

A methodology to predict longitudinal failure in unidirectional composites considering imperfect fiber/matrix interface

José Humberto S. Almeida Jr.¹, Bruna Favoretto², Maísa M. A. D. Maciel², Lars Bittrich¹, Axel Spickenheuer¹, Volnei Tita²

¹Mechanics and Composite Materials Department, Leibniz-Institut für Polymerforschung, Hohe Straße 6, 01069 Dresden, Germany. humberto@ipfdd.de; bittrich-lars@ipfdd.de; spickenheuer@ipfdd.de

²Department of Aeronautical Engineering, São Carlos School of Engineering, University of São Paulo, Av. João Dagnone, 1100, 13573-120 São Carlos, SP, Brazil. bruna.favoretto@usp.br; voltita@sc.usp.br

Abstract: The macroscopic properties of fiber-reinforced polymer composites (FRPC) depend upon the properties and the interfacial bonding conditions of the constituent phases (fiber and matrix) and the microstructure of the composites. In this research, a numerical methodology to model non-perfect interface for a thin interface is presented. A transversely isotropic representative volume element (RVE) with circular fibers embedded into a square bulk polymer matrix was developed in order to calculate all coefficients of the constitutive tensor for several imperfect contact conditions. Later on, the effective coefficients are used as input in a macro-scale model to predict the mechanical response of unidirectional laminates under longitudinal tensile loading.

Keywords: Fiber-matrix interface, micromechanical modeling, longitudinal failure.

INTRODUCTION

Carbon fiber reinforced polymer (CFRP) composites are nowadays widely used in aero-structural components due to their high specific stiffness and strength. CFRPs are well known as hierarchical materials with three structural levels: micro-scale, macro-scale and macro-scale. The micro-scale defines the arrangement of fibers in the fiber bundle; the intermediate level (macro-scale) generally relates to the lamina geometry; and the macro-scale refers to the global structural response of the material. In the framework of a multi-scale simulation of a CFRP, micro-scale approaches are usually applied to predict the effective stiffness and strength properties of transversely isotropic constitutive properties of composites, serving as theoretical tools for engineering structure design (Wang et al., 2016).

Failure mechanisms of CFRPs still is challenging issue, mainly because the anisotropic nature of the carbon fiber complicates the numerical modeling. Unidirectional (UD) CFRPs subjected to transverse tensile loads often fail by two different failure mechanisms: one is associated with matrix damage and the other is caused by micro-cracks growing at the fiber/matrix interface. For longitudinal loading, matrix and fiber cracking are the most often seen failure modes. Some investigations focus on micro-cracks growing at the fiber/matrix interfaces under longitudinal and transverse loads (Vajari et al., 2013).

Yang et al. (2012) developed a micromechanical damage model considering random fiber distribution in order to reveal the failure mechanisms of unidirectional (UD) CFRP composites under transverse tension and compression. It was concluded that the tensile failure initiated as interfacial debonding and evolved as a result of interactions between interfacial debonding and matrix plastic deformation, while the compressive failure was dominated by matrix plastic damage. Totry et al. (2010) studied the effect of fiber, matrix and interface properties on the in-plane shear response of CFRP laminates experimentally and numerically. It was found that in-plane shear behavior of cross-ply laminates was controlled by the matrix yield strength and the interface strength was independent of the fiber properties. Vaughan and McCarthy (2011) presented a micromechanical damage model to assess the influence of intra-ply properties on the transverse shear deformation of a CFRP laminate. The fiber/matrix interface strength was found to control transverse shear strength, while the interface fracture energy had marked effect on the strain to failure and the interaction of damage mechanisms during fracture.

