

This is a postprint version of the following published document:

Naya, F., González, C., Lopes, C., van der Veen, S. & Pons, F. (2017). Computational micromechanics of the transverse and shear behavior of unidirectional fiber reinforced polymers including environmental effects. *Composites Part A: Applied Science and Manufacturing*, 92, 146–157.

DOI: [10.1016/j.compositesa.2016.06.018](https://doi.org/10.1016/j.compositesa.2016.06.018)

© 2016 Elsevier Ltd. All rights reserved.



This work is licensed under a [Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License](https://creativecommons.org/licenses/by-nc-nd/4.0/).

# Computational micromechanics of the transverse and shear behaviour of unidirectional fiber reinforced polymers including environmental effects

F. Naya<sup>a</sup>, C. González<sup>a,b,\*</sup>, C.S. Lopes<sup>a</sup>, S. Van der Veen<sup>c</sup>, F. Pons<sup>c</sup>

<sup>a</sup>*IMDEA Materials Institute, C/Eric Kandel, 2, 28906 Getafe, Madrid, Spain*

<sup>b</sup>*Department of Materials Science, Polytechnic University of Madrid, ETS de Ingenieros de Caminos, 28040 Madrid, Spain*

<sup>c</sup>*AIRBUS Structures Research and Integration, ESIRNM. 18 rue Marius Terce, 31300 Toulouse, France*

---

## Abstract

Qualification of Fiber Reinforced Polymer materials (FRP's) for manufacturing of structural components in the aerospace industry is usually associated with extensive and costly experimental campaigns. The burden of testing is immense and materials should be characterized under different loading states (tension, compression, shear) and environmental conditions (temperature, humidity) to probe their structural integrity during service life. Recent developments in multiscale simulation, together with increased computational power and improvements in modeling tools, can be used to alleviate this scenario. In this work, high-fidelity simulations of the material behaviour at the micro level are used to predict ply properties and ascertain the effect of ply constituents and microstructure on the homogenized ply behaviour. This approach relies on the numerical analysis of representative volume elements equipped with physical models of the ply constituents. Its main feature is the ability to provide fast predictions of ply stiffness and strength properties for different environmental conditions of temperature and humidity, in agreement with the experimental results, showing the potential to reduce the time and costs required for material screening and characterization.

*Keywords:* A. Polymer-matrix composites (PMCs), C. Multiscale modelling, C. Finite element analysis (FEA), C. Computational micromechanics

---

## 1. Introduction

Fiber Reinforced Polymers (FRPs) are nowadays extensively used in applications where good mechanical properties are required in combination with weight savings. However, despite all existing information and current knowledge about these materials, the accurate prediction of the failure

---

\*Corresponding author

*Email address:* carlosdaniel.gonzalez@imdea.org (C. González)

5 stress of composite materials and structures has been an elusive task due to the complexity of the  
6 failure mechanisms involved.

7 Various phenomenological and physically-based models have been proposed, whose input pa-  
8 rameters have to be obtained through costly and time-consuming experimental campaigns for each  
9 material system. [1, 2]. Results obtained for a given unidirectional FRP system can not be directly  
10 extrapolated directly to other configurations with different fibre volume fraction or constituent  
11 properties, leading to a massive investment for their physical characterization. This is the case of  
12 material qualification for the aeronautical industry, where the whole process can last well over two  
13 years due to the required tests under different ageing and environmental conditions.

14 Computational micromechanics (based on Finite Elements Analysis) offers a novel approach to  
15 understand the deformation and fracture mechanisms in materials engineering. In the case of uni-  
16 directional fibre-reinforced composites, it has demonstrated high accuracy in the prediction of the  
17 mechanical behaviour, including fracture mechanisms under complex multiaxial loading cases [3–5].  
18 Numerical simulations of Representative Volume Elements (RVE’s) of the composite microstructure  
19 are useful to predict homogenized lamina properties, in close agreement with experimental data [6],  
20 and to provide the necessary input data for mesomechanical analysis at the laminate level. This  
21 bottom-up multi-scale simulation approach might lead in the future to a drastic reduction of the  
22 current costs associated with properties screening and material characterization programs [7]. In ad-  
23 dition, computational simulation of micromechanical RVE’s can be used to reproduce experimental  
24 stress conditions rather difficult to impose experimentally in laboratory, such as biaxial or triaxial  
25 stress states. Moreover, the influence of the microstructure and the constituents properties in the  
26 failure mechanisms can be addressed by means of parametric studies. All these efforts can lead  
27 in the future to the development micromechanical-based failure criteria with physical soundness, a  
28 clear advance in the state-of-the-art, e.g. Puck [8], LaRC [9] and Catalanotti [10] models.

29 Following previous research works [11, 12], herein detailed information of the microstructure  
30 (fiber diameter distribution, volume fraction, fiber clusters and resin pockets) is captured and  
31 included in a computational model of a unidirectional lamina (UD). Several strategies to determine  
32 micromechanical parameters by fitting against experimental results at the ply level, rather than  
33 measuring them with independent tests at the micro level, were developed in the past [13, 14]. In  
34 this work, the behavior of the constituents is obtained from micromechanical experiments on the  
35 material constituents performed under different environmental conditions. The measured properties  
36 are inputs of the constitutive equations of matrix and fiber/matrix interfaces. The RVE is submitted

37 to homogeneous stress states to determine the material failure envelope in the  $\sigma_{22} - \tau_{12}$  plane  
38 under different environmental conditions, including the pure mode ply strengths, namely transverse  
39 tension strength ( $Y_T$ ), transverse compression strength ( $Y_C$ ), and longitudinal shear strength ( $S_L$ ).  
40 The model shows the importance of capturing adequately the competition between the different  
41 failure mechanisms, fiber/matrix debonding and matrix failure, operating at the same time when  
42 the material is subjected to mechanical and environmental loads.

43 This introduction is followed by the description of the computational micromechanics framework,  
44 i.e. of the constitutive equations used to simulate matrix, fiber and interfaces, as well of the  
45 RVE generation procedure and the subsequent construction of the FE models with the specific  
46 loading conditions. The procedures used to characterize the basic ply constituents and model  
47 input parameters are explained then. The results of the uniaxial and biaxial loading simulations  
48 performed on the Hexcel carbon/epoxy AS4/8552 material (fibre volume fraction: 60% ; cured ply  
49 thickness: 0.184mm) are presented and compared with experimental results. The main advantage of  
50 selecting this well-known pre-impregnated material system system is that most of its ply properties  
51 are directly provided by prepreg manufacturer or found in the literature since it has been widely  
52 used in the aeronautical industry and subject of research, e.g. [15, 16].

53 The experimental-computational approach presented in this work constitutes an good comple-  
54 ment to the experimental characterization campaigns of composite materials to reduce time and  
55 costs associated and providing fast screening capabilities to improve material downselection for a  
56 given engineering application.

## 57 **2. Computational micromechanics model**

### 58 *2.1. RVE model set-up and simulation*

59 Computational micromechanics is based on the analysis of a statistically representative volume  
60 element of the material (RVE) subjected to homogeneous stress states (tension, compression and  
61 shear) or temperature increments. The microstructure of the RVE of the unidirectional composite  
62 is idealized as a dispersion of parallel and circular fibers randomly dispersed in the polymer matrix.  
63 A total number of fibers around 50 is enough to capture adequately the essential features of the  
64 microstructure of the material [17] while maintaining reasonable computing efforts. Synthetic fiber  
65 distributions statistically equivalent to the real ones are generated for the analysis. To this end,  
66 several strategies are available in the literature [12, 18, 19] being the Random Sequential Adsorp-  
67 tion (RSA) algorithm [11], probably, the most popular due to the easiness to achieve large volume

68 fraction of fiber reinforcement. In this work, the RSA algorithm was compared with the Nearest  
69 Neighbor Algorithm (NNA) developed by Vaughan and McCarty [12] using the relevant microstruc-  
70 ture statistical information obtained from micrographs of the unidirectional ply cross section. As  
71 shown in Figure 1, the results revealed well-distributed fiber microstructures without significant  
72 fiber clustering or matrix rich regions. Hence, it can be concluded that both algorithms deliver  
73 similar microstructures.

74 Considering its reliability and computing speed, the RSA algorithm was preferred in this work.  
75 Two-dimensional periodic fiber distributions were generated with the RSA algorithm and extruded  
76 along the fiber direction to achieve the final RVE's of the unidirectional composite material. The pe-  
77 riodic RVE's were then discretized using isoparametric wedge and brick finite elements for fibers and  
78 matrix with full integration at Gauss points (C3D6 and C3D8, respectively, in Abaqus [20]). Typi-  
79 cally, each RVE contains approximately  $\approx 40000$  elements representing a discretization fine enough  
80 to capture the large stress gradients between neighboring fibers. Node positions on opposite faces  
81 of the RVE's are identical in order to apply periodic boundary conditions according to the method-  
82 ology developed by Segurado and LLorca [11]. Simulations were carried out with Abaqus/Standard  
83 within the framework of the finite deformations theory with the initial unstressed state as reference.

84 The RVE's were initially subjected to a homogeneous temperature drop of  $\Delta T = -160^\circ C$  from  
85 the curing ( $180^\circ C$ ) to room temperature ( $20^\circ C$ ), hence generating realistic residual stress states in  
86 the material before mechanical loading. In a second step, homogeneous stress states were introduced  
87 by applying the appropriate displacements to the master nodes linked with the periodic boundary  
88 conditions [17]. The displacement and reactions of these master nodes were used to determine the  
89 stress-strain curves under transverse, shear and combined loads, and to derive the corresponding  
90 material stiffness and strength properties.

91 [Figure 1 about here.]

## 92 2.2. Constitutive equations

93 Carbon fibers are modeled in this work as linear, elastic and transversally isotropic solids. The  
94 anisotropy is taken into account by defining five independent elastic constants ( $E_{f1}, E_{f2}, \nu_{f12}, G_{f12}, G_{f23}$ )  
95 and two different thermal expansion coefficients ( $\alpha_{f1}, \alpha_{f2}$ ).

