MICROMECHANICAL MODELLING OF DAMAGE PROCESSES IN COMPOSITE MATERIALS

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1 Introduction

Damage processes of heterogeneous materials are determined by processes at the micromechanical level. As to include these effects in the numerical simulation of engineering problems, finite element solvers need to be coupled to micromechanical models. This work features an example of the application of the multiscale method on the problem of failure and damage analysis of unidirectional composite materials. The simultaneous analyses in the presented methodology have been achieved by using the Abaqus/Explicit solver for the macro-scale problem, while the High Fidelity Generalized Method of Cells (HFGMC) is used to evaluate the stress and strain state at the micromechanical level, as illustrated in Fig. 1. The micro-scale analysis determines the stress and strain field within the unit cell, which is a periodically repeating volume that characterizes the micro-structure of the heterogeneous material. Effective mechanical properties of the composite material are calculated based on the unit cell morphology and the constitutive behavior of its constituents. As the stress distribution within the unit cell is known, calculation of failure criteria and constitutive response of the composite material are performed on the micro-level. Furthermore, degradation of material properties due to damage effects is also being modeled on the micromechanical level by decreasing constituent mechanical properties at the subcell level. The described methodology is still in the development phase, in which different composite failure criteria and degradation models are being evaluated. This work features the results of the comparison of micromechanical failure criteria.

2 High Fidelity Generalized Method of Cells

The discretization scheme of the applied micromechanical model is shown in Fig. 2. As the theoretical background of the HFGMC model is relatively complex, only the basic information, which are needed to understand this paper, are given here. More details about HFGMC models and their implementation into this methodology can be found in [1-6]. Some more recent and interesting applications of micromechanical models based on the Method of Cells model are provided in [7-8]. The representative volume element of the composite material is discretized using $N_p \times N_f$ rectangular subcells. The number of different material phases within the unit cell as well as the number of subcells is arbitrary. The particular version of the HFGMC model used in this work is the reformulated HFGMC, which has been introduced in [2-4]. The reformulation enhances the computational effectiveness of the model and simplifies the unit cell modeling by departing of the generic cells concept of the original HFGMC model [1]. Since the applied model is a two-dimensional micromechanical model, it is suitable only for unidirectional composite materials. The doubly periodic unit cell is modeled with fibers oriented in the $x_1$ direction and arranged in a doubly periodic array in the $x_2$ and $x_3$ directions. The displacement field within the unit cell is approximated using Legendre-type polynomial expansion, after [1,2]:

$$ u^{(\beta,\gamma)}_i = \bar{e}_{ij} x_j + W^{(\beta,\gamma)}_{(00)} + \bar{y}_{ij}^{(\beta)} W^{(\beta,\gamma)}_{(10)} + \frac{1}{2} \left( 3 \bar{y}_{ij}^{(\beta)} - \frac{h_j^2}{4} \right) W^{(\beta,\gamma)}_{(20)} + \frac{1}{2} \left( 3 \bar{y}_{ij}^{(\beta)} - \frac{h_j^2}{4} \right) W^{(\beta,\gamma)}_{(20)} + (1) $$

where $i, j = 1, 2, 3$. ...
The first step of the micromechanical model is calculation of the subcell local stiffness matrices based on the subcell mechanical properties and dimensions. The stiffness matrices are merged into the global system of equations by application of displacement and traction continuity conditions between the subcells, and periodicity conditions in the $x_2$ and $x_3$ directions on the unit cell boundaries. Additionally, four displacement components are constrained in order to prevent unit cell rigid body motion as displayed by the four arrows at the unit cell borders in Fig. 2. The solution of the global system of equations enables calculation of the strain concentration tensor which relates the macroscopic strain tensor $\varepsilon$ to the microscopic strain state of each subcell $\varepsilon^{(\beta,\gamma)}$, after Eq. 2.

$$\varepsilon^{(\beta,\gamma)} = A^{(\beta,\gamma)} \varepsilon$$

In order to be able to evaluate different micromechanical failure and degradation models, a standalone application has been developed which simulates input from the Abaqus/Explicit analysis to the HFGMC/VUMAT material model for various macroscopic load cases. The results given in this work are obtained using this standalone HFGMC model. As the structure of HFGMC subroutines is the same for the standalone application as for the multi-scale environment, the secondary role of the standalone application is the testing and debugging of the HFGMC subroutines.

