Simulation of the Mechanical Behaviour of Metal Matrix Composites

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Abstract. A model based on the geometry of the phases is introduced in order to investigate the mechanical properties of interpenetrating microstructures. In order to characterize the elastic and elastic-plastic properties of the composite a self consistent unit cell model is applied on a wide range of volume fractions for an Al/TiO\textsubscript{2} composite. Besides the volume fraction a microstructural based parameter is used, the matricity, to describe the mutual circumvention of both phases. Computations are carried out for different temperatures and void volume fractions. In addition a conservative fracture criterion based on critical normal stresses is applied to derive realistic stress-strain curves.

Introduction
The prediction of the overall elastic-plastic behaviour of metal matrix composites with interpenetrating phases is a research topic since long time. Different numerical approaches exist to achieve this goal. The method which costs the most effort is using real microstructures which have to be meshed and calculated in 3D. This approach requires high computation times. Therefore, there had always been intentions to reduce the computational effort especially for parametric studies. A advanced method for time efficient simulations of the mechanical behaviour of MMC-materials is based on unit cell models. They have been developed by simplifying the microstructures to spherical inclusions embedded in a matrix. In the present work a parametric study is carried out to calculate the material response of a wide range of composite materials with interpenetrating microstructures. The aim is to identify the most favourable material properties which could be obtained in TiO\textsubscript{2}-AlSi9Cu3 system automotive applications. The composite manufacturing route selected is the infiltration of a ceramic preform by squeeze casting. The low wettability of the ceramic material was met by the application of pressure during the infiltration process. Therefore, preheating of the melt as well as of the ceramic is of influence on the infiltration and the solidification of the metal. Furthermore the infiltration path of the melt has to be taken into account to reduce the porosity in the MMC-material. Manufacturing of the calculated composites is not part of the present paper.

Nomenclature
matricity
a microstructure dependent parameter which describes the matrix character of a phase
skeleton line
a line that will stay if from a binary image of a microstructure step by step the outer pixels are removed
representative volume element
a cut out of a real microstructure which possesses the same overall distribution of the inclusion as the bulk material
unit cell a simplified simulation cell representing the material behaviour of the bulk material

Unit Cell Models

The embedding of the inclusions in the matrix is described by self consistent unit cells [1, 2]. Even though these models are based on spherical inclusions in a matrix, they have been proven to predict the properties of statistically distributed inclusions. These self consistent unit cell models can be extended to take into account the geometrical mutual circumvention of both phases which will occur to different degrees, for different volume fractions of ceramic and materials (see next section).

The reduction of computing time for the prediction of stress – strain curves is a reason why unit cell models are often used. In these models a representative volume element (RVE) is transferred into a geometry as simple as possible which usually is a sphere of the inclusion material, surrounded by a cylinder of the matrix material. From such unit cells the behaviour of the composite can be studied. By using special rotational symmetric boundary conditions and appropriate elements it is possible to mesh these unit cell models with a 2D FE-mesh. Further reductions of computing time can be achieved by using of geometric symmetries. Self consistent unit cells (Fig. 1) extend this approach by enclosing the inclusion and the matrix, which form the inner cell, with an outer surrounding homogenized material. The mechanical properties of the embedding composite are computed through an iterative approach to the behaviour of the inner cell. Therefore, the elastic-plastic behaviour of the homogenised material can be calculated. Unmodified unit cell models can be applied for all sizes and shapes of reinforcement phases above a size of two microns. Below this size the “Mechanism-based Strain Gradient (MSG) Plasticity Theory” [3, 4] has to be considered to take the geometric necessary dislocations into account. Recent work implemented this approach in a unit cell model to describe the properties of a dual phase steel which contains martensitic particles in a ferritic matrix [5].

