2014 / Published online: 15 August 2014
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Abstract In this work, the local fracture initiation behaviour of an Al₂O₃/6061Al composite is studied numerically. The damage behaviour of the microstructure is evaluated in consideration of the path and the amount of damage as well as the stress–strain performance of the microstructure. The damage behaviour of the ductile matrix has been simulated using the damage parameter D . For the simulation of fracture of the ceramic particles, a normal stress criterion is applied. For the analysis of the damage behaviour of the transition zone between particulate and matrix, both damage models (D parameter and normal stress criteria) are applied in this region. Parameter studies of crack propagation prediction in the Al₂O₃/6061Al composite on the basis of an Element Elimination technique have been performed for two differently heat-treated variants resulting in different mechanical properties. In addition, residual stress effects on the damage behaviour are examined for various microstructural situations.

KEY WORDS: Metal matrix composites; Simulation; Crack propagation; Finite element method; Element elimination technique

1 Introduction

Various techniques for the production and design of composite materials have been developed over the last years in order to improve their mechanical properties and thus to obtain a more effective outcome: low cost and a weight reduction in structural applications.

Metal matrix composites (MMCs) on the basis of aluminium alloys reinforced by elastic ceramic inclusions such as Al₂O₃ particles possess high specific strength and moduli at room temperature and at elevated temperatures and, thus, also improved fatigue strength. They also show excellent wear

resistance [1], high thermal conductivity [2], low thermal expansion [3] and good dimensional stability [4]. These properties make this type of composite attractive for a wide-range of application fields such as automotive, electronics and aerospace industries. For these reasons, MMCs reinforced with ceramic particles are used extensively as electrical contacts, cutting tools, space applications, brake rotors, etc. [3].

MMCs are basically defined as a ductile matrix reinforced by brittle fibres or particles [6]. Thus, under external loading conditions, the overall response of this material is elasto-plastic. However, the accurate modelling of the mechanical behaviour of actual heterogeneous materials is not an easy task due to their complex microstructure.

The strength of the composite is limited by failure of the particles, failure of the interface between particles and matrix or by yielding of the matrix, depending on the precise loading of the material. A considerable volume of research work has been undertaken to understand the effect of failure of these materials under loading [4–6].

Available online at <http://link.springer.com/journal/40195>

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Table 1 Elastic properties and thermal expansion coefficient used in the FE simulations

Material	Elastic modulus, E (MPa)	Poisson's ratio, ν	Thermal expansion coefficient, α ($10^{-6}/\text{K}$)
6061Al matrix	66,000	0.33	23.87
Al_2O_3 particles	380,000	0.22	2.60

Fig. 1 Stress–strain curves for the 6061Al-T6 matrix, ductile transition phase and brittle Al_2O_3 inclusion. The elastic–plastic stress–strain curves are used alternatively for both Al-matrix and interface

Since the transition phase between the reinforcement and the matrix plays an important role primarily for damage initiation and propagation [1, 3], it should be also analyzed carefully and their impact on damage of MMCs ought to be clarified in all important aspects during external loading. Furthermore, residual stresses are present in the matrix and the inclusions owing to the difference of thermal expansion coefficients between ductile matrix and brittle inclusions.

Taking the aforementioned into account, a damage study for $\text{Al}_2\text{O}_3/6061\text{Al}$ MMC (10 vol% Al_2O_3) microstructures considering the roles of matrix, inclusion and interface phases with accounting for residual stress effects is carried out in this work.

2 FE Simulation and Real Microstructure Modelling

Two-dimensional (2D) FE models based on the “intact” real microstructure of the $\text{Al}_2\text{O}_3/6061\text{Al}$ MMCs have been created. In reality, some broken Al_2O_3 particles exist in the material after extrusion [6]. FEM simulations of crack propagation in the cut-out of the real microstructure have

been performed with different parameters of intermediate layer (transition zone between the matrix and Al_2O_3 -inclusion) with and without residual stresses, and the effect of these variations has been analyzed. The mechanical and physical input data are presented in Table 1 and were taken from Ref. [7], while stress–strain correlations for the matrix, inclusion and transition phase have been taken from the experiment (Fig. 1).