### 4 Failure criteria and damage models

The first step in the process of micromechanical damage modeling of composite materials is the application of failure initiation criteria. These criteria, at the micro-scale, indicate initiation of degradation processes at the subcell level within the HFGMC model. As a subcell, in the simplest case of HFGMC, is occupied by either fiber or matrix material, the stress or strain state within the unit cell is compared with the constituent stress or strain allowable values. In order to obtain the micromechanical failure curves of the complete composite material, fiber and matrix failure has to be taken into account simultaneously, as failure initiation in the constituents occurs under different loading conditions. This work features the comparison of three failure initiation models applied at the micromechanical level:

a) The first failure model is taken from [9]. Failure initiation in matrix subcells is calculated using the 3D Tsai Hill criterion defined as
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\[
\left( \sigma_{11}^{(1,2)} \right)^2 + \left( \sigma_{22}^{(1,2)} \right)^2 + \left( \sigma_{33}^{(1,2)} \right)^2 + \frac{-\sigma_{11}^{(1,2)} \sigma_{22}^{(1,2)} - \sigma_{11}^{(1,2)} \sigma_{33}^{(1,2)} - \sigma_{22}^{(1,2)} \sigma_{33}^{(1,2)}}{Y^2} + \frac{\left( \sigma_{12}^{(1,2)} \right)^2 + \left( \sigma_{13}^{(1,2)} \right)^2 + \left( \sigma_{23}^{(1,2)} \right)^2}{T^2} = d_m^2,
\]

where \( Y \) is the matrix transverse strength and \( T \) is matrix shear strength. The value of the matrix strength used in Eq. 3 depends on the type of the applied transverse stress, after \[9\]

\[
Y = Y_r, \quad \sigma_{22} < 0 \quad Y = Y_r, \quad \sigma_{22} > 0.
\]

The criterion indicates initiation of failure processes when the right-hand side term \( d_m \) takes values greater than 1. Failure initiation in fiber subcells is indicated using the maximal strain criterion, which is formulated as

\[
\left( \varepsilon_{11}^{(1,2)} \right)^2 = d_f^2, \quad \varepsilon_{11} > 0.
\]

\( \varepsilon_{11}^{(1,2)} \) denotes the subcell strain in the fiber direction while \( \varepsilon_{11}^{(1,2)} \) is the ultimate fiber strain in the fiber direction which can be calculated from tensile and compressive strength properties provided in Table 1. Similarly to the matrix criterion, failure is initiated if the right-hand side term \( d_f \) reaches values above 1.

b) The second failure model which has been investigated in this work employs the failure criteria applied by the Multicontinuum Theory (MCT) \[10\]. The fiber and matrix failure criteria have been used on the micro-scale for the World Wide Failure Exercise (WWFE) within a finite element micromechanical model. As opposed to the original MCT, the failure criteria in this work have been applied to the HFGMC micromechanical model, consequently taking into account the stress variations within the unit cell instead of dealing with averaged constituent values. The expressions for the criteria have been derived from the quadratic interaction failure criterion, by taking into account assumptions on the failure modes for the fiber and matrix constituents. Failure initiation in the matrix is predicted if the stress state satisfies the relation

\[
K_{3m} I_3 + K_{4m} I_4 = 1, \quad (6)
\]

where

\[
K_{3m} = \frac{1}{S_{22m}^2 + S_{33m}^2}, \quad (7)
\]

\[
K_{4m} = \frac{1}{S_{12m}^2}, \quad (8)
\]