As can be seen, there are numerous works dealing with micromechanical modeling of composite laminates under transverse loads. For longitudinal loads, for simplification purposes, maximum stress criterion is often used. However, local or partial debonding of the fiber/matrix interface might play a key role (Shari et al., 1995). For instance, when a UD laminate is under longitudinal tension, whether some non-linearity throughout the loading history appears, it can be attributed splitting of some bundles, fiber pull-out or imperfect fiber/matrix contact. The interface is a transition zone between the fiber (first phase) and the matrix (second phase). This third phase may result from the manufacturing

process for most fiber-reinforced composites. Although the thickness of interface is very small, this third phase plays a vital role in the reliability of CFRPs and affects their global mechanical response considerably. For instance, if the fiber/matrix adhesion is imperfect, then the continuity conditions for stresses and displacements are not satisfied (Tita et al., 2015).

In this context, this investigation proposes a numerical methodology to predict the mechanical response of UD composite laminates under longitudinal tensile loading accounting for different degrees of fiber/matrix imperfection. For that, a micromechanical model is developed in order to determine the effective coefficients of the constitutive matrix. A reverse methodology is proposed, in which an energy-based method is used, where the energy from the load *vs.* displacement curves of a UD specimen under tensile loading is calculated and used to find the required load (*l*) to generate the experimental displacement (*d*) based on the energy released from any particular point throughout the σ *vs.* ε curve.

Micromechanical modeling

The first objective of the micromechanical modeling is to determine the effective properties for UD periodic laminate, considering individual properties of the constituent materials (fiber and matrix) and of the composite (e.g. fiber geometry, fiber volume fraction and imperfect contact). For that, firstly, a representative volume element (RVE) is generated via *Python* and analyzed numerically via finite element (FE) analysis in Abaqus package.

The first step is to determine the fibers arrangement. In this case, a square arrangement chosen: the RVE is a 1 mm³ cube, and the fiber is a centered cylinder, as shows Figure 1. The V_f must be exactly the same as before ($V_f = 62\%$). In addition, a thin layer is added at the boundary between the fiber and the matrix to represent the interface. Based on “Tita et al., 2015”, the interphase volume fraction (I_f) must be determined based on the following relation:

$$\frac{t}{a} = 0.001 \quad (1)$$

where t is the interface thickness and a is the fiber radius. It leads to an I_f of 0.12%.

The next step is to define the material properties separately. Each element (fiber, matrix and interface) is considered as being isotropic and homogenous. Particularly in the case of the interface, the shear modulus (G_i) is a parameter related to the fiber/matrix contact. For high G values, the contact is perfect, so the stress is transferred from the matrix to the fiber. The higher the G_i , the greater the interfacial contact. When G_i reaches very small values (i.e. 1), there is no fiber/matrix contact anymore. The idea is then to vary the G_i values (that physically represents the transition from a perfect interface to a non-perfect one) in order to understand how it will affect the CFRP properties. Essentially, the idea is to incorporate the fiber/matrix adhesion characteristics obtained via this current micromechanical model into a progressive damage model that will be herein later explained. At the end, a micro-to-macro methodology will be proposed, in which the macro model will be able to incorporate and consider the fiber/matrix interface behavior in the analysis.

The constitutive equation of the composites studied can be written as follow (generalized Hook’s law):

$$\sigma_{ij} = c_{ijkl} \varepsilon_{kl} \quad (2)$$

where σ_{ij} and ε_{ikl} are the stress and infinitesimal strain tensors. For a transversally isotropic composite laminate, this constitutive relation can be written in the matrix form:

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{23} \\ \varepsilon_{13} \\ \varepsilon_{12} \end{Bmatrix} \quad (3)$$

where the contracted Voigt notation is used.