2.1 Modelling of Damage Initiation of $\text{Al}_2\text{O}_3/6061\text{Al}$ Composites with an Element Elimination Technique

The main objective of this section is to investigate the crack initiation in the $\text{Al}_2\text{O}_3/6061\text{Al}$ MMCs with different properties of constituents and with and without heat treatment. The composite microstructure was considered to consist of three phases: matrix, inclusion and the transition phase at the interface between matrix and inclusion.

2.1.1 Material Parameters

The mechanical behaviour of the $\text{Al}_2\text{O}_3/6061\text{Al}$ MMCs has been simulated using experimental curves which were obtained from tensile tests for the 6061Al alloy matrix after T6 heat treatment and for Al_2O_3 , as depicted in Fig. 1. The transition phase was assumed to be brittle (black curve in Fig. 1) or ductile (pink curve in Fig. 1).

When both inclusion and transition phases were taken to be brittle, they differ by the value of critical normal tensile strength (see Table 2).

A small 2D cut-out of a typical microstructure has been selected from the microstructure [6], and with the help of a specially developed programme [8] a finite element-mesh based on triangular elements has been generated (Fig. 2).

2.1.2 Damage Parameter Concept

The stress–strain state of the solid can be described by the equivalent plastic deformation ε_{pl} and the stress triaxiality η . There is an interrelation between ε_{pl} and η [9]:

$$\eta(\varepsilon_{\text{pl}}) = P \cdot \frac{\varepsilon_{\text{pl}}}{\varepsilon_{\text{pl,c}}}, \quad (1)$$

where P is the influence parameter, $\varepsilon_{\text{pl,c}}$ is the critical equivalent plastic strain.

It is necessary to define the influence parameter P and the critical equivalent plastic strains $\varepsilon_{\text{pl,c}}$ in order to define the connection between the plastic strain and triaxiality. For the simulations of the ductile matrix behaviour, the damage parameter D was used, which was introduced by Rice and Tracey [9] and modified by Arndt *et al.* [10] and Hönle *et al.* [11]. In the place where the damage parameter

Table 2 Variations of mechanical properties and damage parameters of MMC constituents used in different simulations

Simulation	Properties of the transition phase	Damage criteria			Residual stress
		Transition phase	Matrix	Particles	
No. 1	Brittle, $E = 326$ GPa, $\nu = 0.3$	Normal stress, $\sigma_c = 4,000$ MPa	Rice and Tracey, $A = 2.82$ $B = 2.07$ $D_c = 1$	Normal stress, $\sigma_c = 3,000$ MPa	Yes (cooling down from 500 °C till 20 °C)
No. 2					No
No. 3	Without transition phase	The same criterion as for particle	Rice and Tracey, $A = 2.82$, $B = 2.07$, $D_c = 1$	$\sigma_c = 3,000$ MPa $\sigma_c = 1,500$ MPa	Yes
No. 4	Brittle, $E = 326$ GPa, $\nu = 0.3$	Normal stress, $\sigma_c = 3,000$ MPa	Rice and Tracey, $A = 2.82$, $B = 2.07$, $D_c = 1$	Normal stress, $\sigma_c = 4,000$ MPa	Yes
No. 5	Ductile, harder than matrix	Rice and Tracey, $A = 1.41$	Rice and Tracey, $A = 2.82$, $B = 2.07$, $D_c = 1$	Normal stress, $\sigma_{crit} = 4,000$ MPa	Yes
No. 6		$B = 1.035$ $D_c = 1$			No
No. 7	Ductile, softer than matrix	Rice and Tracey, $A = 2.82$	Rice and Tracey, $A = 1.41$, $B = 1.035$, $D_c = 1$	Normal stress, $\sigma_c = 4,000$ MPa	Yes
No. 8		$B = 2.07$ $D_c = 1$			No

Fig. 2 Boundary conditions and FE-mesh of cut-out of $\text{Al}_2\text{O}_3/6061\text{Al}$ MMC (white represents inclusion, green represents the matrix and dark green represents the transition phase)

achieves a critical value D_c , the crack will be initiated. The damage parameter D according to Eq (2) will be defined through the so-called stress triaxiality $\eta = \sigma_H/\sigma_{eqv}$ [10] and the equivalent plastic deformation ε_{pl} :

$$D = \frac{1}{1.65\varepsilon_0} \int_0^{\bar{\varepsilon}} \exp\left(\frac{3}{2} * \frac{\sigma_H}{\sigma_{eqv}}\right) d\bar{\varepsilon}, \quad (2)$$

where the hydrostatic stress σ_H and the equivalent stress σ_{eqv} are defined from the calculated data for the micro-structure under investigation.