96 The polymer matrix of the composite material is simulated as an isotropic linear and elastic  
97 solid with  $E_m$  and  $\nu_m$  as elastic modulus and Poisson ratio. In addition, the matrix is able to  
98 undergo plastic deformations with the possibility of damage by cracking under tensile loads. This

99 approach has been adopted by other researchers in the literature [14, 21–23] as it represents a  
100 realistic behavior of a polymer [24]. The damage-plasticity model, available in ABAQUS/Standard  
101 [20] and schematically illustrated in Figure 2, is a modification of the Drucker-Prager plasticity  
102 yield surface [25] by including a damage variable in order to capture the quasi-brittle behaviour of  
103 the polymer under dominant tensile loads. The constitutive equation is based on the yield function  
104 proposed by Lubliner et al. [26] including modifications proposed by Lee and Fenves [27] to account  
105 for strength evolution under tension and compressive loads. The yield function defined in terms of  
106 the  $I_1$  and  $J_2$  invariants of the stress tensor is

$$\Phi(I_1, J_2, \sigma_I, \beta, \alpha) = \frac{1}{1-\alpha} \left( \sqrt{3J_2} + \alpha I_1 + B \langle \sigma_I \rangle \right) - \sigma_{myc} = 0 \quad (1)$$

107 wherein  $I_1$  stands for the first invariant of the stress tensor,  $J_2$  is the second invariant of the  
108 deviatoric stress tensor,  $\alpha$  is the pressure-sensitivity parameter of the Drucker-Prager yield criterion,  
109  $\sigma_I$  is the maximum principal stress,  $\langle \cdot \rangle$  the Macaulay brackets (returning the argument if positive  
110 and zero otherwise) and  $B$  is a function of the tensile and compressive yield stresses,  $\sigma_{myt}$  and  $\sigma_{myc}$ ,  
111 defined as

$$B = \frac{\sigma_{myt}}{\sigma_{myc}} (1 - \alpha) - (1 + \alpha) \quad (2)$$

112 Under biaxial compression stress state, with  $\sigma_I = 0$ , equation 1 reduces to the initially proposed  
113 Drucker-Prager yield condition [25], wherein  $\alpha$  can be expressed in terms of the internal friction angle  
114 of the material ( $\beta$ ) according to  $\tan \beta = 3\alpha$ . The internal friction angle controls the hydrostatic  
115 pressure dependence of the plastic behaviour of the material. Simultaneously,  $\alpha$  can be related to  
116 the biaxial compression behavior according to

$$\alpha = \frac{\sigma_{b0} - \sigma_{c0}}{2\sigma_{b0} - \sigma_{c0}} \quad (3)$$

117 After the onset of damage in tension at  $\sigma_{tm}$ , the softening behavior is controlled by an exponential  
118 cohesive law, characterized by a single normalized scalar damage variable, to ensure the correct  
119 energy dissipation of the matrix  $G_m$ . More details about the constitutive model and the numerical  
120 implementation can be found in [20, 28].

121 [Figure 2 about here.]

122 Even though this damaged-plasticity model requires a complex calibration from detailed exper-  
123 iments, good results can be obtained by the assumption of default parameters while measuring the

124 key properties. An experimental micromechanics approach, to be fully detailed in the following  
 125 section, was developed in by [29] to determine the Young modulus  $E_m$ , the compression yield limit  
 126  $\sigma_{myc}$  and the internal friction angle  $\beta$  of amorphous polymers by means of indentation.

127 Fiber-matrix debonding is modelled by means of a surface-based cohesive interaction, ABAQUS/Standard  
 128 [20]. The cohesive constitutive equation relates the displacement jump across the interface to the  
 129 traction vector acting on it for cracking under the full range of mode-mixities as in [30]. The initial  
 130 response of the cohesive interaction is assumed to be linear elastic governed by a contact penalty  
 131 stiffness  $K$ . Such numerical parameter should be large enough to ensure displacement continuity  
 132 in the absence of interface damage while avoiding convergence difficulties due to ill-conditioned  
 133 stiffness matrix. Damage onset is controlled by a quadratic interaction criterion depending on the  
 134 fibre/matrix interface strength (normal -  $\sigma_n$ , shear transversal -  $\tau_T$ , and shear longitudinal -  $\tau_L$ ), as

$$\left(\frac{\langle\sigma_n\rangle}{\sigma_n^0}\right)^2 + \left(\frac{\tau_T}{\tau_T^0}\right)^2 + \left(\frac{\tau_L}{\tau_L^0}\right)^2 = 1 \quad (4)$$

135 wherein only positive normal tractions affect the criterion. Once fiber/matrix debonding is initiated,  
 136 the cohesive tractions transferred through the interface decrease linearly to zero by means of a  
 137 single normalized scalar damage variable. The energy-based Benzeggagh-Kenane (BK) damage  
 138 propagation criterion [31] is used to account for the fracture energy dependence on the mode mixity  
 139 as

$$G_c = G_{Ic} + (G_{IIc} - G_{Ic}) \left(\frac{G_{shear}}{G_I + G_{shear}}\right)^m \quad (5)$$

140 Cohesive interactions were used in the model to include the effect of friction occurring after  
 141 fiber/matrix debonding. The shear stresses caused by friction at the interface are ramped pro-  
 142 gressively and proportional to the degradation of the interface, and thus, once the fiber/matrix  
 143 interface is fully debonded, the surface interaction is uniquely governed by a pure Coulomb model.  
 144 This friction stresses causes an increment of the interface shear resistance proportional to the nor-  
 145 mal compressive loads applied on it, being  $\mu$  the constant of proportionality or friction coefficient.  
 146 It should be mentioned that this affects not only the post-debonding behavior of the interface but  
 147 also the cohesive response as the friction stresses are ramped with the interface damage variable, as  
 148 schematically illustrated in Figure 2.

149 When using the traditional cohesive elements, instead of the surface-based cohesive approach,  
 150 friction can only be included when the cohesive element is totally damaged and removed from the  
 151 finite element mesh. The combined effect of friction with cohesive behavior has been addressed by

152 other authors, e.g. [32, 33]. These works eventually led to the development of a cohesive element  
153 formulation that take both mechanisms into account; a capability similar to the one used in this  
154 work with cohesive surface interactions.

### 155 **3. *In-situ* characterization of microconstituents**

156 In order to capture the influence of environmental conditions and manufacturing processes on the  
157 ply properties, the constitutive equations include a set of properties measured by means of *in-situ*  
158 micromechanical tests that are carried out on the composite coupon. The experimental procedures  
159 and results are briefly summarized in this section for the sake of clarity. Additional details can be  
160 found in Rodríguez et al. [29, 34].

161 Carbon fibres are assumed to behave elastically and properties were not dependent on the  
162 environmental conditions considered in this work. The longitudinal elastic properties of AS4 fibers  
163 at RT/DRY conditions are directly provided by the supplier. The transverse elastic properties and  
164 the thermal expansion coefficients were found in the literature [1] or estimated by means of Chamis  
165 rule of mixtures [35]. The properties required in the simulations are gathered in Table 1.

166 [Table 1 about here.]

167 Matrix and fiber/matrix interface characterization was carried out using small coupons extracted  
168 from an unidirectional AS4/8552 composite laminate. Samples were first cut using a diamond  
169 wire and the cross section perpendicular to the fibers polished using diamond slurry down to  $1\mu\text{m}$   
170 grain size. A typical cross section after polishing is shown in Figure 3. A first set of samples  
171 were totally dried in a stove for testing at room temperature conditions (RT/Dry). A second set  
172 of samples (HOT/WET) were submitted to aging in environmental chamber at  $70^\circ\text{C}$  and 85% of  
173 relative humidity. The aging procedure followed the recommendation of DIN EN2823 standard [36]  
174 although with small size specimens ( $\approx 1\times 1\times 1\text{ mm}^3$ ) rather than the standard travelers. The coupon  
175 weight uptake was regularly measured until saturation ( $\approx 3\%$  of the dry weight) was attained which  
176 occurred typically after three weeks of humid exposure. It is worth to remark at this point that the  
177 use of small size specimens speed up the water uptake process as compared with the typical coupon  
178 size used in the usual practice.

179 [Figure 3 about here.]



180 *3.1. Matrix characterization*

181 Nanoindentation experiments were conducted using a Hysitron TI 950 TriboIndenter equipped  
182 with a Berkovich tip (pyramidal indenter). A set of approximately 30 indentations were performed  
183 for each environmental condition at an equivalent strain rate of  $\dot{\epsilon} = 0.07s^{-1}$ . The material hardness  
184 is computed from the force recorded during the test and the physical imprint introduced in the  
185 material. However, determining the real contact area of the material with the indenter is an ex-  
186 tremely difficult task as sink-in or pile-up phenomena can mask the results. A first estimation of the  
187 real contact area of the indenter is given by Oliver and Pharr [37] from the ratio between the total  
188 elastic and plastic work ( $W_e$  and  $W_p$ , respectively) measured from the load-displacement curves  
189 (see Figure 4). However, there is no analytical method to determine hardness from indentations in  
190 hydrostatic dependent materials and complex numerical models based on the finite element method  
191 should be applied. In this work, the methodology proposed by Rodríguez et al. [29], assuming  
192  $\beta = 29^\circ$  irrespective of the environmental conditions, is used to obtain the elastic modulus and the  
193 compressive yields stress of the matrix ( $E_m$  and  $\sigma_{myc}$ , respectively).

194 [Figure 4 about here.]

195 The value of the Young modulus of the matrix obtained from nanoindentation in the RT/DRY  
196 condition is reported in Table 2 and is in reasonable good agreement with the experimental value  
197 provided by the supplier ( $E_m = 4.67$  GPa) obtained from macroscopic coupons. The slight differ-  
198 ences obtained can be attributed to the constraint effects induced when testing close to fibers. A  
199 way to alleviate such effect is by identifying and indenting on wider rich resin pockets or by reducing  
200 as much as possible the load applied by the indenter obtaining, therefore, a soft imprint as shown  
201 in Figure 3.

202 Testing under HOT/WET conditions was carried out with a special heating device coupled  
203 to the nanoindenter and placed around the Berkovich tip. Specimens were extracted from the  
204 environmental chamber ( $70^\circ C$  and 85% of relative humidity) and placed immediately in the Hysitron  
205 nanoindentator apparatus. The system was equipped with a heating device and the temperature  
206 was controlled and monitored with a thermocouple. The temperature was maintained at  $70^\circ C$   
207 during some minutes. Then, indentations were performed for a limited period of time to avoid  
208 drying of the material surface. The properties of the 8552 epoxy resin measured in RT/DRY and  
209 HOT/WET conditions are reported in Table 2.

