EVALUATION OF THE APPLICABILITY OF THE FIRST PSEUDO-GRAIN FAILURE MODEL FOR SHORT GLASS FIBER REINFORCED POLYPROPYLENE MATERIALS

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Abstract
The mechanical stress-strain behavior of short glass fiber reinforced polymers can accurately be simulated using mean-field homogenization (MFH) methods [1 - 4]. Since, these methods do not take the damage and failure processes that occur in a real material into account, the MFH-models can be extended by the use of various composite failure criteria in order to predict failure for unidirectional fiber orientations. In addition, the first pseudo grain failure (FPGF) model allows for the application of a selected failure criterion on a complex fiber orientation distribution [5]. In this study the applicability of an MFH-model in conjunction with the FPGF-model is investigated on a 32w% short glass fiber reinforced polypropylene material. Both models are implemented in the Digimat Software Environment (e-Xstream engineering, Belgium), which was used as a basis for the simulation. The model was calibrated and validated on highly oriented injection molded specimens. The mechanical properties, the failure behavior as well as the micromechanical characteristics were provided by experiments and compared to the simulation results. Tensile specimens with a nominal fiber orientation of 0°, 45° and 90° and shear specimens were investigated. Different parameter sets for a Tsai-Hill 2D failure criterion were determined and applied to the FPGF-model.

1 Introduction
Due to their advantageous mechanical properties and low manufacturing cost, short glass fiber (sgf) reinforced polymers are widely used in high performance mass products. To tap the full potential of this material class, it is necessary to properly predict the damage behavior in terms of damage initiation, damage evolution as well as ultimate failure.

Various micromechanical approaches are documented in literature, whereas due to its low computational cost mean-field homogenization (MFH) method turns out as a convenient approach for the use in complex component simulations [1 - 4]. This paper focuses on the investigation of the applicability of the first pseudo-grain failure (FPGF) model [5], which allows for applying selected composite failure criteria that were originally proposed for the use on unidirectional laminates (i.e. maximum stress, Tsai-Hill, Tsai-Wu criteria). In addition, the applicability of these models in the FPGF approach is investigated for materials revealing complex fiber orientation distribution (FOD). In order to evaluate the practical applicability of this model and its limitations to engineering components, every modeling step from the matrix material model to the composite microstructure and the damage behavior was carefully validated by experiments.

A focus was put on the possibility to use the FPGF model to properly predict the point of ultimate failure in terms of failure stresses for various fiber orientations.

2.1 Modeling of Uniaxial Tests using Mean Field Homogenization
Short glass fiber reinforced Polypropylene with 32w% fiber content was investigated in this paper as a model material. The mean-field homogenization (MFH) model implemented in the Digimat Software [6] environment was applied to predict the stress – strain behavior. The polymer matrix was modeled by
an elasto-viscoplastic material model, which uses an exponential and linear strain hardening formulation. The hardening stress \( R(p) \) is expressed as a function of the accumulated plastic strain \( p \) with three parameters \( k, R_\infty \) and \( m \) [6].

\[
R(p) = kp + R_\infty (1 - e^{-mp})
\]

(1)

In order to model the strain rate dependence a current yield Norton law viscoplasticity [6] was used as well. The viscoplastic stress \( \dot{\sigma} \) depends on the accumulated plastic strain rate \( \dot{p} \), the yield stress \( \sigma_y \) and the hardening stress \( R(p) \). The two parameters \( \eta \) and \( m \) were identified by a best-fit optimization process.

\[
\dot{p} = \frac{\sigma_y}{\eta} \left( \frac{f}{\sigma_y + R(p)} \right)^m
\]

(2)

This model was calibrated on monotonic uniaxial tensile tests conducted on standardized injection molded specimens of unfilled PP matrix (ISO 527-2) at different loading rates (0.0001s\(^{-1}\), 0.001s\(^{-1}\) and 0.01s\(^{-1}\)). As the second constituents, the glass fibers were modeled as linear elastic and isotropic and the corresponding data were taken from [7].

To support the modeling of short fiber reinforced PP-GF materials, tensile specimens with nominal fiber orientations of 0°, 45° and 90° and with a nominal thickness of 2 mm were used. These specimens were produced by injection molding in a special multi-tool which allows for a controlled fiber orientation with a narrow distribution. The actual microstructure of these specimens was characterized by the fiber length distribution (FLD) and the fiber orientation (FOD) and these are listed in figure 1. These values were determined for each specimen type by computed tomography measurements [8, 9]. Similar to the tensile test on neat PP, uniaxial tensile tests were conducted on these three types of specimens at strain rates of 0.0001s\(^{-1}\), 0.001s\(^{-1}\) and 0.01s\(^{-1}\). In addition, a digital image correlation system was used to record the strain fields and to obtain the true stress – true strain behavior.