\( S_{22m} \) and \( S_{33m} \) are matrix strengths in the 2 and 3 directions, which are dependent on the tensile/compressive character of the loading in the 2 direction \[10\]. The shear strength of the matrix \( S_{12m} \) is not provided in \[11\], therefore its value is estimated to be half of the tensile strength value. This estimation is valid for epoxy matrices, as stated in \[12\]. Fiber failure is predicted using the equation

\[
K_{1f} I_1^2 + K_{4f} I_4 = 1, \quad (9)
\]

where

\[
K_{1f} = \frac{1}{S_{11f}^2}, \quad (10)
\]

and

\[
K_{4f} = \frac{1}{S_{12f}^2}. \quad (11)
\]

The \( S_{11f} \) term denotes the strength in fiber direction, which can be tensile or compressive, while \( S_{12f} \) is the fiber shear strength. The relations in Equations 6 and 9 include the transversally isotropic stress invariants, expressed as \[10\]

\[
I_1 = \sigma_{11},
I_2 = \sigma_{22} + \sigma_{33},
I_3 = \sigma_{22}^2 + \sigma_{33}^2 + 2\sigma_{23}^2, \quad (12)
I_4 = \sigma_{12}^2 + \sigma_{13}^2.
\]

c) The last failure theory examined in this work is the 3D Hashin-type strain based failure criterion for the matrix combined with the maximal strength criterion for the fiber, as used in \[13\]. The damage
The degradation model introduced in [13] has also been incorporated in the presented multiscale procedure. The continuum damage model presented in [13] accounts for multiaxiality and progressive degradation of subcell elasticity properties. The failure criterion for the matrix subcells employs damage strains defined as

$$\varepsilon_1^D = \left( \frac{\varepsilon_{11}}{X_e} \right)^2 + \left( \frac{\varepsilon_{12}}{Y_e} \right)^2 + \left( \frac{\varepsilon_{13}}{Z_e} \right)^2,$$

$$\varepsilon_2^D = \left( \frac{\varepsilon_{22}}{Y_e} \right)^2 + \left( \frac{\varepsilon_{23}}{Q_e} \right)^2 + \left( \frac{\varepsilon_{33}}{S_e} \right)^2,$$

$$\varepsilon_3^D = \left( \frac{\varepsilon_{33}}{Z_e} \right)^2 + \left( \frac{\varepsilon_{23}}{Q_e} \right)^2 + \left( \frac{\varepsilon_{33}}{R_e} \right)^2,$$

where the $X_e$, $Y_e$, and $Z_e$ variables are the normal failure strains while $R_e$, $Q_e$, and $S_e$ are engineering shear failure strains. The damage strains defined in Eq. 13 have the same function as the left-hand sides of commonly used failure criteria for fiber reinforced composite materials, indicating initiation of failure processes if their values reach 1.0.

Failure within fiber subcells is predicted using the maximal strain criterion, defined as

$$\frac{\varepsilon_1^{(t, T)}}{X_e^{t, T}} \geq 1.$$ (14)

If fiber subcells reach failure initiation, mechanical properties are instantaneously set to a very low value (0.0001 times the initial value) thereby simulating complete subcell failure. The damage progression model is applied only for matrix subcells. The degradation processes of matrix subcells are initiated if the damage strains reach values higher than 1.0 or the maximal obtained value during previous load increments. Damage evolution in matrix material is tracked using six different damage variables $D_i$, three for tension and three for compression. The incremental changes of damage variables and associated degradation of mechanical properties during a load increment are calculated using the relation

$$dD_i = (1 - D_i - k_i') \frac{d\varepsilon_i}{\varepsilon_i}, \quad i, j = 1, 2, 3, \quad (15)$$

where $d\varepsilon_i$ is the increment of the damage strain, while $k_i'$ is the modified slope parameter calculated as

$$k_i' = A e^{-\varepsilon_i^{(t, T)/B}}, \quad i = 1, 2, 3,$$ (16)

with $A$ and $B$ as the post-damage slope parameters. The damage model separates degradation processes in tensile and compressive failure modes

$$D_i^T = D_i^{T, old} + dD_i \quad \text{for } \varepsilon_i > 0,$$

$$D_i^C = D_i^{C, old} + dD_i \quad \text{for } \varepsilon_i < 0.$$ (17)