The homogenization approach for composite materials relies on finding dependence between the average variables of the material model, which may represent the coherent physical behavior (Brito-Santana et al., 2016). Based on the theorem of average, the mechanical properties of the RVE are taken from average properties of the composite laminate. It is assumed that the average mechanical properties of a RVE are equal to the average properties of the composite laminate, as follows

$$\langle T_{ij} \rangle = \overline{T_{ij}} \quad (4)$$

where $\langle T_{ij} \rangle$ is the second rank stress tensor and $\overline{T_{ij}}$ is the average stress. In this case, the average stress in the RVE is defined by:

$$\bar{T}_{ij} = \frac{1}{|V|} \int_V T_{ij}^0 dV \quad (5)$$

where $|V|$ is the RVE volume. Using FE analysis, the average results can be calculated via the following relation:

$$\bar{T}_{ij} = \frac{1}{|V|} \sum_{n=1}^{nel} T_{ij}^{(n)} V^{(n)} \quad (6)$$

where nel is the number of elements of the RVE, $T_{ij}^{(n)}$ and $V^{(n)}$ are the evaluated tensor and volume of the n th element.

For a complete description to determine effective material properties, it is necessary to formulate suitable boundary conditions (BCs). Since periodic structures are herein investigated, periodic boundary conditions must be applied to make the RVE representative. Considering the composite as a periodical array of RVEs, periodic BCs must be applied to the RVE models.

Figure 1 presents a periodic FRPC structure with a square arrangement and a circular fiber embedded into a bulk polymer matrix. It is valid to mention that the fiber is aligned with the z-axis (direction 3). A 3D model with fiber and matrix meshed with eight-node linear brick element with reduced integration and hour glass control (C3D8R) is developed. As depicts Figure 2, periodic boundary conditions (PBC) are applied to the RVEs, where a small displacement is applied whereas all other displacements are restricted to calculate the effective coefficients. For example, for calculating c_{11}^{eff} and c_{12}^{eff} , the displacement is applied in x-direction (Figure 2b).

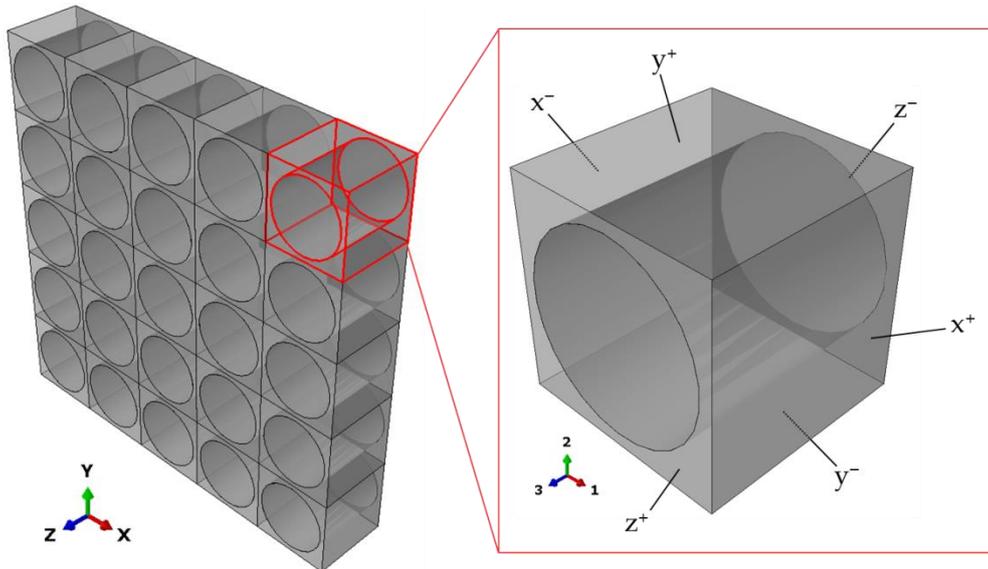


Figure 1 – Periodic FRPC with circular fibers embedded into a square bulk matrix (left) highlighting a unit cell (right).

The set of constitutive matrix (Eq. 3), with prescribed boundary conditions allow the evaluation of the effective material properties. For given particular BCs applied in the RVE, more than one coefficient is obtained for each analysis. Therefore, to calculate all 6 effective coefficients, only 4 analyses are required. Table 1 presents a summary of the loads and BCs used.