210 [Table 2 about here.]

211 The thermal expansion coefficients (CTE) for RT/DRY were obtained from the literature [38].  
212 The mode I fracture toughness of the 8552 resin  $G_m$  was not measured in this work. Typical values  
213 found in the literature for epoxy resins  $G_m$  are in the range of  $40 J/m^2$  and  $400 J/m^2$  depending on  
214 crack propagation speed, as reported in [39]. Taking into account this lack of experimental results,  
215 a value of fracture energy for the 8552 epoxy matrix  $G_m$  in the order of  $\approx 100 J/m^2$  seems to be  
216 reasonable in this case [5, 6]. In any case, the simulations demonstrated that the effect of matrix  
217 toughness on the transverse and shear strengths of the unidirectional material was limited.

### 218 3.2. Fiber/matrix interface characterization

219 The interface strength was determined using the fibre push-in technique described in [34]. In  
220 this test a single fibre is pushed-in by means of a cylindrical flat-tipped nanoindenter until interface  
221 debonding occurs. The load-displacement curves of the push-in tests on individual fibers are linear  
222 and elastic up to a point where the response deviates from the linearity. This behaviour is attributed  
223 to the progressive and stable propagation of a debonding through the fiber/matrix interface. The  
224 mechanics of the push-in test were analyzed in detail in [34] by means of detailed FE simulations  
225 that allowed the determination of the influence of the different mechanical parameters (interface  
226 shear strength, toughness and friction; elastic constants; residual thermal stresses) on the onset of  
227 debonding. It should be mentioned that push-in tests only provide the values of the shear strength of  
228 the interface along the fiber direction  $\tau_L^0$ . The normal strength is assumed equal to  $\sigma_n^0 = 2/3\tau_L^0$  based  
229 on the experimental results obtained by Ogihara and Koyanagi [40] on cruciform E-glass/epoxy  
230 specimens subjected to biaxial loading. In addition, in the absence of reliable experimental results,  
231 the interface transverse shear strength is assumed equal to the longitudinal one ( $\tau_T^0 = \tau_L^0$ ).

232 All push-in tests were carried out using a Hysitron TI 950 TriboIndenter equipped with a  $5\mu m$   
233 diameter flat punch tip. The indentations were centered as much as possible on the  $7\mu m$  AS4  
234 carbon fibers. In order to achieve good reproducibility, fibre push-in tests were performed on the  
235 central fibres of highly-packed fibre clusters with hexagonal symmetry, a feature easily found in  
236 unidirectional AS4/8552 plies, as shown in Figure 3.

237 A total of fifteen push-in tests were carried out at RT/DRY and RT/WET conditions. The  
238 RT/WET condition was used instead the standard HOT/WET previously used for matrix char-  
239 acterization due to experimental difficulties associated with the thermal stability of the indenter  
240 at  $70^\circ C$ . The average values, as well as the standard deviation, are gathered in Table 2. It can  
241 be observed that the interface strength decreases in the RT/WET condition and this value can be

242 considered an upper value of the strength of the interface at  $70^{\circ}C$  and 85% of relative humidity.  
243 The additional effect of temperature on the interface strength can be estimated using the knock-  
244 down factor on matrix compressive strength due to HOT/WET conditions which can be thought  
245 to be entirely due to the temperature increase with respect to RT/DRY conditions. Under this  
246 assumption, the HOT/WET matrix compression strength would be further reduced  $\approx 17\%$  with  
247 respect to a RT/WET environment.

248 The interface fracture energy in mode I,  $G_{Ic}$ , could not be measured experimentally but it is  
249 assumed to be in the range of  $2 - 5J/m^2$ . Similar values were used by other authors and reported  
250 in the literature [5, 12]. In addition, due to the lack of experimental data, the interface fracture  
251 energies in the shear modes were set equal to the matrix cracking fracture energy,  $G_{IIc} = G_{IIIc} =$   
252  $G_m = 100J/m^2$ , a value similar to the one used in [34]. The fracture energy was assumed to be  
253 insensitive to the environmental conditions for the sake of simplicity.

## 254 4. Micromechanical simulation and model validation

### 255 4.1. Pure transverse and shear loading

256 Under pure transverse tension loading, the fracture process is controlled by the fiber/matrix  
257 interface debonding, for both RT/DRY and HOT/WET conditions. Cracks start at the fiber poles  
258 along the loading direction in those regions where the stress concentrations in the fiber/matrix  
259 interface are higher, for instance in a fiber cluster. After failure of the interface, the matrix undergoes  
260 severe plastic deformation, accumulating damage until ultimate failure of the matrix ligaments. The  
261 final failure of the RVE is produced by the development of a crack perpendicular to the loading axis,  
262 as shown in Figure 5. The behaviour is essentially linear an elastic up to failure being the transverse  
263 tension strength of the composite strongly controlled by the fiber/matrix interface strength.

264 [Figure 5 about here.]

265 Under pure transverse compression, the final failure of the composite ply takes place by the  
266 development of matrix shear bands. However, the fiber/matrix interface plays an important role  
267 in the failure initiation process. According to the in-situ nanoindentation tests, the nominal shear  
268 strength of the AS4/8552 fiber/matrix interface is lower than the shear strength of the 8552 resin  
269 matrix, specially under HOT/WET conditions (see Table 2). If these were the only two mechanisms  
270 at play, the simulations show that failure under pure transverse compression would initiate by  
271 interface decohesion at the fibre poles and then propagate in the form of a plastic shear band

272 oriented at  $\theta_{fr} \approx 47^\circ$ . The introduction of frictional effects in the interaction between fiber and  
273 matrix changes this equilibrium between fiber/matrix debonding and matrix shear banding. Friction  
274 leads to the increment of the interface shearing resistance due to the normal compressive stresses at  
275 the interface generated by the thermal and transverse compressive loadings. For significant values  
276 of  $\mu$ , failure under pure transverse compression appears not to be initiated by interface decohesion  
277 but directly by shear banding with orientation  $\theta_{fr} \approx 56^\circ$ . This failure mechanism transition effect  
278 is represented in Figure 6. Values of shear band orientation similar to the later case were reported  
279 in previous research works [41] and are supported by experimental data [42] for similar materials.  
280 Therefore, it can be concluded that friction plays an important role in the failure process. From  
281 a simple parametric study, the threshold value of the friction coefficient that modifies the failure  
282 mechanism from a single plastic shear band at  $\theta_{fr} \approx 47^\circ$  to multiple distributed plastic shear bands  
283 at  $\theta_{fr} \approx 56^\circ$  is in the range  $0.2 < \mu < 0.4$ .

284 [Figure 6 about here.]

285 For a relatively high frictional effects, the composite can sustain a relatively high level of strain  
286 under transverse compression, typically around 4-5%, justified by the high compressive resistance  
287 of the matrix. For low values of  $\mu$ , the premature failure of the fibre/matrix interface leads to the  
288 concentration of plastic strain in a single band inducing the catastrophic failure of the material (see  
289 Figure 6). This might be the case in HOT/WET conditions, as the water absorbed by the polymer  
290 tends to form micro channels around the fibers reducing the friction coefficient [43, 44]. In the  
291 absence of more reliable data, the friction coefficient in HOT/WET conditions was set to  $\mu = 0.01$   
292 leading to failure initiating at the fibre/matrix interface followed by shear banding at  $\theta_{fr} \approx 47^\circ$ , as  
293 shown in Figure 7.

294 [Figure 7 about here.]

295 When pure shear loading is applied to the RVE, different behaviors are found depending on the  
296 shearing direction, parallel or perpendicular to the fibers. If shear is applied parallel to the fibers  
297 ( $\tau_{||}$ ), the failure mechanism is dominated by interfacial decohesion or by matrix yielding, depending  
298 on the interface strength [45]. In the particular case of the AS4/8552 material studied in this work,  
299 the interface strength is slightly lower than the matrix shear limit. Thus, fracture is triggered by  
300 interface debonding rather than by matrix plasticity, similarly to the pure transverse tension case.  
301 As the interface debonds, the matrix holds progressively shear loads and plastic band deformations

302 are formed. On the other hand, if shear is applied in the plane perpendicular to the fibers ( $\tau_{\perp}$ ),  
303 the deformation pattern after matrix yielding is different. Once interface debonding initiates, fiber  
304 rotation starts resulting in a gradually stiffer response of the composite material. The in-plane  
305 shear response of the composite lamina ( $\tau_{12}$ ) was approximated in this work by averaging the values  
306 obtained along the fibers  $\tau_{\parallel}$  and perpendicular to the fibers  $\tau_{\perp}$ , as suggested by Totry et al. [45].

307 The values of the elastic constants (transverse elastic modulus and in-plane shear modulus) as  
308 well as the predictions of the transverse tensile strength, transverse compressive strength and in-  
309 plane shear strength for a AS4/8552 lamina are gathered in Table 3. The reported numerical results  
310 are the average of five different random realizations and are in good agreement with experimentally-  
311 obtained average ply properties reported in the literature [15], specially for RT/DRY conditions.

312 [Table 3 about here.]

#### 313 4.2. Failure envelopes

314 One of the potential applications of computational micromechanics is the prediction of ply failure  
315 envelopes, i.e. the failure loci for the whole range of combined stress states. In this work the focus is  
316 put on the prediction of the intersection of the failure envelope with the  $\sigma_{22} - \tau_{12}$  stress plane. This  
317 is carried by applying different combinations of transverse and in-plane shear loads, as represented  
318 in Figure 8 for RT/DRY and HOT/WET conditions. The numerical results are compared to the  
319 predictions of physically-based Puck ply failure criteria [8] using as model inputs the AS4/8552  
320 material properties available in literature [15] and summarized in Table 3.

321 [Figure 8 about here.]