The dependence between the critical equivalent plastic strain $\varepsilon_{pl,c}$ and the critical stress triaxiality η_c can also be defined based on the modified Rice and Tracey criterion, according to the following equation:

$$\varepsilon_{pl,c} = A \exp(-B\eta_c), \quad (3)$$

where A and B are the material constants. The modified damage parameter denominated by D is described by the following Eq (4) and is calculated in this work for each load increment in the FE simulations [12]:

$$D = \frac{1}{A} \int_0^{\varepsilon_{pl,c}} \exp(B\eta) d\varepsilon_{pl}. \quad (4)$$

Crack formation in the particles is the most frequent mechanism of damage initiation in the composite after T6 heat treatment. The normal stress controlling crack initiation and crack development in the brittle ceramic phase have been used as criteria for this kind of damage in the simulation. The third damage mechanism refers to cracking–delamination interface between the matrix and the particle. The transition phase between matrix and inclusion could be assumed as brittle or ductile, because this phase is usually unknown in its physical parameters. With this in mind, two damage criteria (D parameter and normal stress criterion) are applied for the transition phase.

Fig. 3 Stress–strain curves for the cut-out of the microstructure from Fig. 2 with different properties of the transition phase: **a** without residual stresses; **b** with residual stresses

These two damage criteria models have been implemented in the user-defined subroutine in ABAQUS [13]. The visualization of the damage evolution in the microstructure is done by an in-house developed programme [14]. Finally, this microstructure with different properties of the transition zone was simulated under external tensile loading. Parameter studies concerning the variation of normal stresses used as criterion for the transition phase failure, and the damage behaviour of the microstructure with respect to the crack path, the degree of damage and the stress–strain curve have been performed. Besides, the influence of residual stresses on the damage behaviour is studied.

2.1.3 Element Elimination Technique (EET)

There are different methods for simulating crack propagation in Finite element program ABAQUS. Among them are XFEM [15–17], cohesive zone model [18, 19] and element deletion technique [20]. In the present work, we simulate the crack propagation with element elimination technique. Provided that the criterion of failure is satisfied in an element or at Gauss points, the material stiffness is set to zero at this point or the element is directly removed from the model. The EET has the advantage that the crack path is not predefined by element boundaries.

The possibility of modelling crack growth is provided by USDFIL or UMAT subroutines in ABAQUS [13]. The element is removed from the model and then the simulation can be restarted without the eliminated elements.

In addition, a damage subroutine (URDFIL) is developed using the damage parameter D as criterion for the crack initiation in the ductile phases and the critical normal stress as criterion for breaking of the brittle phases. The

elements are removed from the model when the failure criterion for the phase which is represented by the element has been reached. The variations of mechanical properties and damage parameters of MMC constituents which were used in simulations are listed in Table 2.

3 Results and Discussion

3.1 Effect of Residual Stresses on the Crack Propagation in $\text{Al}_2\text{O}_3/\text{6061Al}$ Composite with Different Material Parameters

Generalizing the work performed for the simulation of damage evolution in the selected $\text{Al}_2\text{O}_3/\text{6061Al}$ cut-out of microstructure, the stress–strain curves for different mechanical and damage parameters (from Table 2) can be depicted, as shown in Fig. 3. As can be seen from the comparison of Fig. 3a and b accounting of residual stresses results in decrease in strain for the initiation of fracture and a step-wise behaviour of stress–strain curve (see Table 2).

Figure 4 shows the damage development in the microstructure of an $\text{Al}_2\text{O}_3/\text{6061Al}$ composite at the gradual deformation steps obtained by simulation No. 1. The simulation results demonstrate that at the beginning the crack starts to develop in the matrix along the phase boundary then extends itself in the brittle Al_2O_3 particle. Parametric studies based on the element elimination technique (EET) showed that the residual stresses can contribute to the failure behaviour of the considered $\text{Al}/\text{Al}_2\text{O}_3$ -composite.

