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Computational Micromechanics of Composites: Debonding Failure and Matrix Cracking Under Transverse Type Load

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Abstract

Composites are widely utilized across various industries due to their exceptional properties, allowing design flexibility and complexity. There are different scales of composites numerical study, and this study aims to understand the damage mechanisms observed in microscale composites undergoing transverse compressive load. This understanding is achieved through prediction via simulation and micromechanical computational analyses. Based on previously conducted experimental studies, Zumaquero et. al. studied different stages of damage progression through microscopical inspection of the tested coupons[1]. The compressive failure behaviour of composites in the transverse direction was observed, revealing the preferential debonding angle is between 70 to 80°. Subsequently, the growth of the interface debonding failure becomes stable, and the kinking angle towards the matrix was found to be between 50 to 60°, consistent with the numerical predictions by Correa et al. using the Boundary Element Method (BEM) [2]. These findings motivate the current study, where a UD RVE model with a periodic boundary condition (PBC) is developed using the random sequential algorithm (RSA) and the angles of debonding and kinking failure are observed. To predict the onset of matrix cracking and the crack propagation, the extended FEM modelling approach [3] is used and the LaRC05 failure criterion is implemented through a compiled UMAT. The Drucker-Prager model served as the constitutive law for matrix yielding behaviour, while cohesive elements were assigned to predict the debonding failure of the fibre-matrix interface. In addition, the Phase-Field Fracture (PF) method is also used to predict matrix cracking behaviour and the results from both LaRC05 and PF are compared to investigate the efficiencies of both methods. The study concludes that the initial direction of failure predicted agrees with that microscopically observed in experiments. This research aims to contribute to the development of computational tools leading eventually to more resilient and precisely engineered composites for diverse applications.

Keywords: *Micromechanical modelling; Debonding; Matrix cracking; LaRC05; Drucker-Prager model; cohesive elements, Phase-field.*

1 Introduction

The computational modelling of failure in composite materials is a challenging task as it involves various complex failure mechanisms, regardless of the model scale. In this paper, the study aims to investigate the formation of debonding at the interface and the initiation and propagation of matrix cracks in microscale composites under transverse type load. The investigation implements two different failure criteria to compare the differences in the failure behaviour in the composites. The cohesive zone model (CZM) is used to capture the interface debonding phenomena in an RVE model. As the debonding failure tends to grow along the interface and propagate towards the matrix region, the LaRC05 and Phase-field (PF) model is then used to investigate the crack behaviour in the matrix. This viewpoint of computational micromechanics allows prediction of material performance, optimization of material properties, insights into complex failure mechanisms as well as provide validation to experimental findings.

2 Interface debonding and matrix cracking phenomena

Fibre-matrix interface debonding

The debonding failure of the interface is implemented using the CZM method. CZM is a modelling method widely used to predict the onset and propagation of fibre-matrix interface debonding failure. This approach is defined by a bi-linear traction separation law, as can be seen in Figure 1. In a bilinear traction separation law, K represents the initial elastic stiffness, N_{max} is the maximum traction or, in this case, represents the interface strength while δ_n^{fail} is the critical interface separation, and δ_n^{init} indicates the displacement or small debonding at damage initiation.

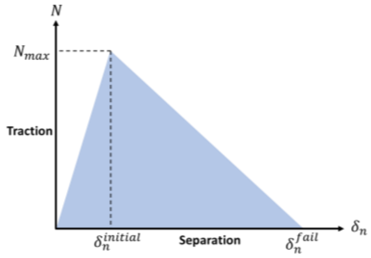


Figure 1. A bi-linear cohesive law to describe the behaviour of CZM in the interface.

Predicting Matrix Crack Initiation and Propagation

LaRC05 failure criterion

LaRC05 is reliable and accurate in predicting the strength value of a matrix dominated failure with its ability to provide the plane of the fracture angle which is crucial in XFEM modelling method. This failure criterion enables the assumption that the matrix failure may appear on an arbitrary plane parallel to the fibre direction. The failure is controlled by the combination of both transverse and longitudinal shear (τ_{nT} , τ_{nL}), as well as normal tractions (σ_n) on the corresponding plane. Two failure modes are considered in which these modes rely on the value of normal traction and the failure index as per equation (1) below.