The progressive degradation model modifies only matrix subcell mechanical properties. The elasticity properties are degraded using

$$E_i = dE_i^0 \quad \text{for } i = 1, 2, 3,$$ (18)

$$\nu_{ij} = d\nu_{ij}^0 \quad \text{for } i, j = 1, 2, 3.$$ (19)

The $d_i$ variables are calculated as

$$d_i = \begin{cases} 1 - b_i^T D_i^T & \text{for } \sigma_i > 0 \\ 1 - b_i^C D_i^C & \text{for } \sigma_i < 0 \end{cases} \quad i = 1, 2, 3 \quad (20)$$

where $b$ parameters are the scaling parameters. The final failure of matrix subcells is predicted using damage energy principles. The strain energy density is calculated using the relation

$$dW_i = \frac{1}{2} \left[ \sigma_i (\varepsilon_i + d\varepsilon_i) - \varepsilon_i (\sigma_i + d\sigma_i) \right] \quad i = 1, 2, 3. \quad (21)$$

Table 1. Constituent properties as listed in [11]

<table>
<thead>
<tr>
<th>Fiber</th>
<th>$E$ (GPa)</th>
<th>$\nu$ [-]</th>
<th>$X^t$ [MPa]</th>
<th>$X^c$ [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-glass fiber</td>
<td>74</td>
<td>0.2</td>
<td>2150</td>
<td>1450</td>
</tr>
<tr>
<td>Epoxy matrix</td>
<td>3.35</td>
<td>0.35</td>
<td>80</td>
<td>120</td>
</tr>
</tbody>
</table>

The final failure criterion is associated with the loading modes - Mode I (opening), Mode II (in-plane shear) and Mode III (out of plane shear). The mode-specific strain energy density release rates, after [13], are

$$dW_i = \frac{1}{2} \left[ \sigma_i (\varepsilon_i + d\varepsilon_i) - \varepsilon_i (\sigma_i + d\sigma_i) \right] \quad i = 1, 2, 3.$$ (21)
The associated strain energy release rates are
\[ G_i^1 = \frac{l_i}{b_{11}} \frac{dW_i^1}{dD_1}, \quad G_i^m = \frac{l_i}{b_{11}} \frac{dW_i^m}{dD_1}, \]
\[ G_i^m = \frac{l_i}{b_{22}} \frac{dW_i^m}{dD_1}, \quad G_i^2 = \frac{l_2}{b_{22}} \frac{dW_i^2}{dD_2}, \]
\[ G_i^3 = \frac{l_3}{b_{23}} \frac{dW_i^3}{dD_3}, \quad G_i^3 = \frac{l_3}{b_{33}} \frac{dW_i^3}{dD_3}. \] (23)

where \( b_{ij} \) denote scaling parameters, while \( l_i \) is the characteristic material length. Complete degradation of matrix subcells properties in tensile loading modes is determined if the mode-specific strain energy release rates reach the material critical strain release rate.

\[ G_M^i \geq G_M^C, \quad M = I, II, III. \] (24)

For failure prediction in compressive loading modes a criterion based on the total dissipated energy has been employed. The criteria have the form
\[ (W_i^1 + W_i^m + W_i^m) V = W^C, \quad i = 1, 2, 3, \] (25)

where \( V \) is the volume of the material and \( W^C \) is the critical compressive strain energy. An example of the properties for the degradation model is provided in Table 3, after [13].

5 Results
Fig. 3 shows the visualization of the matrix failure initiation criteria in the \( \sigma_{22} - \sigma_{33} \) plane. The mechanical properties of the matrix for this study are taken from [11] for the MY750/HY917/DY063 epoxy matrix and are listed in Table 1. The discontinuities in the 3D Tsai-Hill and MCT curves arise from the difference between the compressive and tensile strengths of the matrix. The comparison of the three failure curves shows that the 3D Tsai-Hill and the Hashin curve match reasonably well, while the MCT curve deviates from the other two curves in some regions of the stress space. This deviation can be explained by the fact that the MCT matrix failure criterion, defined in Eq. 6, has been derived with the assumption that the matrix is used within a fiber reinforced material. The complete derivation of the MCT failure criteria, along with the modified mechanical properties for matrices used in the WWFE can be found in [10].