The crack evolution represented in Fig. 4 is accompanied by stress drops at the stress–strain curve (Fig. 3b). When the crack enters the brittle inclusion (segments c and d in Fig. 4), a sharp stress drop at the stress–strain curve is

Fig. 4 Damage evolution in $\text{Al}_2\text{O}_3/6061\text{Al}$ composite microstructure obtained by simulation No. 1 at the following deformation steps: **a** strain is 0.5%; **b** strain is 1.1%; **c** strain is 2.0%; **d** strain is 2.8%; **e** strain is 3.8%; **f** strain is 4.5%

observed (black curve in Fig. 3b). This sharp stress drop is explained by the high level of residual stress in the inclusion after the heat treatment. A pronounced stress drop on the curve is caused apparently by the fact that the inclusion occupies the biggest part of our modelled cut-out. During the following crack propagation in the ductile matrix, the stress keeps at the same level (black curve in Fig. 3 and segments e and f in Fig. 4).

The same simulations have been performed without residual stresses, i.e. the initial and the final temperatures were taken to be equal to 20 °C, the simulation results are represented in Fig. 5. The comparison of the crack path development for both cases (with and without residual stresses in Figs. 4, 5, respectively) shows that the residual

stresses after the heat treatment result in cracking of the large inclusion. In the absence of residual stresses, cracks propagate only in the ductile matrix. This observation is due to the fact that the particles are under compressive stresses in the presence of residual thermal stresses. Another behaviour of the stress–strain curve is also observed (black curve in Fig. 3a).

Taking the residual stresses into account, similar simulations have been performed for two different values of critical normal stresses (1,500 and 3,000 MPa) for the brittle Al_2O_3 inclusion in order to investigate the influence of this parameter on the behaviour of stress–strain curve (Fig. 6).

The stress–strain curves are identical till the deformation of 1.5%. After achieving this value of deformation, a very

Fig. 5 Damage evolution in the model of the $\text{Al}_2\text{O}_3/6061\text{Al}$ composite microstructure obtained by simulation No. 1 at the following macroscopic deformation steps: **a** strain is 0.5%; **b** strain is 2.0%; **c** strain is 3.8%; **d** strain is 4.5%

Fig. 6 Stress–strain curves for the small cut-out from the microstructure of the specimen under tensile loading with accounting of residual stresses with different values of critical normal stress damage criterion (simulation No. 3 in Table 2)

pronounced stress drop is observed at the stress–strain curves. For the lower critical normal stress value (1,500 MPa), the stress–strain curve decreases to a lower value of stress in comparison with the one for the higher critical stress value. The drop observed in the curve for 1,500 MPa can be explained by a larger amount of broken particles or longer cracks compared to the case of

3,000 MPa. This stress drop is observed because the number of failed elements significantly increases, when a lower critical normal stress value for the inclusion is used.

For the case of a brittle transition phase with $\sigma_c = 3,000$ MPa, the cracks nucleate simultaneously in the brittle transition phase and in the ductile matrix (Fig. 7a, b). During the following steps of deformation, the crack propagates between two smaller inclusions (Fig. 7b–d) and along the transition phase, which results in delamination of the Al_2O_3 inclusion from the matrix.

For the investigation of the behaviour of a ductile transition phase, two cases have been considered: (1) the case of a ductile transition phase with the stress–strain curve being harder than for the ductile matrix (Fig. 7); (2) a ductile transition layer with a stress–strain curve, which is softer than that for the ductile Al6061-alloy matrix (Fig. 8).

As can be seen from a comparison of Figs. 8 and 9, accounting for the ductile behaviour of a transition phase results in different mechanisms of damage in the Al6061 alloy with the brittle ceramic Al_2O_3 -inclusions. In the case of the ductile transition phase with the lower stress–strain curve, the delamination of the particles from the matrix is observed. As for the ductile transition phase with a higher stress–strain curve, cracking of the matrix is observed.

