High-fidelity micro-scale modeling of the thermo-visco-plastic behavior of carbon fiber polymer matrix composites

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Abstract

An experimentally validated micro-scale analysis of the visco-thermo-mechanical behavior of polymer matrix composites under different loads is proposed. A new constitutive law for the matrix material is developed taking into account the pressure dependence of the material as well as strain-rate and temperature dependence. Capturing the matrix behavior under multi-axial stress states is concluded to be essential to accurately predict the composite material behavior, even when considering simple load cases such as transverse compression and/or shear. Without any calibration procedure at the composite level, good agreement with the experimental data is observed for different loading conditions, including strain-rate dependency.

Using this validated micro-scale model, a three-dimensional simulation of the formation of a kink band under longitudinal compression of the composite is conducted. A new evidence at micro-scale is found supporting the hypothesis that shear stresses transferred between fibers and matrix are particularly important in the formation of the kink band.

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1. Introduction

There is an increasing demand for accurate predictive models of the inelastic and fracture behavior of fiber reinforced polymer matrix composites due to the wide spread of applications where these materials are being used, especially in the transportation industry. However, accurately modeling the thermo-mechanical behavior of these materials remains a difficult challenge due to various factors, namely: 1) the matrix material is usually a highly cross-linked glassy polymer (e.g. epoxy resin) that shows rate- and thermal-dependent inelastic response [1]; 2) the high strength and brittleness of the fibers associated to the high fiber volume fraction of the composite (typically around 60%) leads to large three-dimensional strain concentrations in the matrix [2]; 3) the fiber distribution is non-uniform [3]; and 4) the manufacturing process introduces thermal residual stresses [4] and different defects such as voids, fiber waviness and fiber misalignment [5].

These factors limit the applicability of analysis models based on the homogenized behavior of the composite, denominated here by macro- and meso-scale models. Macro-scale models deal with the entire laminate as homogeneous continuum and therefore are capable of doing structural analysis and preliminary design and optimization [6, 7]. Meso-scale models improve the predictive capabilities of the macro-scale models by analyzing individual plies as a homogeneous continuum [8–15] and by modeling the delamination between the different plies via cohesive models [16–18]. The recent work of Camanho et al. [19] presented a meso-scale model that coupled a fully three-dimensional damage model with a new plasticity law developed by Ref.[20] that led to accurate predictions for non-trivial experimental tests.

Since the macro- and meso-scale models rely on the description of the polymer composite as a homogeneous continuum, they inevitably lead to complex

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9 constitutive and damage laws that require a large number of experimental in-
10 puts [7, 9, 10]. Furthermore, the analyses obtained at these scales do not provide
11 enough detail about the mechanical processes that explain the inelastic behavior
12 of the material. This motivated efforts for the development of micro-scale mod-
13 els, where the highest level of detail in modeling the different failure mechanisms
14 of polymer composites under different load cases has been reached. Significant
15 progress was obtained by using different constitutive models for each constituent
16 in the composite. Since fibers are very brittle, the constitutive law can be as-
17 sumed as transversely isotropic linear elastic. However, the polymeric matrix
18 constitutive law is significantly more challenging, as highlighted by several au-
19 thors [4, 21–26]. In fact, the polymeric matrix can exhibit strong nonlinear
20 behavior under general load cases, as well as thermal and strain-rate depen-
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25 In this article the authors present a micro-scale analysis that will be shown
26 to lead to accurate predictions of the behavior of the composite material. The
27 presented model is validated experimentally not only at the level of the single
28 constituents but also at the composite level by comparing its homogenized re-
29 sponse with published experimental data. This contrasts with previous works
30 where direct comparison with experimental data was not shown. A new con-
31 stitutive model for polymer matrix is proposed and validated in Section 2 and
32 Section 3. Section 4 discusses the micro-scale model for composite materials
33 and the validation of the predicted response for a carbon fiber polymer matrix
34 composite. Section 5 is dedicated to the prediction of a particularly complex
35 failure mechanism of composite materials under longitudinal compression: the
36 formation of a kink band.
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50 **2. Constitutive model for polymer matrix**

51 *2.1. A modified paraboloid yield criterion*

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53 The motivation for developing a new constitutive law for the matrix material
54 stems from the fact that even the simplest loading conditions applied to the
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composite produce general stress states that are far from the uniaxial loading conditions under which the bulk matrix material is typically tested [1]. Previous works used constitutive models that are known to be unable to describe such general stress states, as the Mohr-Coulomb elasto-plastic model [4, 21–23], or the Drucker-Prager model [24–26]. The inadequacy of these models was pointed out by different authors [2, 27, 28], who proposed the paraboloidal criterion as an alternative.