<table>
<thead>
<tr>
<th>Fiber Orientation</th>
<th>( \bar{a}_{11} )</th>
<th>( \bar{a}_{22} )</th>
<th>( \bar{a}_{33} )</th>
<th>( \bar{a}_{12} )</th>
<th>( \bar{a}_{13} )</th>
<th>( \bar{a}_{23} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>0.86</td>
<td>0.11</td>
<td>0.03</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>45°</td>
<td>0.56</td>
<td>0.41</td>
<td>0.03</td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>90°</td>
<td>0.20</td>
<td>0.78</td>
<td>0.02</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Fig. 1: Measured fiber orientation tensors of the specimens with a nominal fiber orientation of 0°, 45° and 90°.

Although, the MFH-model is able to predict the stress strain behavior sufficiently for low strains (~ up to 1%), it overestimates the stresses for higher strains (Fig. 2). This is mainly due to the fact that this modeling approach does not take the damage process (interface debonding, void formation, etc.) into account [10, 11]. Therefore, the matrix material model parameters for the plastic region were altered in order to obtain an appropriate MFH-model which is able to reproduce the stress-strain behavior of the composite up to the point of ultimate failure. These parameters were optimized to best-fit the experiments for the 0°, 45° and 90° specimens under all applied loading rates. The stress-strain curves for both the original MFH using the neat PP data and the reverse engineered data from the fiber reinforced specimens are shown in figure 2. It must be emphasized here, however, that these data were derived based on a combination of manually driven parameter fit and optimization routine implemented in DigimatMX [6]. The optimization process was finished if the deviation between the experimental and the homogenized curves at the maximum stress was lower than 2 %. As relevant experimental curve, the average curve of 3 single tensile experiments was used. For further calculations the PP matrix data determined by this reverse method were used.
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Fig. 2: True stress-true strain diagram for the 45° specimen comparing the experimental measurement and the simulation with and without the adapted matrix material model at 0.001s⁻¹

The parameters of the optimized elasto-viscoplastic matrix material model are shown in figure 3.

<table>
<thead>
<tr>
<th>Elasticity</th>
<th>Strain hardening</th>
<th>Viscoplasticity</th>
</tr>
</thead>
<tbody>
<tr>
<td>E 1990 MPa</td>
<td>k 1.04</td>
<td>η 607</td>
</tr>
<tr>
<td>σᵧ 5.6 MPa</td>
<td>R∞ 8 MPa</td>
<td>m 3.3</td>
</tr>
<tr>
<td>ν 0.42</td>
<td></td>
<td>m 1400</td>
</tr>
</tbody>
</table>

Fig. 3: Table of the optimized matrix material parameter for the MFH-model

The comparison of the MFH-model simulations using the optimized matrix and the experimental results at an exemplary strain rate of 0.001s⁻¹ for all fiber orientations is shown in figure 4. With these modified matrix material parameters an acceptable prediction quality (deviation is less than ± 2% regarding the maximum stress value) could be achieved for the different specimen orientations and loading rates.

These models, however, assume perfectly bonded interface and the applicability of them is limited to low strains.

2.2 Experimental determination of the ultimate failure

Prior to the implementation of a failure model the onset of failure was experimentally determined. The onset of failure was defined by a critical stress or strain level. Although various experimental methods were carried out and a number of onset points were defined, for simplicity the maximum stresses as well as the maximum strains were extracted from the uniaxial tensile tests and are used in this study. For more information regarding the experimental techniques please refer to [12, 13].

In addition to the three tensile specimen types with different fiber orientations, shear specimens were milled from injection molded plates with dimensions of 60mm x 60mm x 2mm. This plate was molded in the same multi-tool as the tensile specimens and reveal a nominal fiber orientation of 0° at the range of interest (location of the shear zone at the mid of the plate). The shape and the size of this new specimen are shown in figure 5. These specimens were loaded under uniaxial tension and the nominal shear stress was calculated by dividing the applied force by the initial cross-section (6mm x 2mm) of the shear region. Furthermore the shear strength in the relevant cross-section was determined.
The maximum values of all stress-strain curves for all parameter combinations are shown in figure 6. As expected, these maximum stress values reveal both a clear dependence of the fiber orientation and the strain rate. The 0° specimens show the highest failure stresses, whereas the shear specimens show the lowest stresses, which were slightly under those of the 90° specimens.