Fig 3. Failure curves in \( \sigma_{22} - \sigma_{33} \) stress space for the MY750/HY917/DY063 stress matrix, in MPa.

The investigated composite micromechanical failure models have been validated on a composite material consisting of the Silenka E-glass fiber and the MY750/HY917/DY063 epoxy matrix with 60% fiber volume fraction, as used in the WWFE [11]. Visualization of the evaluated failure models for fiber reinforced composite materials in the homogenized \( \sigma_{11} - \sigma_{22} \) stress plane is shown in Fig. 4. The failure curves have been predicted using a 40 x 40 HFGMC model with a single fiber at the unit cell centre. All results shown in this work have been derived using the standalone application as described in Section 3.

At the micromechanical level the fiber and matrix constitutive relations can be approximated by an
isotropic material model which is a common assumption used in micromechanical analyses as suggested in [9,13-15]. The homogenized mechanical properties calculated using the HFGMC differ from the composite ply properties provided in [11], as listed in Table 2. Differences between micromechanically calculated and experimentally obtained composite properties are often encountered in the literature e.g. [10, 13, 14]. These differences are explained by the assumption that the constituent properties in a composite material differ from the original constituent properties. Therefore, micromechanical analyses use modified constituent mechanical properties, which are selected as to match homogenized properties with experimentally obtained results.

### Table 2. Composite lamina properties

<table>
<thead>
<tr>
<th>Provided in [11]</th>
<th>40 x 40 HFGMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$ [GPa]</td>
<td>45.6</td>
</tr>
<tr>
<td>$E_2 = E_1$ [GPa]</td>
<td>16.2</td>
</tr>
<tr>
<td>$G_{12}$ [GPa]</td>
<td>5.832</td>
</tr>
<tr>
<td>$\nu_{12}$ [-]</td>
<td>0.278</td>
</tr>
<tr>
<td>$\nu_{21}$ [-]</td>
<td>0.4</td>
</tr>
</tbody>
</table>

The discontinuities of matrix failure curves, observable in Fig. 3, are also present in the results for the composite material. The three evaluated failure curves compare reasonably well to each other, especially for the fiber failure loading modes (compressive loading in the fiber direction). The largest differences occur in the $\sigma_{22}$ loading curves, where the MCT failure theory is the most conservative by predicting lower values at which failure occurs. The 3D Tsai-Hill criterion, on the other hand, predicts failure initiation at significantly higher load states.

The failure curves in Fig. 4 show the loading state at which the HFGMC model indicates failure of the first subcell. As to get insight into the real differences between the evaluated failure models, Fig. 5 shows the distribution of the value of matrix failure criteria at the tensile load state at which the MCT criterion indicates failure initiation.

![Fig. 4 Failure curves in the macro-level $\sigma_{11} - \sigma_{22}$ plane, in MPa.](image)

The distribution of the MCT criterion shows that the failure initiation state is reached in a relatively large area of the unit cell at the same load increment. The maximal values of the other criteria for this loading state are 0.763 and 0.915 for the 3D Tsai-Hill and Hashin criterion, respectively.

Fig. 6 shows the comparison of the matrix failure criteria for the load state at which the 3D Tsai-Hill reaches the failure state. The damage degradation effects have been neglected for this comparison. The results show that at this load state failure initiation has been predicted in a large number of subcells for the MCT and the Hashin criteria.

![Fig. 6. Comparison of failure criteria distribution for the load state at which the 3D Tsai-Hill matrix failure criterion reaches the critical value.](image)

The results of the progressive damage degradation model are shown in Fig. 7. For this analysis the constituent mechanical properties have been modified as to be able to compare the implementation of the model with the results.
provided in [13]. The modified mechanical properties are listed in Table 3. The final failure criterion of the complete unit cell is not specified in [13]. The final failure curve in Fig. 7 has been constructed by setting the complete degradation of the unit cell to occur when 10% of the total number of matrix subcells fails. The unit cell failure criterion is very important since the failure of the unit cell indicates the failure of the material point for the case in which the HFGMC is applied within the multiscale environment, as explained in Section 3. Therefore, this parameter controls the element deletion criterion in the FE analysis. The initial subcell failure curve is very close to the final unit cell failure curve, thus only the final unit cell curve is shown in Fig. 7. The HFGMC model used for this analysis is discretized using 30x30 subcells.