In order to predict the longitudinal tensile failure of UD composites, a reverse methodology is herein proposed. The whole methodology is hereafter described, as follows:

- i. Develop the RVE and apply adequate BCs for calculating specific effective coefficients;
- ii. Calculate the effective coefficients through Python scripts collecting the stress and strain tensors numerically by running the Python script in Abaqus FE package;
- iii. For a $[0]_5$ laminate under experimental tensile loading (from Tita, 2003), calculate the released energy at each point (see Table 2) of the σ vs. ε curve, i.e. from macro scale;
- iv. Impose strain on the RVE (micro scale) and calculate stress on the RVE, which promotes the same released energy calculated in iii) (macro scale), and by using theorem of average, inverse analyses and an optimization process compute G_i (shear interface modulus) for that energy level;
 - a. Repeat this step for the 8 points shown in Table 2);

- v. The obtained relationship between G_i and imposed local strain will allow knowing the degree of fiber/matrix adhesion imperfection for each point;
- vi. A relationship between a calibrated value of \bar{E}_{11} vs. \bar{G} ($G_i + G_f$) can be established by using different values for the degree of imperfections in the interface of the RVE;
- vii. Based on the relation between G_i and imposed local strain, it is possible determine G_i for a given strain level. Then, based on the relationship between \bar{E}_{11} vs. \bar{G} ($G_i + G_f$), it is possible to calculate \bar{E}_{11} . Thus, these effective properties are transferred to a macro-based scale numerical model of a $[0]_5$ laminate under longitudinal tensile loading;
- viii. Calibrating the elastic portion through the steps above described, an efficient and fast degradation model is applied to accurately predict the non-linear portion of the curve.

Table 1. Loadings and boundary conditions (BCs) for calculating all effective coefficients.

Equation	Displacement field (m)	Loading field (N)	Displacement BCs (m)
$c_{11}^{eff} = \frac{\bar{T}_{11}}{\bar{\epsilon}_{11}}$ & $c_{12}^{eff} = \frac{\bar{T}_{22}}{\bar{\epsilon}_{11}}$	Positive u_x : face x^+	---	Zero normal displacement at faces: x^-, y^+, y^-, z^+, z^- $\epsilon_{22} = \epsilon_{33} = \epsilon_{12} = \epsilon_{23} = \epsilon_{31} = 0$
$c_{13}^{eff} = \frac{\bar{T}_{11}}{\bar{\epsilon}_{33}}$ & $c_{33}^{eff} = \frac{\bar{T}_{33}}{\bar{\epsilon}_{33}}$	Positive u_z : face z^+	---	Zero normal displacement at faces: x^+, x^-, y^+, y^-, z^- $\epsilon_{11} = \epsilon_{22} = \epsilon_{12} = \epsilon_{23} = \epsilon_{31} = 0$
$c_{66}^{eff} = \frac{\bar{T}_{12}}{\bar{\epsilon}_{12}}$	---	$+F_y$ & $-F_y$ at faces x^+ & x^- $+F_x$ & $-F_x$ at faces y^+ & y^-	Zero y-displacement at faces: x^+ & x^- Zero x-displacement at face: y^- Uniform x-displacement at face: y^+
$c_{44}^{eff} = \frac{\bar{T}_{23}}{\bar{\epsilon}_{23}}$	---	$+F_y$ & $-F_y$ at faces z^+ & z^- $+F_z$ & $-F_z$ at faces y^+ & y^-	Zero y-displacement at faces: z^+ & z^- Zero z-displacement at face: y^- Uniform z-displacement at face: y^+