$$f_{mat} = \begin{cases} \left(\frac{\tau_{nT}(\theta)}{S_T - \mu_T \sigma_n(\theta)}\right)^2 + \left(\frac{\tau_{nL}(\theta)}{S_L - \mu_L \sigma_n(\theta)}\right)^2 + \left(\frac{\sigma_n(\theta)}{Y_T}\right)^2, & \sigma_n(\theta) \geq 0 \\ \left(\frac{\tau_{nT}(\theta)}{S_T - \mu_T \sigma_n(\theta)}\right)^2 + \left(\frac{\tau_{nT}(\theta)}{S_L - \mu_L \sigma_n(\theta)}\right)^2, & \sigma_n(\theta) < 0 \end{cases} \tag{1}$$

The failure index value indicates the failure state where; the matrix is predicted to be undamaged when $f_{mat} < 1$ and failed when $f_{mat} = 1$.

$$\mu_T = -\frac{1}{tan(2\emptyset_0)}, S_T = \frac{Y_C}{2tan(\emptyset_0)}, \mu_L = S_L \frac{\mu_T}{S_T} \tag{2}$$

Y_T, Y_C, S_L and S_T represent the failure strength of UD composites under transverse tensile, transverse compressive, longitudinal shear and transverse shear loads, respectively. LaRC05 criterion also enable the implementation of the friction effect into the model, represented by μ_L and μ_T for friction coefficients under longitudinal shear stress and transverse shear stress [4]. Lastly, $\emptyset$ is the through-the-thickness direction and the general value for composites is $53\pm 2°$ obtained via experimental study in [5]. The matrix crack initiation and the direction of the crack propagation are defined by this failure criterion, which was implemented through the UDMGINI user subroutine.

Phase-field fracture method

The Phase-field fracture (PF) allows the capture of complex fracture phenomena such as the merging of cracks, nucleation, and crack branching in composites. This method was first mentioned by Griffith in [6] based on the thermodynamical analysis, where, according to the first law of thermodynamics, growth of a crack can only occur if a process implies that the total energy of a system decreases or remains constant with an increase in the crack area. The thermodynamic balance was used in the PF formulations (i.e. AT1, AT2, and PF-CZM) where normalization parameter, C_w, degradation function, $g(\boldsymbol{\phi})$ and geometric functions, $\alpha(\boldsymbol{\phi})$ define the specific PF (Table 1). This formulation represents the total potential energy, Π, in a domain of an elastic body, Ω, and evolving internal discontinuities, Γ (see Figure 2).

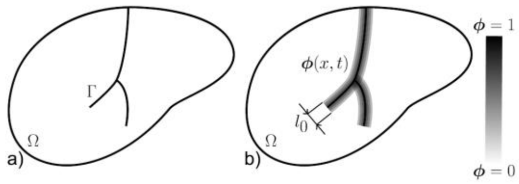


Figure 2. (a) Schematic representation of a body with an internal discrete continuity, (b) Schematic representation of a Phase-field approximation of a similar discontinuity pattern.

The AT1 model, uses a quadratic degradation function and a linear geometric function, while the AT2 model uses quadratic functions for both geometric and degradation functions. The Phase-Field Cohesive zone model (PF-CZM) uses a quadratic geometric function and a rational degradation function [7]. The use of PF to investigate the decohesion of the interface will be considered as part of the future scope. The length scale parameter is used to control the material strength in AT1 and AT2 formulations, while in the PF-CZM model, the strength is explicitly defined and is not affected by the length scale parameter.

Model	$\alpha(\boldsymbol{\phi})$	$g(\boldsymbol{\phi})$	Cw	l^0
AT1	$\boldsymbol{\phi}$	$(1-\boldsymbol{\phi})2$	$\frac{2}{3}$	$\frac{8\text{GcE}}{3\sigma_c^2}$
AT2	$\boldsymbol{\phi}2$	$(1-\boldsymbol{\phi})2$	$\frac{1}{2}$	$\frac{27\text{GcE}}{256\sigma_c^2}$
PF-CZM	$2\boldsymbol{\phi}-\boldsymbol{\phi}2$	$\left(\frac{(1-\phi)^p}{(1-\phi)^p+Q(\phi.)}\right)$	$\frac{\pi}{4}$	[-]

Table 1. Geometric and degradation functions for AT1, AT2 and PF-CZM models

3 Numerical example: 3D RVE under transverse compressive load with cohesive zone model, phase-field and LaRC05 criteria[1]

In this study, a periodic 3D RVE subjected to remote transverse load is developed. The fibre and matrix region were meshed using a 6-node linear triangular prism (C3D6) and 8-node linear brick (C3D8R) respectively. A periodic boundary condition is applied to the model to ensure the continuity of displacements across the RVE boundaries. The angle of initial debonding and the matrix cracking is observed.