Fig. 1. Schematic model of a self consistent embedding cell [6].
Matricity Model

The matricity model is a combination of two self consistent unit cells, which consider the enclosure of the phases of a two-phase structure [6 - 8]. Thereby, in every cell, depending on the volume fraction, every phase is once considered as the matrix and as inclusion. Thus, there are two stress-strain characteristics for the composite material. With the aid of a weighting function, which depends on volume fraction and the topology of the microstructure (matricity), the stress-strain curve is calculated. For the derivation of the microstructure parameter, matricity, which was introduced in [9], the length of the skeleton lines (Fig. 2) of the two phases has to be compared (Eq. 1). The matricities of both phases are complementary to each other and sum up to one. If a phase has a matricity of zero, it is in a globular shape and is totally enclosed by the other phase (matricity one).

\[
M_\alpha = \frac{S_\alpha}{S_\alpha + S_\beta} \\
M_\beta = \frac{W_2\left(\sqrt{1-f_\beta} + 1\right)}{W_2\left(\sqrt{1-f_\beta} + 1\right) + W_1\left(\sqrt{f_\beta} + 1\right)}
\]

Fig. 2. Two-phase microstructure with skeleton lines for each phase [6].

Fig. 3 shows the two self consistent unit cells. The volume fractions of both phases \(\alpha\) and \(\beta\) are the same, but the arrangement of the phases \(\alpha\) and \(\beta\) is interchanged, so that every phase once appears as “inclusion” and once as “matrix”. Since the volume fractions \(f_\alpha\) and \(f_\beta\) of the phases are the same in both unit cells, the matricities \(M_\alpha\) and \(M_\beta\) can be represented in terms of \(W_1\) and \(W_2\) (Eq. 2).

In Fig. 4 an iterative approach to the composite behaviour of an interpenetrating microstructure with a phase composition of 50 vol.% metal and accordingly ceramic can be seen. The diagram intentionally shows results for strain levels which the composite is not likely to reach because of failure initiation. However, by displaying results for larger strain levels, the changes appearing in higher iteration steps can be seen. The default for the iteration step of a volume fraction of 50% ceramic was close to the stress-strain behaviour of the metal phase. Therefore, the stress-strain curve after the first iteration shows a stiffer material behaviour than before. The slope of the elastic part of the curve is after one iteration similar to the one after the last iteration. In this case the plastic part of the phase composition can be sufficiently exact approximated after about seven iteration steps.
In Fig. 4 the stress stain curves for the 7th up to the 15th iteration are marked with “higher iterations”. At these iterations the curves only differ in stress- and strain-levels that are no more relevant for the composites on hand. Hence, the underlying convergence criterion, which finishes the calculation if successive iteration curves differ by less than 3%, can be used without any loss in quality.

The model was applied to calculate the mechanical properties of different interpenetrating microstructures. In [10 - 12] the model was applied to W/Cu and Ag/Fe composites, where the comparison with experimental results showed good agreement. Furthermore the model was used successfully to calculate the material response for composite materials with randomly distributed particle reinforcements [13].
Elastic Modulus and Thermal Expansion

With the aid of an analytical approach for linear material characteristics, boundaries for the composite modulus can be defined. The calculated elastic modulus must be within the area between the boundaries. Otherwise the chosen preconditions for the simulation are not appropriate. The analytical calculation of an upper and lower value boundary for the elastic modulus is derived by using rules of mixture. As shown in Fig. 5, the upper boundary is obtained by the rule of mixture for a model of both materials, the lower boundary is obtained from a serial arrangement of the materials. These two assemblies represent the extreme combinations of two material phases in a composite C. Hence, it is possible to determine the upper and lower boundary for the elastic modulus through their extreme arrangement relative to the direction of loading. The distance between the two limiting curves gets larger, the more the quotient $E_A/E_B$ differs from 1.

Fig. 5. Young’s modulus of interpenetrating microstructures versus the ceramic content.