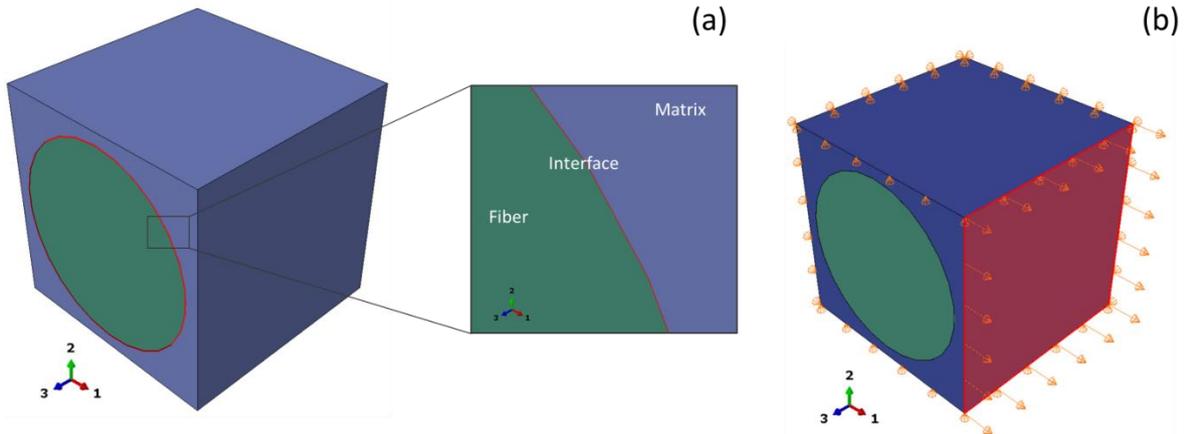


Figure 2 - Unit cell illustrating the three different phase of a RVE (a) and BCs for determining c_{11}^{eff} and c_{12}^{eff} .

Table 2. Experimental stress and strain values collected from 2 specimens (macro-level) under longitudinal tensile loading used to calculate the released energy at each point.

Point	Stress (MPa)	Strain ¹ (%)	Strain ² (%)
1	250	0.200	0.250
2	500	0.380	0.500
3	750	0.647	0.760
4	1000	0.900	1.050
5	1250	1.200	1.320
6	1500	1.500	1.617
7	1750	2.000	2.000
8	2000	2.500	2.500

PRELIMINARY RESULTS

Following the methodology previously described, the step i), which consists on developing the RVEs, have been already described in the Methodology section. The effective coefficients are also calculated after applying suitable loading and BCs, and they are shown in Figure 3. Considering that this is an ongoing research, all other results listed in the previous section will be presented in the final version of this article. At the final submission, it is expected to have more accurate predictions of the mechanical response of UD composites under longitudinal tensile loading, in which the non-linear portion of experimental curves will be associated with imperfect fiber/matrix adhesion.

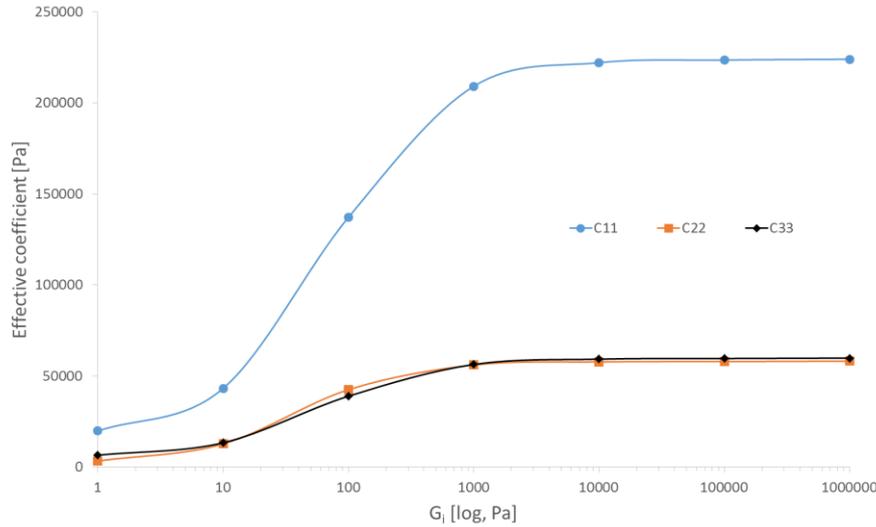


Figure 3. Variation of three effective coefficients with the shear interface modulus (G_i).