322 The effect of friction between fibres and matrix is clearly visible on the shape of the failure  
323 envelopes mainly on the transverse compression quadrant. The results reported in this work suggest  
324 that fiber/matrix friction controls the transition between interface-dominated failure in pure shear  
325 loading to matrix-dominated failure for pure compression loading. Shear hardening under moderate  
326 transverse compression has been observed experimentally (e.g. [42]) and is predicted by Puck's  
327 criteria [8]. If fibre/matrix friction is omitted, or the friction coefficient is low, no change in the  
328 failure mechanism is obtained and no shear hardening is predicted by computational micromechanics  
329 as reported in other works [5, 46]. Other authors assumed an arbitrarily large fiber/matrix interface  
330 strength in order to capture this effect [3] leading to unrealistic predictions of the in-plane and  
331 transverse tension strengths. The results of a parametric analysis of the effect of the friction

332 coefficient on the shape of the failure envelope for the RT/DRY conditions are shown in Figure 9a.  
 333 There is a threshold value of the friction coefficient in the range  $0.2 < \mu < 0.4$  that triggers the  
 334 transition of the fracture mechanism. Increasing  $\mu$  above this value leads to no significant change  
 335 in the material response except for the increase in the slope of the shear hardening curve.

336 [Figure 9 about here.]

337 The transition between interface-dominated shear failure to matrix-dominated occurs when the  
 338 interface shear strength, including the friction effects, overcomes the matrix shear strength. As  
 339 failure of the matrix under compression loading starts to dominate the ply failure process, the  
 340 fracture angle also starts to change from  $\theta_{fr} = 0^\circ$  to approach a typical shear fracture. Figure 10  
 341 shows how that transition is produced in the  $\sigma_{22} - \tau_{12}$  frame with increasing ratios of transverse  
 342 compression over shear loads.

343 [Figure 10 about here.]

344 This whole range of processes of ply fracture under transverse compression ( $\sigma_{22} < 0$ ) can be  
 345 described by a single criterion from the set of Puck failure criteria for plane stress cases [8]:

$$\left( \frac{\tau_T}{S^T - \eta^T \sigma_n} \right)^2 + \left( \frac{\tau_L}{S^L - \eta^L \sigma_n} \right)^2 = 1 \quad (6)$$

346 wherein the tractions on a possible fracture plane with angle  $\theta$  are obtained from the components  
 347 of the stress tensor defined in the material coordinate system (see Figure 11) as:

$$\begin{aligned} \sigma_n &= \sigma_{22} \cos^2 \theta \\ \tau_T &= -\sigma_{22} \sin \theta \cos \theta \\ \tau_L &= \tau_{12} \cos \theta \end{aligned} \quad (7)$$

348  $S^L$  and  $S^T$  are, respectively, the material shear strengths in fibre and transverse-to-fibre directions  
 349 while  $\eta^L$  and  $\eta^T$  are the corresponding internal friction coefficients acting on the fracture plane. The  
 350 prediction of the correct  $\theta_{fr}$  for each biaxial load ratio requires the criterion to be maximised for the  
 351 whole range of possible fracture angles. Following this procedure will dictate that the fracture angle  
 352 evolves from  $\theta_{fr} = 0^\circ$ , for transverse tension and moderate transverse compression, to  $\theta_{fr} \approx 53^\circ$   
 353 for pure transverse compression. A remarkably similar trend is suggested by the computational  
 354 micromechanical results presented above and by experimental observations [42], with sensible dif-  
 355 ferences being that the increase of  $\theta$  predicted by Equation 6 is continuous and progressive up to

356  $\theta_{fr} \approx 53^\circ$  while in micromechanics the increase is in discrete steps and up to  $\theta_{fr} \approx 56^\circ$ , a value that  
357 matches experimental observations [42] more accurately. These differences are likely to be related  
358 to the discreteness of the microstructure which is not taken into account in the ply failure model.

359 [Figure 11 about here.]

360 The effect of friction on ply failure for transverse compression is also taken into account in Puck's  
361 criterion wherein the shear strengths are affected, i.e. increased, by negative normal tractions acting  
362 on the fracture plane on  $\eta^L$  and  $\eta^T$  proportions (note that Equation 6 is only valid for  $\sigma_{22} < 0$ ).  
363 For  $\theta = 0^\circ$ ,  $\eta^L$  defines the slope of the shear hardening region in the failure envelope. A linear  
364 interpolation of the micromechanical simulations in this range, for a fibre-matrix friction coefficient  
365 of  $\mu = 0.4$ , results in  $\eta^L = 0.22$  (see Figure 9a), a value close to the one experimentally observed by  
366 Koerber et al. [42] ( $\eta^L = 0.26$ ) for a similar CFRP system (IM7/8552). Given these correlations,  
367 the parametrically-obtained friction coefficient  $\mu = 0.4$  is adopted at this point and used in the  
368 following predictions.

369 For a HOT/WET environment, ply fracture seems to be controlled by interface failure in the  
370 whole range of transverse biaxial loads. Hence, no shear hardening should be observed in moderate  
371 compression. As the drop of friction coefficient due to water uptake is not perfectly defined, two  
372 failure envelopes, corresponding to  $\mu = 0.01$  and  $\mu = 0.4$ , are represented in Figure 8 in order to  
373 establish lower and upper bounds for the failure envelope for HOT/WET conditions.

374 Given the importance of the hydrostatic pressure in the behavior of polymers and the uncertainty  
375 about the model parameters that control its effect, namely the internal friction angle, a parametric  
376 study on the variation of this parameter on the behaviour of the composite was carried out. The  
377 internal friction angle ( $\beta$ ) is related to the coefficient of the hydrostatic term of constitutive equa-  
378 tion of the epoxy matrix (Equation 1) and its variation implies a change in the material biaxial  
379 compressive response (Equation 3). The influence of the polymer matrix plastic behaviour in the  
380 global composite microstructure can be assessed by comparing three failure envelopes corresponding  
381 to values of  $\beta = 22^\circ$ ,  $29^\circ$  and  $36^\circ$  and a fixed value of the friction coefficient ( $\mu = 0.4$ ), as shown  
382 in Figure 9b. The curve for  $\beta = 29^\circ$  corresponds to the material properties gathered in Table 1  
383 and represents the baseline configuration. The other values considered herein represent a lower and  
384 upper bound for most of epoxy resins [29].

385 As observed in Figure 9b, the material pure transverse compressive strength ( $Y_C$ ) and the slope  
386 of the shear hardening curve ( $\eta^L$ ) increase for  $\beta = 22^\circ$ . However, this effect is not symmetric, i.e.

387  $Y_C$  and  $\eta^L$  do not significantly decrease for an equivalent increase of  $\beta$  to  $36^\circ$ . In addition, the ply  
388 fracture angle for pure transverse compression ( $\theta_{fr}$ ) is kept constant regardless the internal friction  
389 angle of the polymer, as shown in Figure 12. It appears that decreasing  $\beta$  from the baseline value of  
390  $29^\circ$  results in a pronounced increase of the matrix yield load with a direct effect on  $Y_C$ . Indirectly,  
391 a stronger matrix allows the increase of the normal stresses on the fiber/matrix interface and, as a  
392 consequence of friction, an increase on its shear resistance. In other words, decreasing the friction  
393 angle of the polymer increases its compressive strength [29] and hence of the friction shear load  
394 transferred between the fibers and the polymer. On the other hand, increasing  $\beta$  above  $29^\circ$  appears  
395 not to have a significant impact on matrix compressive yielding and neither on  $\eta^L$ , i.e. the effect of  
396 this parameter is nonlinear. Hence, in the absence of more objective information, a value of  $\beta \approx 29^\circ$   
397 seems to be appropriate to characterize the 8552 epoxy resin behaviour as it results in values of  $Y_C$ ,  
398  $\eta^L$  and  $\theta_{fr}$  coherent with experimental data.

399 The results and correlations made in this section lead to the hypotheses that  $\eta^L$  may be regarded  
400 as a ply-homogenized combination of the effects of fibre/matrix interface friction and matrix internal  
401 friction, while  $\eta^T$  would better correspond to matrix internal friction only. The confirmation of these  
402 hypotheses would require further investigation.

403 [Figure 12 about here.]

## 404 5. Conclusions

405 In this work, the transverse tensile strength, transverse compressive strength and in-plane shear  
406 strength of a unidirectional AS4/8552 lamina under both RT/DRY and HOT/WET environmental  
407 conditions have been determined using computational micromechanics. The main parameters of the  
408 constitutive equations of the microconstituents, including the fiber/matrix interface and polymer  
409 plastic behavior, were obtained experimentally by means of *in-situ* nano-indentation tests. Using  
410 only micromechanical properties, the model reproduces the ply stress-strain behavior and fracture  
411 mechanisms observed experimentally [17, 23, 45], both for uniaxial and biaxial stress states. Hence,  
412 this paper suggests that virtual ply characterization tests, based on reliable properties of the micro-  
413 constituents, can replace the physical experiments, at least for material screening purposes. These  
414 virtual tests provide full control of the composite microstructure and constituent properties, al-  
415 lowing microstructural optimization to be performed in the future [47]. Moreover, complex stress  
416 states, not possible to be applied experimentally, can be simulated. Finally, this work shows that



417 there is a need to improve existing ply failure criteria that rely only on ply properties [8, 9]. Without  
418 exception, these assume microstructures containing perfect fiber-matrix bonding and do not take  
419 into account important micromechanical parameters such as fibre/matrix interface strength and  
420 interface friction.

## 421 **Acknowledgments**

422 The authors would like to acknowledge the support provided by AIRBUS SAS through the  
423 project SIMSCREEN (Simulation for Screening Composite Materials Properties). Additionally,  
424 C.S. Lopes acknowledges the support of the Spanish Ministry of Economy and Competitiveness  
425 through the *Ramón y Cajal* program. The help of Dr. Miguel Monclús and Dr. Jon Molina in the  
426 experimental work is also gratefully acknowledged.