Table 3. Modified constituent properties and parameters of the degradation model as specified in [13]

<table>
<thead>
<tr>
<th>Material</th>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silenka E-glass properties</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E$ [GPa]</td>
<td>$v$ [-]</td>
<td>$X^T$ [MPa]</td>
</tr>
<tr>
<td>74</td>
<td>0.2</td>
<td>2110</td>
<td>1290</td>
</tr>
<tr>
<td>MY750/HY917/DY063 epoxy properties</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E$ [GPa]</td>
<td>$v$ [-]</td>
<td>$X_i^T$ [-]</td>
</tr>
<tr>
<td>3.7</td>
<td>0.35</td>
<td>0.0125</td>
<td>0.0287</td>
</tr>
<tr>
<td>Post-damage slope parameters</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A^T = 0.7$</td>
<td>$A^C = 2.0$</td>
<td>$B^T = 0.82$</td>
<td>$B^C = 0.96$</td>
</tr>
<tr>
<td>$b_i^T = b_i^C = 1.32$</td>
<td>$b_{ii} = b_{ii} = b_{iii} = 0.50$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Critical energy release rates</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mode I SERR</td>
<td>$G_i^C$</td>
<td></td>
<td>800 J/m$^2$</td>
</tr>
<tr>
<td>Mode II and III SERR</td>
<td>$G_{ii}^C = G_{ii}^C$</td>
<td>2400 J/m$^2$</td>
<td></td>
</tr>
<tr>
<td>Critical compressive strain energy</td>
<td>$W_{S}^C$</td>
<td>$1.86 \times 10^{-6}$ J</td>
<td></td>
</tr>
<tr>
<td>Material length</td>
<td>$l_i$</td>
<td></td>
<td>$9.0 \times 10^{-3}$ m</td>
</tr>
</tbody>
</table>

Fig. 8 shows the evolution of the subcell failure process for loading in the tensile $\sigma_{22}$ direction. The damage strain in the 2 direction indicates initiation of degradation processes in the first subcells at 33.5 MPa. The first subcells in this load case fail at the $\sigma_{22}$ loading of 36.4 MPa, and the contour of the failed subcells compares well to the $e_{22}^D$ distribution shown in Fig. 5 and Fig. 6. The 10% matrix failure condition is reached at 36.6 MPa.

Fig. 7: Initial and final failure curves of the E-glass epoxy composite with the failure and degradation model provided in [13].

Fig. 8. Subcell failing process in the $\sigma_{22}$ loading direction.

6 Conclusions

The three evaluated failure criteria compare reasonably well to each other. Currently, a sophisticated damage progression model has been implemented into the model. The literature survey on micromechanical failure models shows the need for progressive degradation models. As indicated in e.g. [16], the sudden loss of mechanical properties is a too conservative approach to micromechanical damage modeling and the progressive nature of damage has to be taken into account as to be able to replicate experimental results. The progressive damage model within the HFGMC framework employs continuum damage principles at the subcell level, which enables the variation of matrix mechanical properties within the unit cell.
A limitation of the presented damage modeling procedure is that it is not applicable to a localized damage effects within the composite material due to the periodicity conditions on the unit cell boundaries. As a result, the model indicates that the calculated damage repeats itself in the unit cell plane which contradicts the physical behavior of damage in composite materials. A further drawback of the applied damage model is the strong dependence of the load increment on damage progression. The failure curves obtained with 30x30 unit cell model are very close to finer unit cells, indicating that damage processes of simple unit cells can be efficiently modeled using relatively coarse unit cell models. Although micromechanical failure criteria predict the onset of damaging processes in only a single subcell, the obtained results show that a large number of the subcells satisfy the failure initiation criterion at the same load state. Consequently, damage processes are initiated in a large part of the unit cell for the same macroscopic loading condition.

References