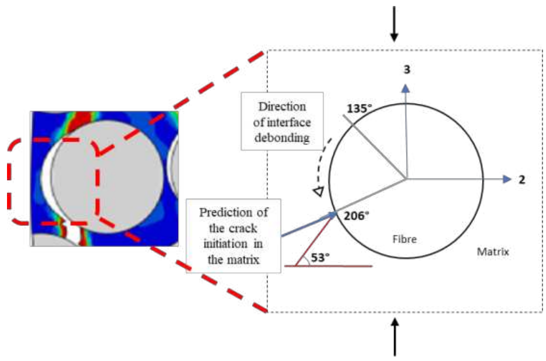
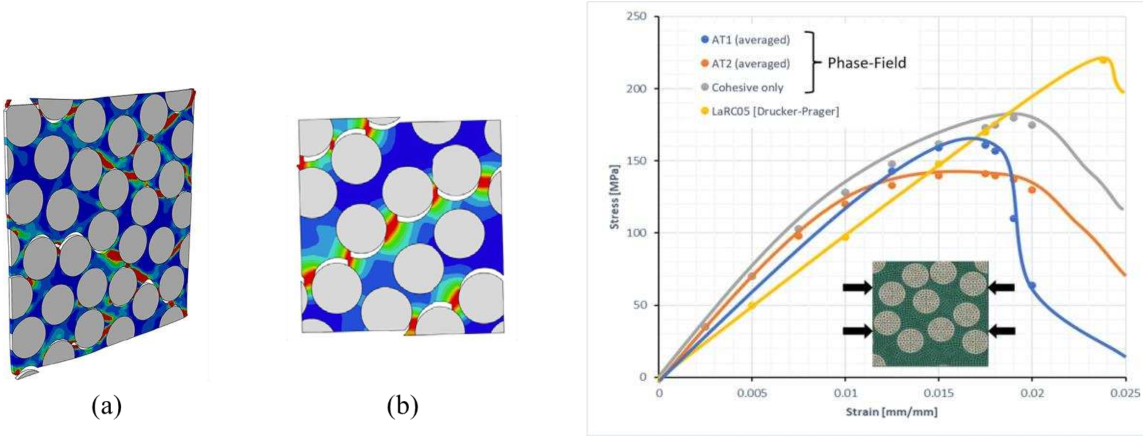


Figure 3. The debonding failure of the interface and predicted crack initiation angle in the matrix

A detailed investigation of the progress of failure and cracks within the micromechanical models reveals the different phases of failure processes. The initiation of the fibre-matrix interface debonding due to the high shear stress was first observed, at around 45° (or 130°- 140°) in the transverse direction to the fibre (see Figure 3). Due to the matrix undergoing shear plastic deformation and maximum stiffness degradation, the debonding of the interface grows until it reaches an angle of ~206° [1], [8]. It is expected that one will observe similarities between the LaRC05 and the phase-field model by examining the crack development under compression, Figure 4 (a) and (b). An example of a stress-strain graph comparison between LaRC05 and PF is shown in Figure 4 (c).



(a) (b) (c)

Figure 4. (a) RVE-LaRC05 [4] *and (b) RVE-PF*[7] *shows the similarities of the debonding failure and crack pattern in the matrix. (c) shows the example of stress-strain graph comparison between Phase-field (PF) methods and LaRC05 with Drucker-Prager criterion extracted from* [7], [9].

4 Conclusions

Computational micromechanics was employed to simulate the mechanical response of a fibre-reinforced composite subjected to transverse compression at the microscale level by implementing different failure criteria. In general, it was observed that microscale failure within the composites initiated at the interface due to the concentration of stress around the fibre and weak properties of both the matrix and the interface. The predicted debonding expanded to the cracking of the matrix. The observed debonding failure demonstrates good agreement with experimental results. The comparison between LaRC05 and the Phase-field fracture (PF) method is investigated. The accuracy of PF is found to be highly affected by the loading scenario. According to [7] Further investigation on both methods shows great potential and significance of both LaRC05 and PF methods could become highly profound in expanding areas of computational micromechanics of composites.

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