## 427 **References**

## 428 **References**

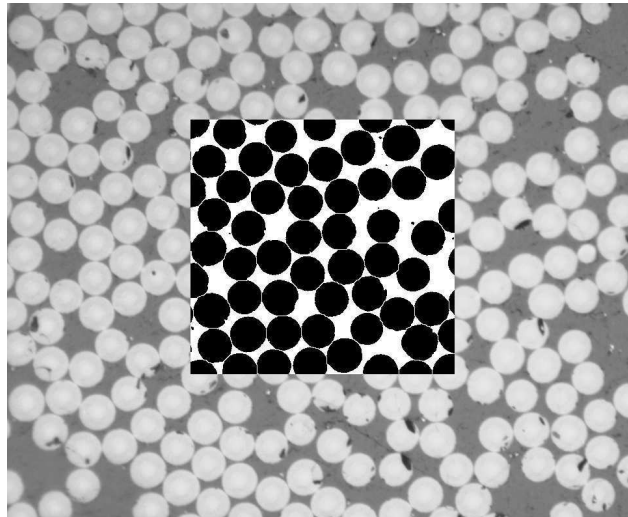
- 429 [1] M. Hinton, A. Kaddour, P. Soden, A further assessment of the predictive capabilities of current  
430 failure theories for composite laminates: comparison with experimental evidence, *Composites*  
431 *Science and Technology* 64 (2004) 549–588.
- 432 [2] I. M. Daniel, J.-J. Luo, P. M. Schubel, B. T. Werner, Interfiber/interlaminar failure of compos-  
433 ites under multi-axial states of stress, *Composites Science and Technology* 69 (2009) 764–771.
- 434 [3] E. Totry, C. González, J. LLorca, Failure locus of fiber-reinforced composites under transverse  
435 compression and out-of-plane shear, *Composites Science and Technology* 68 (2008) 829–839.
- 436 [4] M. Romanowicz, A numerical approach for predicting the failure locus of fiber reinforced  
437 composites under combined transverse compression and axial tension, *Computational Materials*  
438 *Science* 51 (2012) 7–12.
- 439 [5] A. Melro, P. Camanho, F. Andrade Pires, S. T. Pinho, Micromechanical analysis of polymer  
440 composites reinforced by unidirectional fibres: Part II ??? Micromechanical analyses, *Interna-*  
441 *tional Journal of Solids and Structures* 50 (2013) 1906–1915.
- 442 [6] L. P. Canal, C. González, J. Segurado, J. LLorca, Intraply fracture of fiber-reinforced compos-  
443 ites: Microscopic mechanisms and modeling, *Composites Science and Technology* 72 (2012)  
444 1223–1232.

- 445 [7] J. LLorca, C. González, J. M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket,  
446 M. Rodríguez, S. Sádaba, R. Muñoz, L. P. Canal, Multiscale modeling of composite mate-  
447 rials: a roadmap towards virtual testing., *Advanced materials* 23 (2011) 5130–47.
- 448 [8] A. Puck, H. Schürmann, Failure analysis of FRP laminates by means of physically based  
449 phenomenological models, *Composites Science and Technology* 62 (2002) 1633–1662.
- 450 [9] C. Davila, P. Camanho, C. A. Rose, Failure Criteria for FRP Laminates, *Journal of Composite*  
451 *Materials* 39 (2005) 323–345.
- 452 [10] G. Catalanotti, P. P. Camanho, A. Marques, Three-dimensional failure criteria for fiber-  
453 reinforced laminates, *Composite Structures* 95 (2013) 63–79.
- 454 [11] J. Segurado, J. LLorca, A numerical approximation to the elastic properties of sphere-reinforced  
455 composites, *Journal of the Mechanics and Physics of Solids* 50 (2002) 2107–2121.
- 456 [12] T. Vaughan, C. McCarthy, A combined experimental???numerical approach for generating  
457 statistically equivalent fibre distributions for high strength laminated composite materials,  
458 *Composites Science and Technology* 70 (2010) 291–297.
- 459 [13] S. T. Pinho, L. Iannucci, P. Robinson, Physically based failure models and criteria for lami-  
460 nated fibre-reinforced composites with emphasis on fibre kinking. Part II: FE implementation,  
461 *Composites Part A Applied Science and Manufacturing* 37 (2006) 766–777.
- 462 [14] A. Melro, P. Camanho, F. Andrade Pires, S. T. Pinho, Micromechanical analysis of polymer  
463 composites reinforced by unidirectional fibres: Part I ??? Constitutive modelling, *International*  
464 *Journal of Solids and Structures* 50 (2013) 1897–1905.
- 465 [15] K. Marlett, Y. Ng, J. Tomblin, E. Hooper, NCAMP Test Report: CAM-RP-2010-002 Rev A,  
466 Technical Report, National Institute for Aviation Research, 2011.
- 467 [16] C. Lopes, S. Sádaba, C. González, J. LLorca, P. Camanho, Physically-Sound Simulation of Low-  
468 Velocity Impact on Fibre Reinforced Laminates, *International Journal of Impact Engineering*  
469 (2015) 1–15.
- 470 [17] C. González, J. LLorca, Mechanical behavior of unidirectional fiber-reinforced polymers un-  
471 der transverse compression: Microscopic mechanisms and modeling, *Composites Science and*  
472 *Technology* 67 (2007) 2795–2806.

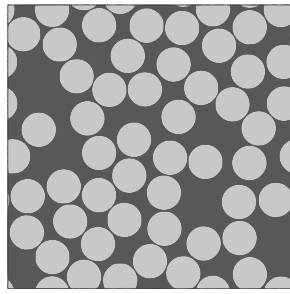
- 473 [18] D. Trias, J. Costa, a. Turon, J. E. Hurtado, Determination of the critical size of a statistical  
474 representative volume element (SRVE) for carbon reinforced polymers, *Acta Materialia* 54  
475 (2006) 3471–3484.
- 476 [19] A. R. Melro, P. P. Camanho, S. T. Pinho, Generation of random distribution of fibres in  
477 long-fibre reinforced composites, *Composites Science and Technology* 68 (2008) 2092–2102.
- 478 [20] Dassault Systèmes, Abaqus 6.13 Documentation, 2013.
- 479 [21] L. Yang, Y. Yan, Y. Liu, Z. Ran, Microscopic failure mechanisms of fiber-reinforced polymer  
480 composites under transverse tension and compression, *Composites Science and Technology* 72  
481 (2012) 1818–1825.
- 482 [22] D. Ashouri Vajari, C. González, J. Llorca, B. N. Legarth, A numerical study of the influence  
483 of microvoids in the transverse mechanical response of unidirectional composites, *Composites  
484 Science and Technology* 97 (2014) 46–54.
- 485 [23] L. P. Canal, J. Segurado, J. Llorca, Failure surface of epoxy-modified fiber-reinforced com-  
486 posites under transverse tension and out-of-plane shear, *International Journal of Solids and  
487 Structures* 46 (2009) 2265–2274.
- 488 [24] B. Fiedler, M. Hojo, S. Ochiai, K. Schulte, M. Ando, Failure behavior of an epoxy matrix under  
489 different kinds of static loading, *Composites Science and Technology* 61 (2001) 1615–1624.
- 490 [25] D. C. Drucker, W. Prager, Soil mechanics and plastic analysis for limit design, *Quarterly of  
491 Applied Mathematics* 10 (1952) 157–165.
- 492 [26] J. Lubliner, J. Oliver, S. Oller, E. Oñate, A plastic-damage model for concrete, *International  
493 Journal of Solids and Structures* 25 (1989) 299–326.
- 494 [27] J. Lee, G. L. Fenves, Plastic-Damage Model for Cyclic Loading of Concrete Structures, *Journal  
495 of Engineering Mechanics* 124 (1998) 892–900.
- 496 [28] L. P. Canal, C. González, J. M. Molina-Aldareguía, J. Segurado, J. Llorca, Application of  
497 digital image correlation at the microscale in fiber-reinforced composites, *Composites Part A:  
498 Applied Science and Manufacturing* 43 (2012) 1630–1638.

- 499 [29] M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca, Determination of the mechan-  
500 ical properties of amorphous materials through instrumented nanoindentation, *Acta Materialia*  
501 60 (2012) 3953–3964.
- 502 [30] A. Turon, P. Camanho, J. Costa, C. Dávila, A damage model for the simulation of delamination  
503 in advanced composites under variable-mode loading, *Mechanics of Materials* 38 (2006) 1072–  
504 1089.
- 505 [31] M. L. Benzeggagh, M. Kenane, Measurement of mixed-mode delamination fracture toughness  
506 of unidirectional glass/epoxy composites with mixed-mode bending apparatus, *Composites*  
507 *Science and Technology* 56 (1996) 439–449.
- 508 [32] G. Alfano, E. Sacco, Combining interface damage and friction in a cohesive-zone model,  
509 *International Journal for Numerical Methods in Engineering* 68 (2006) 542–582.
- 510 [33] I. Guiamatsia, G. D. Nguyen, A thermodynamics-based cohesive model for interface debonding  
511 and friction, *International Journal of Solids and Structures* 51 (2014) 647–659.
- 512 [34] M. Rodríguez, J. M. Molina-Aldareguía, C. González, J. LLorca, A methodology to measure the  
513 interface shear strength by means of the fiber push-in test, *Composites Science and Technology*  
514 72 (2012) 1924–1932.
- 515 [35] C. Chamis, *Mechanics of Composite Materials: Past, Present, and Future*, ASTM 11 (1989).
- 516 [36] Beuth, DIN EN 2823 - Aerospace series - Fibre reinforced plastics - Determination of the effect  
517 of exposure to humid atmosphere on physical and mechanical characteristics, 1999.
- 518 [37] W. Oliver, G. Pharr, An improved technique for determining hardness and elastic modulus  
519 using load and displacement sensing indentation experiments, *Journal of Materials Research* 7  
520 (1992) 1564–1583.
- 521 [38] M. Herráez, D. Mora, F. Naya, C. S. Lopes, C. González, J. LLorca, Transverse cracking of  
522 cross-ply laminates: A computational micromechanics perspective, *Composites Science and*  
523 *Technology* 110 (2015) 196–204.
- 524 [39] E. H. Andrews, A. Stevenson, Fracture energy of epoxy resin under plane strain conditions,  
525 *Journal of Materials Science* 13 (1978) 1680–1688.