When using the simple forms of the mixture rules it is obvious that they only allow a very rough estimation of the composite behaviour since in the present case of an interpenetrating microstructure a rather inhomogeneous arrangement of the phases prevails. From the shape of the Young’s modulus-curve of the composite the area by area classification of the composite material can also be derived. Up to a ceramic volume fraction of 30% the material behaviour is mainly based on the logic of the series connection of the phases in the stress-strain behaviour. As soon as the rise of ceramic material in the composite has limited the plastic deformability of the metallic parts, the increase of the Young’s-moduli is orientated to the conditions of a parallel assembly of the phases. For more than 40% of ceramic the Young’s modulus increases stronger with increasing ceramic phase fraction as compared to a ceramic volume fraction of less than 40%. The simulations show that the change of the Young’s modulus is by far not directly proportional to the volume fraction of the ceramic phase. For this reason composite models based on the rules of mixture can only be used as a rough approximation, while self-consistent unit cell models are capable to represent the actual material behaviour of the composites with interpenetrating microstructures.
Fig. 6. Young’s modulus of Al/ceramic interpenetrating microstructures at room temperature and 200°C versus the ceramic volume fraction.

Fig. 6 shows the dependence of the Young’s modulus and the volume fraction of ceramic at a temperature of 200°C. To compare the dimensions, the dependence of the Young’s modulus at room temperature is also shown. This comparison demonstrates that the development of material properties, depending on the composition of the material, follows the same tendency even at different temperatures.

Fig. 7. Coefficient of thermal expansion drawn against the ceramic content for two temperatures (room temperature and 200°C).

As can be seen from Fig. 7, there are differences in the coefficient of thermal expansion (CTE) depending on the temperature. From above simulations, however, it is known that the thermal expansion coefficients only slightly changes between 400°C and room temperature. This constancy also exists in the simulation, which only considers cooling form 400°C to 200°C.
Stress-Strain Curves

In Fig. 8 simulation results for different ceramic volume fractions are shown. For each simulation the convergence criterion was met and the iteration process stopped. Thereby the phase compositions in the simulations have been changed in 10% steps to allow a continuous evaluation of the change in mechanical behaviour depending on the phase composition. The shown stress-strain curves are simulation results in which no fracture criterion has been used.

The material behaviour in this combination group can be divided into three areas. Microstructures with a ceramic phase fraction up to 30 vol.% show distinctive plastic behaviour. In this combination area the properties of the metallic phase are dominant.

In the second area the change in deformation behaviour from metallic dominated to ceramic dominated takes place. In this area, microstructures with about 40% ceramic can be assigned. From 50% ceramic phase on the plastic part in the stress-strain behaviour gets noticeably smaller and the deformation behaviour of the composite approaches the one of ceramics. In principle according to Fig. 8 there will be no proportional transition of material behaviour from the pure metal phase to the pure ceramic phase with increasing ceramic volume fraction.

Conservative Fracture Criteria

Fig. 9 shows the application of the fracture criterion. For this conservative criterion the maximal shear stress criterion is applied to the metal phase of the model and the maximum stress theory is applied to the ceramic phase of the model. Due to the incremental analysis of the stresses and strains within each model phase it is possible to determine which criterion is reached first. If one of the criterions is met the composite is considered at its failure strength.

The straight lines in Fig. 9 connect the failure criterion of the Aluminium and the Failure criterion of the ceramic for each phase composition. From the slope of the lines the external stress and strain distribution on each phase of the microstructure can be derived. At low ceramic volume fractions the strains within the metallic phase will be much higher than in the ceramic phase at similar stress levels. This can be explained by the inclusion of the ceramic within a metal matrix: In this...
It is possible for the metallic phase to absorb the appearing load through plastic deformation, whereas the brittle ceramic parts of the composite interfere in this yielding process at first only slightly and with increasing volume fraction more and more. Up to compositions of 30% the material reacts to the applied loads in this way. A ceramic volume fraction of over 30% leads to the formation of a ceramic network within the composite material. The deformation of the metallic phase is therefore restrained and the same strain level in both phases is assumed.

Fig. 9. Realisation of the fracture criterion.