In addition, the maximum strains were also determined for the tensile specimens. A variation of the maximum strains for the different orientations is shown in figure 7. In contrary to the maximum stresses, the strains at the maximum stresses do not reveal clear strain rate dependence. Due to the character of all stress-strain curves measured, the strain-at-maximum stress is nearly perfectly coincided with the maximum strains. The majority of the failure criteria are based on relevant stress values and only the “maximum strain criteria” utilizes critical strain values in fiber reinforced composites [7, 14]. In a more general experimental situation the user has two options: (1) use the maximum measured stress values and (2) and use the maximum measured strain values and calculate the maximum stress values. Latter requires, however, the accurate determination of local strain near to the failure region. Hence, stress based failure criteria were combined with the FPGF technique in this study.

Furthermore, the experimentally determined maximum strains were taken and the corresponding stresses were calculated using the previously defined MFH-model. In order to estimate the deviation between the real and predicted stress strain behavior, experimentally obtained maximum stresses and calculated stresses at maximum strains are compared in figure 8.

![Fig. 5: Geometry of the shear specimen](image1)

![Fig. 6: Maximum stresses of monotonic tensile tests of the 0°, 45° 90° and shear specimens at strain rates of 0.0001 s⁻¹, 0.001 s⁻¹ and 0.01 s⁻¹](image2)

![Fig. 7: Maximum strains of monotonic tensile tests of the 0°, 45° 90° at strain rates of 0.0001 s⁻¹, 0.001 s⁻¹ and 0.01 s⁻¹](image3)

![Fig. 8: Simulated maximum stresses of monotonic tensile tests of the 0°, 45° and 90° specimens at strain rates of 0.0001 s⁻¹, 0.001 s⁻¹ and 0.01 s⁻¹](image4)
2.3 First pseudo grain failure model

In order to predict the onset and development of failure, the FPGF model was additionally implemented in the MFH. The main goal of this model is to link the actual local fiber orientation state of a component to unidirectional composite failure criterion. Since this model requires a certain failure criterion, the Tsai-Hill 2D criterion (3) \cite{14} was chosen as a practicable model for these investigations. It must be emphasized here, however, that in principle all composite failure models might be applied and some of these models have already been implemented in DigiMat MF. The failure indicator, $f_A$ of the Tsai-Hill 2D model is expressed as:

$$f_A = \frac{\sigma_{11}^2}{X_t^2} - \frac{\sigma_{11}\sigma_{22}}{X_t^2} + \frac{\sigma_{22}^2}{Y_t^2} + \frac{\sigma_{12}^2}{S^2}$$

(3)

Where $X_t$ is the tensile strength in fiber direction, $Y_t$ is the transverse tensile strength and $S$ is the in-plane shear strength. The FPGF model mathematically separates the fiber orientation distribution function into several pseudo fiber orientations termed as pseudo grains (PG). A pseudo grain reveals a specific unidirectional fiber orientation. Furthermore, a certain weight value is addressed to each pseudo-grain and this value corresponds to the size of the PG. Consequently, the selected failure criterion is applied to each pseudo grain. As the local failure indicator reaches the critical value of 1, the pseudo grain fails and therefore the software increases the global pseudo grain failure indicator by its weight. This global pseudo grain failure indicator can also exhibit a value between 0 and 1. The onset of failure is now defined by a critical failure fraction (cff), which is a critical value of the global pseudo grain failure indicator (defined as PGA value). As these cff values are of crucial importance for characterizing the failure process, the sensitivity was analyzed in this paper. Hence, three different cff values of 0.5, 0.7 and 0.9 were selected for the further modeling. According to these values, Tsai-Hill parameter were determined by mathematical optimization in order to match the measured maximum stresses for all four specimens (tensile 0°, 45° and 90° and shear). These Tsai-Hill parameters, $X_t$ - the tensile strength in fiber direction, $Y_t$ – the

<table>
<thead>
<tr>
<th>cff</th>
<th>$X_t$ [MPa]</th>
<th>$Y_t$ [MPa]</th>
<th>$S$ [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>112.0</td>
<td>21.5</td>
<td>13.0</td>
</tr>
<tr>
<td>0.7</td>
<td>103.0</td>
<td>21.5</td>
<td>12.0</td>
</tr>
<tr>
<td>0.9</td>
<td>101.0</td>
<td>18.5</td>
<td>11.5</td>
</tr>
</tbody>
</table>

Fig. 9: Tsai-Hill failure parameter at a strain rate of 0.0001 s$^{-1}$

Moreover, strain rate dependence was also introduced to the Tsai-Hill parameters. This was realized with a piecewise linear scaling function, which was taken from the experimentally measured maximum stresses. The scaling function of the 0° specimen was applied to $X_t$, the one of the 90° specimen to $Y_t$ and the one of the shear specimen to the parameter $S$. The strain rate dependence of scaling functions for all specimen configurations is shown in figure 10.