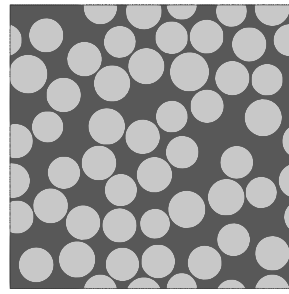
- 526 [40] S. Oghihara, J. Koyanagi, Investigation of combined stress state failure criterion for glass  
527 fiber/epoxy interface by the cruciform specimen method, *Composites Science and Technology*  
528 70 (2010) 143–150.
- 529 [41] C. González, J. LLorca, Multiscale modeling of fracture in fiber-reinforced composites, *Acta*  
530 *Materialia* 54 (2006) 4171–4181.
- 531 [42] H. Koerber, J. Xavier, P. Camanho, High strain rate characterisation of unidirectional carbon-  
532 epoxy IM7-8552 in transverse compression and in-plane shear using digital image correlation,  
533 *Mechanics of Materials* 42 (2010) 1004–1019.
- 534 [43] G. Huang, H. Sun, Effect of water absorption on the mechanical properties of glass/polyester  
535 composites, *Materials and Design* 28 (2007) 1647–1650.
- 536 [44] J. Wang, B. Chen, N. Liu, G. Han, F. Yan, Combined effects of fiber/matrix interface and wa-  
537 ter absorption on the tribological behaviors of water-lubricated polytetrafluoroethylene-based  
538 composites reinforced with carbon and basalt fibers, *Composites Part A: Applied Science and*  
539 *Manufacturing* 59 (2014) 85–92.
- 540 [45] E. Totry, J. M. Molina-Aldareguía, C. González, J. LLorca, Effect of fiber, matrix and interface  
541 properties on the in-plane shear deformation of carbon-fiber reinforced composites, *Composites*  
542 *Science and Technology* 70 (2010) 970–980.
- 543 [46] P. P. Camanho, a. Arteiro, a. R. Melro, G. Catalanotti, M. Vogler, Three-dimensional invariant-  
544 based failure criteria for fibre-reinforced composites, *International Journal of Solids and Struc-*  
545 *tures* 55 (2014) 92–107.
- 546 [47] M. Herráez, C. González, C. S. Lopes, R. Guzmán de Villoria, J. Llorca, T. Varela, J. Sánchez,  
547 Computational micromechanics evaluation of the effect of fibre shape on the transverse strength  
548 of unidirectional composites: an approach to virtual materials design, Submitted to *Composites*  
549 *Part A: Applied Science and Manufacturing* (2015).



(a)



(b)



(c)

Figure 1: (a) AS4/8552 cross-section micrograph.(b) NNA virtual microstructure.(c) RSA virtual microstructure

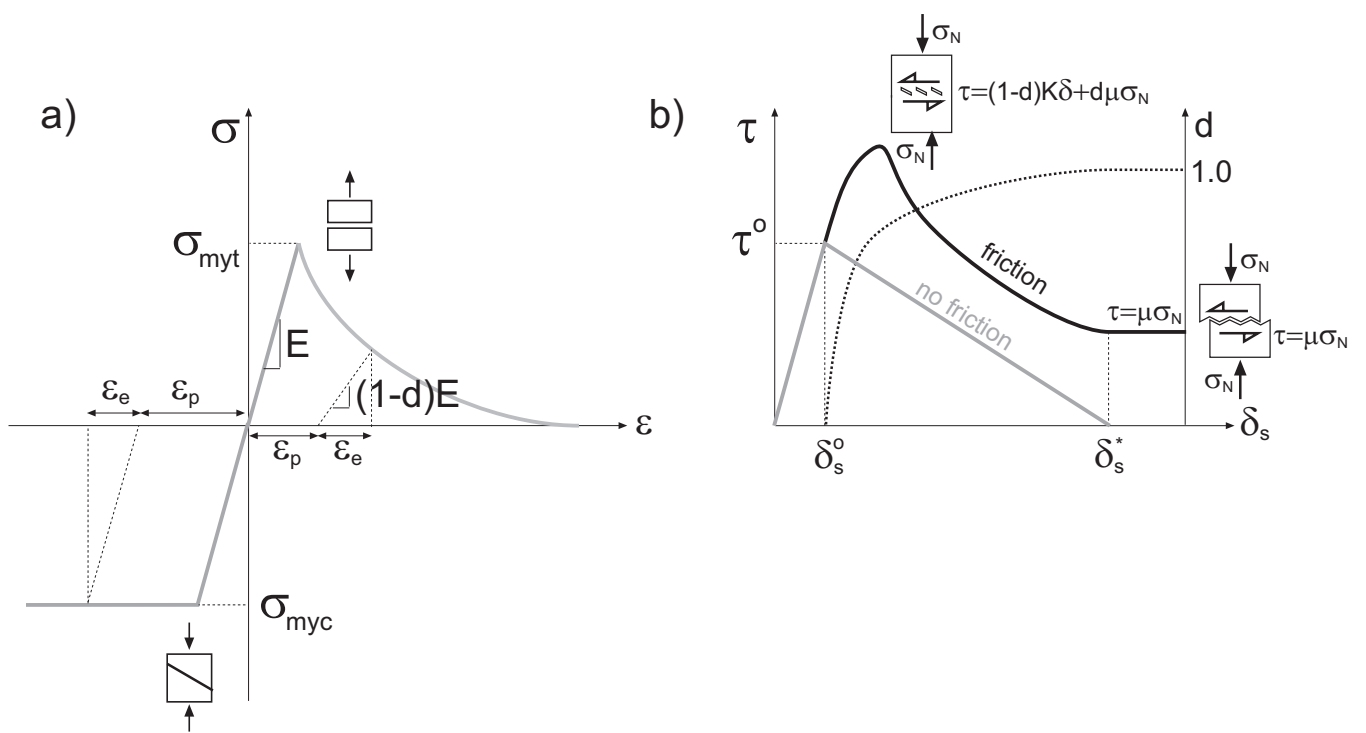


Figure 2: a) Schematic of the uniaxial tension-compression response of the epoxy matrix according to the damage-plasticity model for quasi-brittle materials, b) Schematics of the shear response of the damage-friction model for fiber/matrix interfaces.

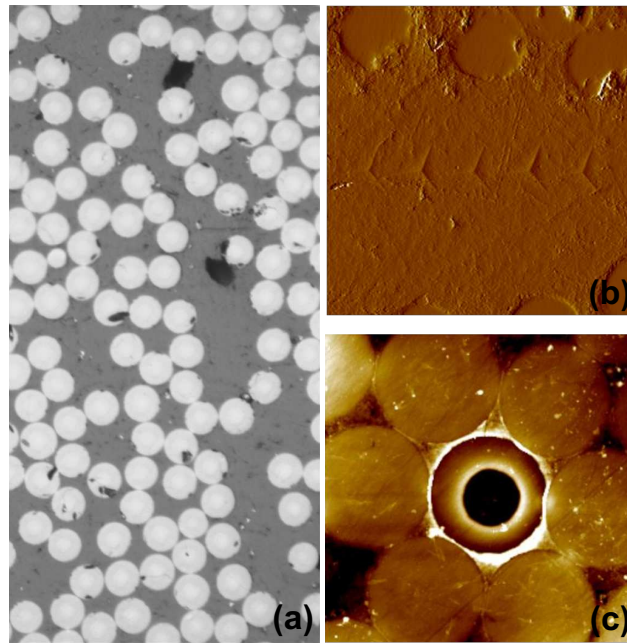


Figure 3: Micromechanical tests.(a) AS4/8552 cross section showing matrix rich regions. Atomic Force Microscope (AFM) image showing (b) the Berkovich pyramidal indenter footprint on a polymer matrix and (c) the flat punch tip footprint on a carbon fiber



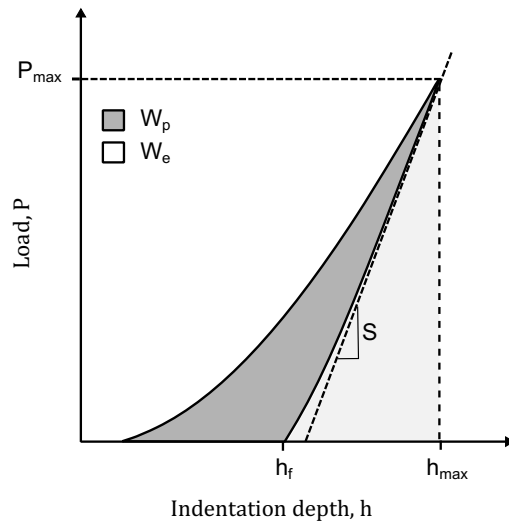


Figure 4: Typical load-displacement curve resulting from the nanoindentation test (adapted from [29])

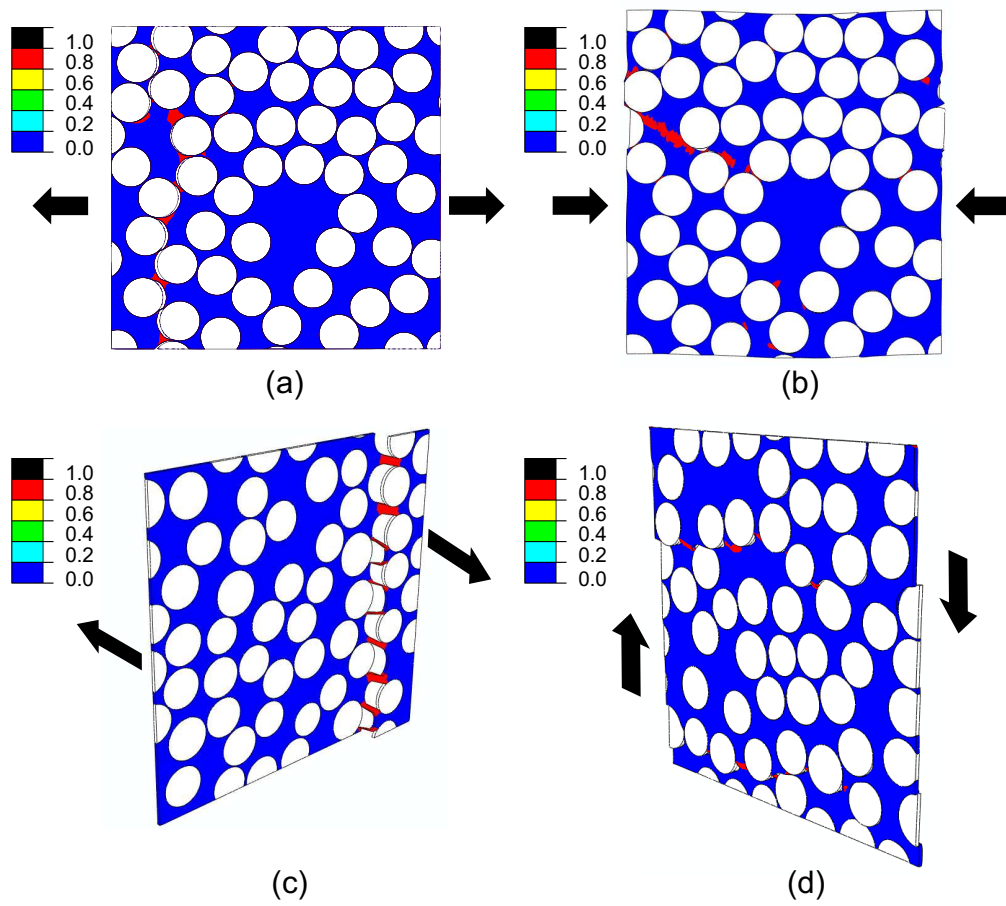


Figure 5: Predicted failure modes in a AS4/8552 ply. Tensile damage for transverse tension (a), parallel shear (c) and perpendicular shear (d). Compression damage for transverse compression (b)