CONCLUSION

In the final version of this work, a complete methodology to predict longitudinal tensile failure of UD composites will be proposed. For that, an association between FE micromechanical and FE macromechanical models is proposed. The RVEs, with periodic boundary conditions, are subjected to several BCs and loading conditions in order to calculate the effective coefficients. Then, based upon the released energy collected from experimental curves, this energy is used as input in the micromechanical models to understand the relation between the interfacial adhesion and the RVE strain based on the released energy. At last, these data are used as input into macromechanical analysis in which a progressive degradation law will be applied.

ACKNOWLEDGMENTS

J.H.S. Almeida Jr. is grateful for CAPES and Alexander von Humboldt for the financial support; Volnei Tita is thankful to National Council for Scientific and Technological Development (CNPq process number: 401170/2014-4 and 310094/2015-1).

REFERENCES

- Brito-Santana, H., Medeiros, R., Rodriguez-Ramos, R., Tita, V., 2016, "Different interface models for calculating the effective properties in piezoelectric composite materials with imperfect fiber–matrix adhesion", *Composite Structures*, Vol. 151, pp. 70-80.
- González, C. and Llorca, J., 2007, "Mechanical behavior of unidirectional fiber-reinforced polymers under transverse compression: microscopic mechanisms and modeling", *Composites Science and Technology*, Vol. 67, pp. 2795–2806.
- Shari H.Z. and Chou T.W., 1995 "Transverse elastic moduli of unidirectional fiber composite with fiber/matrix interfacial debonding", *Composites Science and Technology*, Vol. 53, pp. 383–391.
- Tita, V., 2003, "Contribuição ao estudo de danos e falhas progressivas em estruturas de material compósito polimérico", Tese (Doutorado) – Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos
- Tita, V., de Medeiros, R., Marques, F.D., Moreno, E.M., 2015, "Effective properties evaluation for smart composite materials with imperfect fiber–matrix adhesion", *Journal of Composites Materials*, Vol. 49(29), pp. 3683-3701.
- Totry, E., Molina-Aldareguía, J.M., González, C., et al., 2010, "Effect of fiber, matrix and interface properties on the in-plane shear deformation of carbon-fiber reinforced composites", *Composites Science and Technology*, Vol. 70, pp. 970–980.

- Vajari, D.A., Legarth, B.N., Niordson, C.F., 2013, “Micromechanical modeling of unidirectional composites with uneven interfacial strengths”, *European Journal of Mechanics A/Solids*, Vol. 42, pp. 241-250.
- Vaughan, T.J. and McCarthy, C.T., 2011, “A micromechanical study on the effect of intra-ply properties on transverse shear fracture in fibre reinforced composites”, *Composites Part A*, Vol. 42, pp. 1217–1228.
- Wang, W., Dai, Y., Zhang, C., Gao, X., Zhao, M., 2016, “Micromechanical modeling of fiber-reinforced composites with statistically equivalent random fiber distribution”, *Materials*, Vol. 9, pp.624.
- Yang, L., Wu, Z., Cao, Y., Yan, Y., 2015, “Micromechanical modelling and simulation of unidirectional fibre-reinforced composite under shear loading”, *Journal of Reinforced Plastics and Composites*, Vol. 34(1), pp. 72-83.
- Yang, L., Yan, Y., Liu, Y.J., et al, 2012, “Microscopic failure mechanisms of fibre-reinforced polymer composites under transverse tension and compression”, *Composites Science Technology*, Vol. 72, pp. 1818–1825.

RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.