![Scaling function](image)

Fig. 10: Piecewise linear scaling functions for the different failure parameters

The Tsai-Hill failure envelopes for tensile and shear loading are visualized for the three parameter sets of cff in figure 11a, b and c. These envelopes represent the maximum multiaxial stresses in $\sigma_{11}$-$\sigma_{22}$ plane that can be applied to a specimen with unidirectional fiber orientation until failure occurs. The axis in $\sigma_{11}$ direction equals the fiber axis. Using the cff values both a self-similar and an uneven shift of these envelopes was realized. That is, lower cff values
results in higher safety. At low cff value less pseudo grains must fail until the ultimate failure occurs.

Using the MFH-model in conjunction with the FPGF failure model the tensile tests of the 0°, 45° and 90° specimen as well as the shear tests could be simulated and the onset of failure could be predicted. Stress - strain curves of the 0° and 90° specimens are plotted in figures 12 and 13 for different strain rates. It can also be shown how the damage of the pseudo grains evolves until it reaches the cff-value, which was defined as 0.5 in this particular case.

Fig. 11: Tsai-Hill failure envelope for UD-fibers for a strainrate of 0.0001 s⁻¹; (a) $\sigma_{11} - \sigma_{22}$; (b) $\sigma_{22} - \sigma_{12}$; (c) $\sigma_{11} - \sigma_{12}$

As expected, the rate dependence of the failure process can be simulated (see figures 12 and 13).

Fig. 12: Simulated stress – strain curves and PGA-value for the 0° specimen for different strain rates

Fig. 13: Simulated stress – strain curves and PGA-value for the 90° specimen for different strain rates

Figure 14 and figure 15 illustrates how the pseudo grains fail for the three different Tsai-Hill parameter sets according to the cff-values of 0.5, 0.7 and 0.9.
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Although, minor differences were observed both regarding the start and the ultimate failure values for all cff sets, no clear tendency could be recognized.

To more strikingly visualize the differences, all results are summarized in figure 16. As clearly shown the fiber orientation has a major influence on the strength. The experimental values are in good agreement with the predicted values based on the Tsai-Hill criterion. Clear strain rate dependence was also observed over the strain rate range investigated. For all cff values used a corresponding set of Tsai-Hill parameters was found. The predictions were for all cff values in the range of the experimental results. The accuracy of the strength prediction does not depend on the cff values. A minor shift in the prediction can be realized towards a more conservative estimation in the Tsai-Hill failure indicators with higher cff values. This is however an apparent phenomenon. Using higher cff values the more pseudo grains must fail up to ultimate failure occurs. That is there is a higher probability for a convenient fiber orientation which does not fail. This effect may results in unreasonable high fracture strain prediction.

3 Conclusions

In a first step a MFH-model was set up based on microstructure parameters, which were derived from computed tomography experiments, elastic-viscoplastic matrix material data from uniaxial tensile tests and linear elastic fiber properties. A good agreement was found between the calculated and the experimental stress-strain curves up to a nominal strain value of 0.01 by using proper material data for the constituents and adequate microstructure. For larger strains, however, the MFH model overestimates the stress both for the 0° and the 90° specimens. These calculations do not include any kind of damage and the divergence of the experimental and the calculated curves may indicate changes in the material behavior. In order to bring the stress-strain behavior of the MFH-model in concordance with the experiments the plasticity material parameters were adapted.

To predict the point of ultimate failure, the MFH-model was extended by a FPGF approach. The
pseudo-grain technique was used to simplify the actual FOD of the specimens. The material is considered as failed, if the pseudo grain failure indicator, which equals the weighted amount of failed grains, reaches a critical level. For this critical failure fraction (cff) value characteristic values of 0.5, 0.7 and 0.9 were selected. To obtain the proper point of ultimate failure for the different cff-values adequate Tsai-Hill parameters were identified. It could be shown that suitable Tsai-Hill parameters could be found for all selected cff-values.

Based on the experimentally measured strain rate dependence of the maximum stress values strain rate dependent Tsai-Hill parameters were also implemented using piecewise linear scaling functions. It must be pointed out that for all failure parameters similar strain rate dependence was observed.

The damage calculations using the Tsai-Hill 2D failure criterion were carried out on each pseudo grain and the kinetics of the failed pseudo-grains was calculated. Although, three different parameters sets leads to a slightly different damage kinetic, a similar point of ultimate failure could be detected. This point of ultimate failure could be properly predicted in the tensile and shear regime. Since in this first approach the tension and compression region are considered to be symmetric, additional experiments must be carried out in order to reliably predict a compressive failure.

In an upcoming work this model will be applied to a component simulation and the models should be validated under multiaxial loading conditions.

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