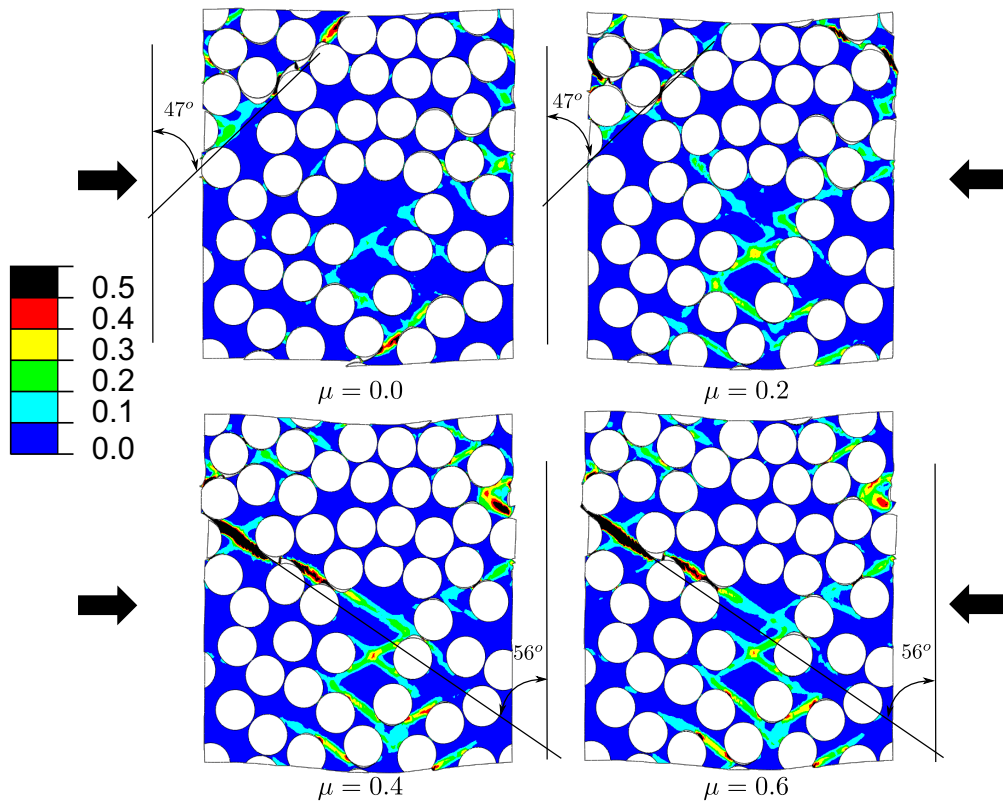


Figure 6: Effect of the friction coefficient,  $\mu$ , in the transverse compression loading when  $\epsilon = 5\%$ . Prediction of accumulated plastic strain (PEEQ)

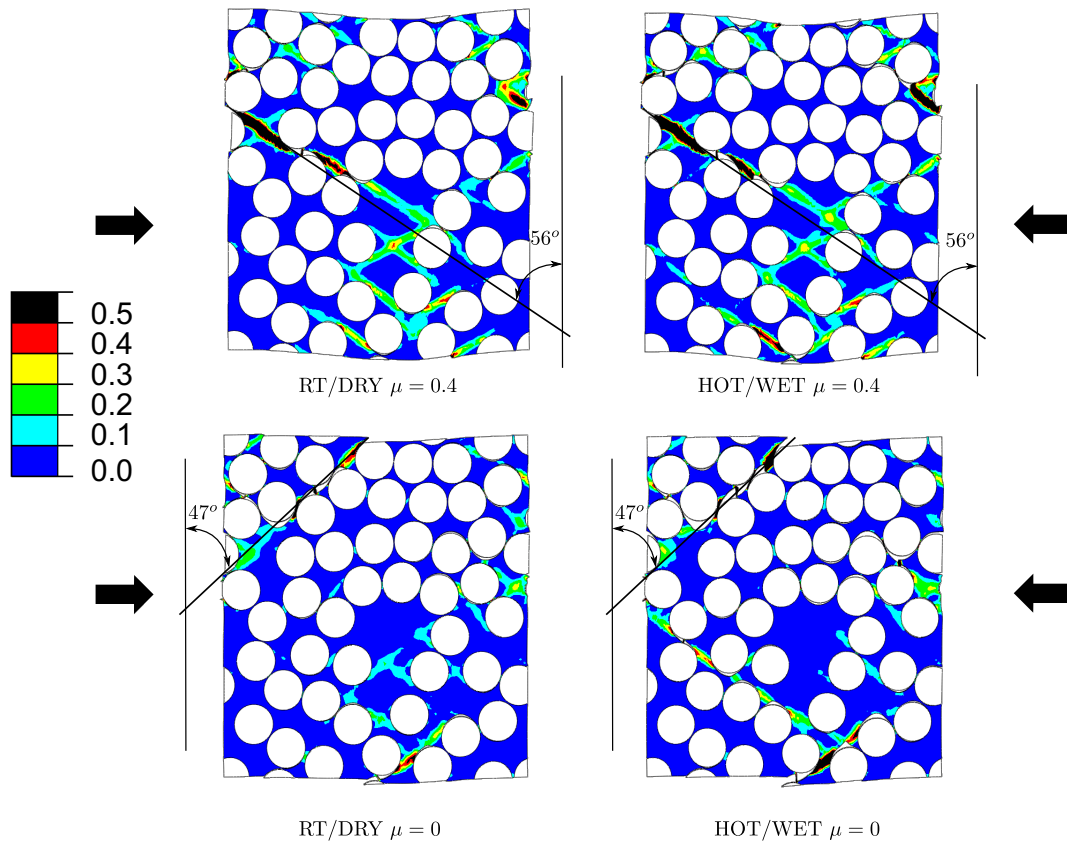


Figure 7: Effect of the environmental conditions in the transverse compression loading. Predicted accumulated plastic strain (PEEQ) at  $\epsilon = 5.5\%$  for  $\mu = 0.4$  and  $\mu = 0.0$  under RT/DRY environment. Predicted accumulated plastic strain (PEEQ) at  $\epsilon = 4.8\%$  for  $\mu = 0.4$  and  $\mu = 0.0$  under HOT/WET environment

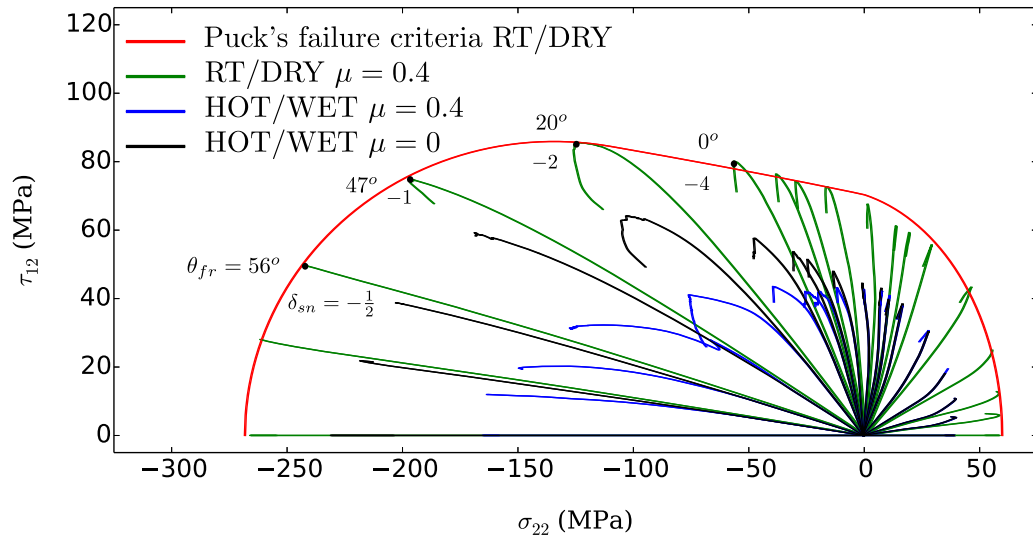


Figure 8: Predicted failure locus in a AS4/8552 ply under combined transverse stress and in-plane shear for RT/DRY and HOT/WET conditions(with and without friction)