Fig. 7 Damage evolution in the model of the $\text{Al}_2\text{O}_3/6061\text{Al}$ composite microstructure obtained by simulation No. 4 at the following macroscopic deformation steps: **a** strain is 0.5%; **b** strain is 2.0%; **c** strain is 3.8%; **d** strain is 4.5%

Fig. 8 Damage evolution in the model of the $\text{Al}_2\text{O}_3/6061\text{Al}$ composite microstructure obtained by simulation No. 5 at the following macroscopic deformation steps: **a** strain is 0.5%; **b** strain is 2.0%; **c** strain is 2.8%; **d** strain is 4.5%

Fig. 9 Damage evolution in the model of the $\text{Al}_2\text{O}_3/\text{6061Al}$ composite microstructure obtained by simulation No. 7 at the following macroscopic deformation steps: **a** strain is 0.5%; **b** strain is 1.1%; **c** strain is 2.0%; **d** strain is 2.8%

Fig. 10 Stress–strain curve for the microscopic cut-out of the microstructure from Fig. 2 under tensile loading after cooling down from 500 to 200 and 100 °C, respectively

Fig. 11 Stress–strain curve for the microscopic cut-out of the microstructure from Fig. 2 under tensile loading after cooling down from 500, 200 and 100 °C to room temperature

3.2 Influence of the Value of the Residual Stresses in $\text{Al}_2\text{O}_3/\text{6061Al}$ MMC on the Stress–Strain Behaviour under Tensile Loading

The existence of residual stresses in MMCs after manufacturing has been recognized for many years [2]. Typical undesirable effects associated with residual stresses are reinforcement delamination [21], diminished fatigue

resistance [22], shape distortion [23] and accelerated stress corrosion [24]. Furthermore, mechanical properties such as yield strength or fracture toughness can be affected by the presence, sign and magnitude of residual stresses.

6061Al alloy possesses a higher coefficient of thermal expansion than Al_2O_3 . This mismatch in CTE results in that at room temperature and without loading most parts of the reinforcements are under compression and most parts of the matrix phase are under tension [2]. Thus, it is

extremely crucial to consider residual stresses and its effect on the damage behaviour of the microstructure including the transition phases.

To investigate the influence of residual stresses on the crack propagation, two different temperature models have been applied to the structural cut-out before the tensile loading: cooling down from the temperature 500 to 200 and 100 °C (Fig. 10); cooling down from 500, 250 and 100 °C to the room temperature (Fig. 11). It can be seen from Fig. 10 that under the influence of higher residual stresses (cooling down to 100 °C) fracture occurs at lower stresses in comparison with the lower residual stresses (cooling down to 200 °C). Under cooling down to the room temperature from different initial temperatures (100, 250 and 500 °C), the similar tendency as in the previous case (Fig. 10) is observed. The increased difference between the initial and final temperatures results in more pronounced steps on the stress–strain curves and the increasing segment on the stress–strain curve decreases. As can be seen from Figs. 10 and 11, the simulation result leads to the following conclusions. At the higher starting temperature of cooling down, damage starts at the higher stress but is accompanied by clearly pronounced stress drops in steps and the oscillations at the stress–strain curve are more pronounced at the higher start temperature. This can be explained by the fact that by cooling down from higher temperature the more residual stresses accumulate in the material, and the less external applied stress is necessary to achieve the critical stresses in material, which result in fracture.

4 Conclusions

The 2D-FE-simulations of crack propagation cut-out of real microstructure of $\text{Al}_2\text{O}_3/6061\text{Al}$ MMC are performed with ABAQUS using the Element Elimination Technique and the following conclusions have been reached.

- (1) The damage development in the MMC in the case of the presence of residual stresses is visible as steps in the stress–strain curve. Brittle cracking of the inclusions is accompanied by sharp stress drops, and the following ductile fracture in the matrix corresponds to the plateau on the stress–strain curve.
- (2) For the case of the absence of residual stresses, there exist no clear pronounced steps in the stress–strain curve, the damage occurs at higher stresses, and cracking of the inclusion is not observed in the model.
- (3) The influence of the value of residual stresses on the damage behaviour in MMCs has been studied by simulating cooling down from different annealing temperatures prior to external loading of the

specimen. It was found that the influence of residual stress values only depends on the temperature difference ΔT . Not taking into account the presence of residual stresses in FEM simulations does not result in particle fracture because in that case the overall stresses are not high enough to be critical for particle fracture.

Acknowledgments The authors are thankful for the financial support from German Research Foundation (DFG), under project Schm 746/55-1.

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