These principles can be applied for the present composite materials in the way that at high volume fractions of ceramic the strain in the metallic parts of the microstructure is restrained. In the extreme case of a metallic inclusion in a ceramic surrounding the metal is separated from the applied loads since only strains according to the ceramic surrounding are conveyed to the metal, which lead to small stresses in the metal. The influence of the ceramic phase on the stress-strain ratio in the metallic phase is very noticeable at more than 50 vol.% ceramic. The change between the model representation of the series connection to the parallel connection takes place at a ceramic volume fraction of 30% to 50%.

After the evaluation of the fracture criterion for each microstructural composition the stress-strain-ratio is shown in Fig. 10. For its determination the intersection points of the stress-strain curves with the lines, that represent the stress distribution between the two phases and were shown in Fig. 9, must be defined. The intersection points also stand for the failure of the phase compositions. It becomes obvious that interpenetrated microstructures with a ceramic volume fraction of up to 30% can take large plastic deformations, which are much higher than expected for a composite with a TiO$_2$ structure. The striking influence of the ceramic part to the behaviour of the whole microstructure with a ceramic volume fraction of more than 50% is a result of the restrained plastic deformation in the metal phase. Because of the pure elastic characteristic of the ceramic the restrained deformation of the aluminium through the ceramic phase is approved.
After the application of the fracture criterion, which applies the maximal shear stress criterion to the metal phase and the maximum stress theory to the ceramic phase, stress-strain curves for 200°C shown in Fig. 11. In comparison with the stress-strain curves at room temperature in Fig. 11 it can be seen, that the overall strain is higher for the temperature of 200 °C.
This change in the behaviour of the composite is together with the lower fracture stresses a result of the decreasing strength of the metal at elevated temperatures. The material behaviour of the ceramic phase is not changed by the higher temperature which was applied in this study.

The stress-strain curves in Fig. 12 show that the influence of porosities only applies to metal dominated microstructures. From the figure it can be seen that the development of the stress-strain behaviour according to the applied loads and depending on the composition of the microstructure in principle stays the same as without pores. Porosities show an influence on the macroscopic material behaviour for microstructures with less than 50% of ceramic phase. In the material system at hand, the interpenetrating microstructures react very sensitive to changes of the volume fractions of the phases. Microstructures with a ceramic volume fraction up to 30% show metal dominated behaviour, which are displaced at lower stress levels in comparison to the calculations of the aluminium/ceramic interpenetrating microstructure with ceramic volume fractions between 50% and 70%.

The increased plasticity of the microstructure induced by pores may not distract from the problematic impact of the porosities. Because of their properties porosities will not take part in the transmission of loads. Thus, they reduce the load carrying area of the Material. Hereby the stress levels are increased regarding to the macroscopic loads. Furthermore, porosities induce strong notch effects which additionally increase the stress levels.

The effects of virtual lowering the elastic modulus of the ceramic to 60% of its value are shown in Fig. 13. It displays the stress-strain curves for the phase compositions from 30% to 60% ceramic for both the base value for the Young`s modulus for the ceramic (250 GPa) and the reduced Young`s modulus for the ceramic (150 GPa). Despite the more elastic composition of the ceramic phase the plastic part of the stress-strain curves has been reduced compared to the original calculation with 250 GPa. For all phase compositions the material behaviour is almost purely elastic. This is the result of a reduced stress loading of the metal phase during deformation. The fracture criterion in the ceramic phase is reached as the strain level increases and due to the restricted deformation of the metal phase the load is not distributed to the metal but rather has to be carried by the ceramic.

Fig. 12. Stress-strain curves after the application of the presented fracture criterion for porous Al/ceramic interpenetration microstructures at room temperature.
Conclusion

The described self-consistent approach shows a good possibility to predict a wide range of composite properties including the Young’s modulus, plastic behaviour and the coefficient of thermal expansion. Moreover this model applies to a wide range of temperatures and different phase distributions, which is achieved by introducing the matricity microstructure parameter, and volume fractions. By applying the conservative fracture criteria, which represents the maximal shear stress criterion the metal phase and the maximum stress theory phase, is a way to approximate the material failure.

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