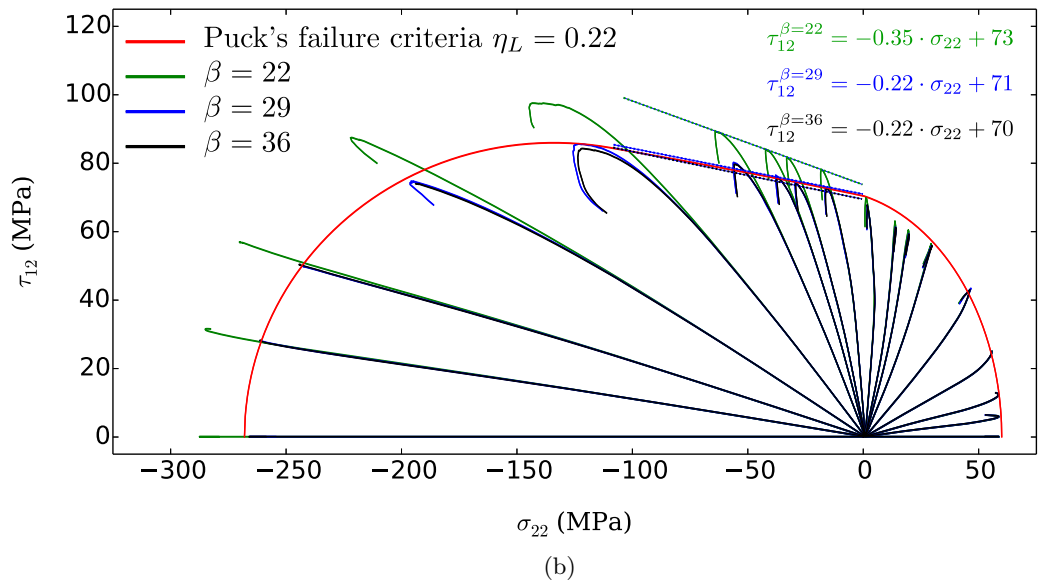
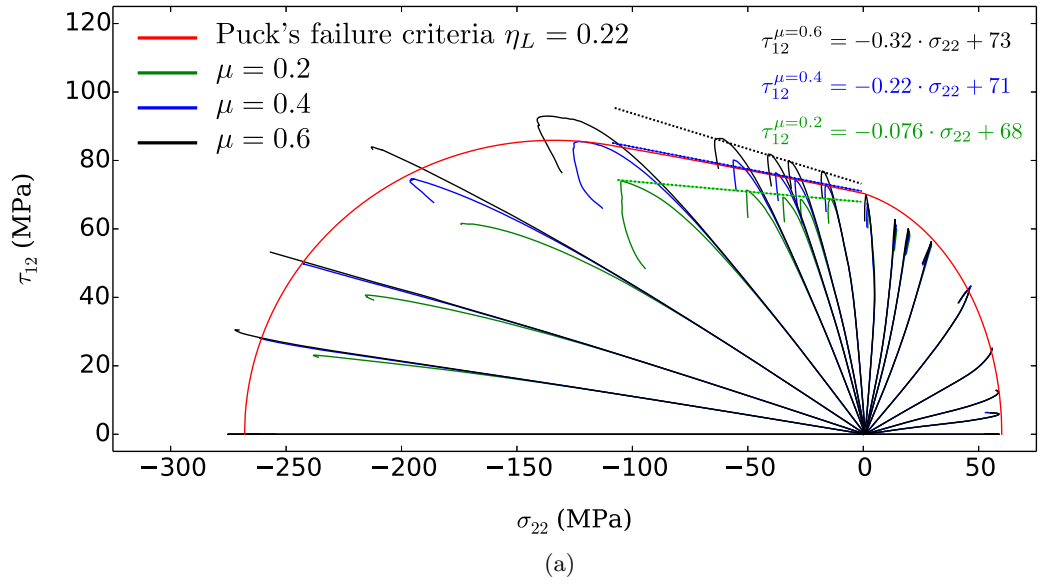


Figure 9: Effect of model parameters on the predicted failure locus in a AS4/8552 ply under combined transverse stress and in-plane shear: a) Effect of the friction coefficient between fiber and matrix; b) Effect of polymer matrix internal friction angle.

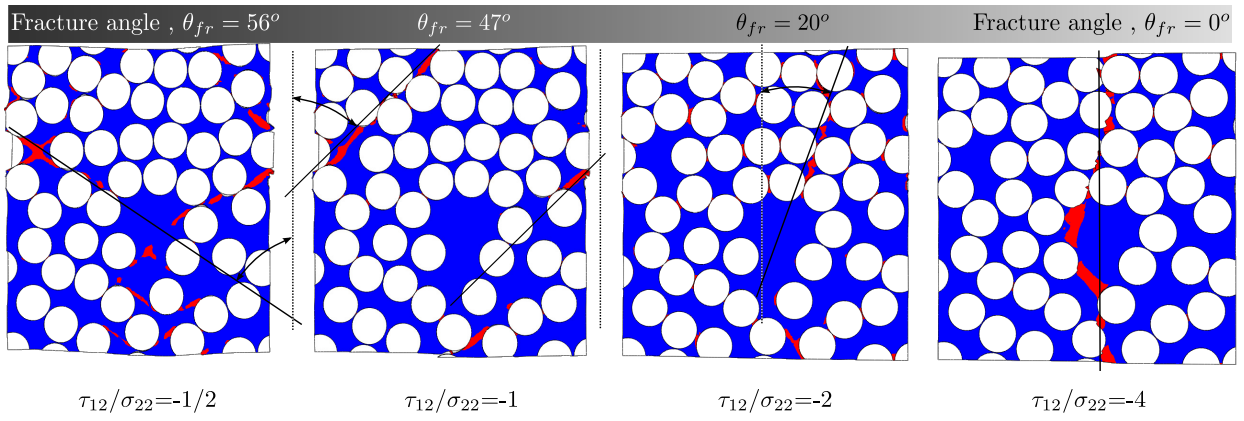


Figure 10: Predicted fracture angles for different load combinations and RT/DRY conditions ( $\mu = 0.4$ ). The image show the concentration of accumulated plastic strain (PEEQ) for the different biaxial loading states

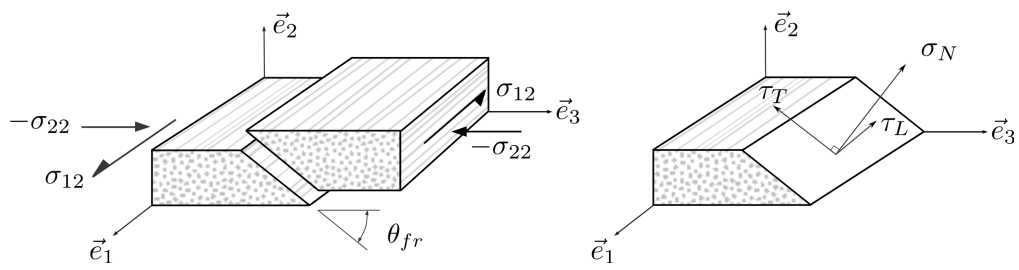


Figure 11: a) Fracture plane for a ply subjected to transverse compression and in-plane shear; b) Stresses in the fracture plane.



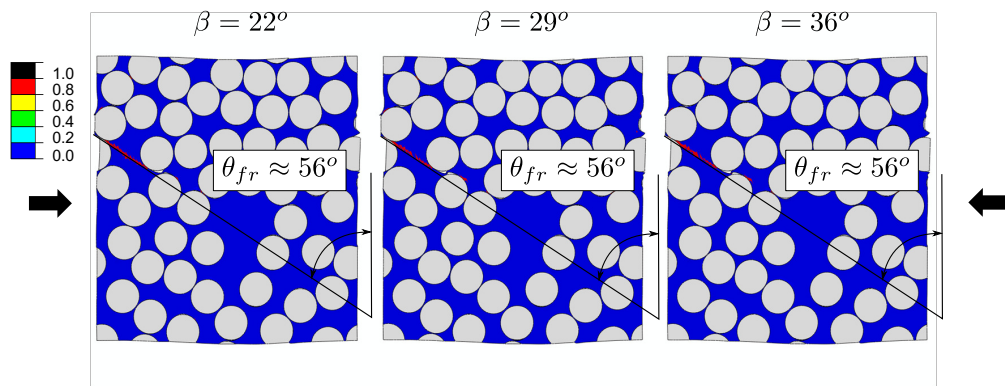


Figure 12: Predicted compression damage and fracture angle in a AS4/8552 ply under a pure transverse compressive stress state for different polymer matrix internal friction angles,  $\beta$

Table 1: Properties of the AS4/8552 material constituents used in the FE simulations. Polymer fracture energy, tensile strength, Poisson ratio and internal friction angle are taken from [38]. Carbon fiber elastic properties are also extracted from [38]

AS4 carbon fiber properties							
	$E_{f1}(GPa)$	$E_{f2}(GPa)$	$G_{f12}(GPa)$	$G_{f23}(GPa)$	$\nu_{f12}$	$\alpha_{f1}(K^{-1})$	$\alpha_{f2}(K^{-1})$
	231	12.97	11.28	4.45	0.3	-0.9e-6	7.2e-6
8552 epoxy matrix properties							
Condition	$E_m(GPa)$	$\nu_m$	$\sigma_{myt}(MPa)$	$\beta$	$\sigma_{myc}(MPa)$	$\mathcal{G}_m(J/m^2)$	$\alpha_m(K^{-1})$
RT/DRY	5.07	0.35	121	29	176	100	52e-6
HOT/WET	4.28	0.35	104	29	152	100	1.5e-6
AS4/8552 fibre/matrix interface properties							
Condition	$\sigma_N(MPa)$	$\tau_T(MPa)$	$\tau_L(MPa)$	$\mathcal{G}_{Ic}(J/m^2)$	$\mathcal{G}_{IIc}(J/m^2)$	$\mathcal{G}_{IIIc}(J/m^2)$	
RT/DRY	42	64	64	2	100	100	
HOT/WET	30	45	45	2	100	100	

Table 2: 8552 epoxy resin indentation and AS4/8552 interface push-in tests results under RT/DRY and HOT/WET (70C/85%) conditions

Condition	$\beta(^{\circ})$	$\sigma_{myc}(MPa)$	$E(GPa)$	$\tau_d(MPa)$
RT/DRY	29	$176 \pm 17$	$5.07 \pm 0.3$	$63.77 \pm 2.64$
HOT/WET	29	$152 \pm 08$	$4.28 \pm 0.2$	$44.55 \pm 2.72$

Table 3: Numerically-predicted vs. experimentally-obtained elastic constants, transverse and shear strengths for a AS4/8552 ply (ply thickness  $t=0.184\text{mm}$ )

Property	RT/DRY		HOT/WET	
	Micromechanics	Literature [15]	Micromechanics	Literature [15]
$E_2(\text{GPa})$	9.2	9.6	8.3	8.4
$G_{12}(\text{GPa})$	4.8	4.8	3.1	2.3
$Y_T(\text{MPa})$	$61\pm 3$	63.9	$36\pm 2$	24.1
$Y_C(\text{MPa})$	$290\pm 30$	268.0	$141\pm 7$	136.0
$S_L^{0.2\%}(\text{MPa})$	$55\pm 1$	55.2	$34\pm 1$	23.2
$S_L^{5\%}(\text{MPa})$	$88\pm 3$	91.6	$55\pm 3$	38.0