Here an extension to the paraboloidal model is proposed so that the predictive ability of the micro-scale analyses is improved. The classical paraboloidal yield criterion [29, 30] can be written as:

$$f(\boldsymbol{\sigma}, \sigma_{Y_C}, \sigma_{Y_T}) = 6J_2 + 2(\sigma_{Y_C} - \sigma_{Y_T}) I_1 - 2\sigma_{Y_C} \sigma_{Y_T} \quad (1)$$

where σ_{Y_C} and σ_{Y_T} are the absolute values of compressive and tensile yield stresses, $I_1 = \text{Tr}(\boldsymbol{\sigma}_{ij})$ is the first stress invariant, and $J_2 = \frac{1}{2} \boldsymbol{s}_{ij} \boldsymbol{s}_{ij}$ is the second invariant of the deviatoric stress tensor $\boldsymbol{s}_{ij}$.

Observing Eq. (1), one sees that this yield surface is determined uniquely by the two parameters σ_{Y_C} and σ_{Y_T} . However, this yield surface leads to inaccurate predictions for the response of the bulk matrix under pure shear case, as demonstrated by the results presented in Section 3.

The following modification to the paraboloidal yield criterion is proposed here to include the shear yield behavior:

$$f(\boldsymbol{\sigma}, \sigma_{Y_C}, \sigma_{Y_T}, \sigma_{Y_S}) = a(J_2^3 + bJ_3^2)^{1/3} + 2(\sigma_{Y_C} - \sigma_{Y_T}) I_1 - 2\sigma_{Y_C} \sigma_{Y_T} \quad (2)$$

where the third deviatoric stress invariant $J_3 = \det(\boldsymbol{s}_{ij})$ and two inter-dependent parameters a and b are introduced. These parameters can be determined with only one additional experimental test.

The relationship between a and b can be determined from the uniaxial tensile test by considering $\sigma_2 = \sigma_3 = 0$ in Eq. (2) to obtain:

$$a = 6 \left(\frac{27}{4b + 27} \right)^{1/3} \quad (3)$$

Since this modified paraboloidal yield criterion has only one additional independent parameter, the pure shear experimental test of the matrix is sufficient to

calibrate the constitutive law. This is achieved by considering the pure shear stress state $\sigma_1 = -\sigma_2$ and $\sigma_3 = 0$ in Eq. (2) and relating the parameter b with the shear yield strength σ_{Y_S} :

$$b = \frac{1}{4} \left(\frac{(3\sigma_{Y_S})^6}{(\sigma_{Y_C} \sigma_{Y_T})^3} - 27 \right) \quad (4)$$

The derivation of a and b can be found in APPENDIX A. The effect of the third invariant J_3 is modulated by the parameter b as illustrated in Fig.1 and Eq.(5)

$$\begin{cases} b = 0 & \Rightarrow \text{Classical paraboloidal model} \\ b > 0 & \Rightarrow \text{Increase shear yield stress} \\ b < 0 & \Rightarrow \text{Decrease shear yield stress} \end{cases} \quad (5)$$

It is also observed that the variation of b has no effect on the compressive, tensile and biaxial yield strengths. The added term has an influence on the shear yield strength, the asymmetry of the yield function and its evolution, which will be shown to lead to accurate predictions for the material response with particular impact on the predictions of the response for the composite material.

A non-associative flow rule [31] was used to prevent positive volumetric plastic strain under hydrostatic pressure

$$g = \sigma_{vm}^2 + \alpha p^2 \quad (6)$$

where $\sigma_{vm} = \sqrt{3J_2}$ is the von Mises equivalent stress, $p = 1/3I_1$ is the hydrostatic pressure, and the parameter α is given as:

$$\alpha = \frac{9}{2} \frac{1 - 2\nu_p}{1 + \nu_p} \quad (7)$$

with ν_p being the plastic Poisson's ratio that can be determined from the uniaxial tensile test. From the above results one can write the increment in plastic deformation via the flow rule that uses the plastic potential given in Eq. (6):

$$\Delta \varepsilon^p = \Delta \lambda \frac{\partial g}{\partial \boldsymbol{\sigma}} \quad (8)$$

with $\Delta \lambda$ being the plastic multiplier, subjected to the Kuhn-Tucker consistency conditions and to be updated via the return mapping algorithm [32].

2.2. Thermo-visco-plastic hardening

Since the proposed yield criterion depends on the compressive, tensile and shear yield strengths these three values need to be updated according to the corresponding hardening laws that depend on the equivalent plastic strain:

$$\sigma_{Y_C}^* = h_C(\varepsilon_e^p), \quad \sigma_{Y_T}^* = h_T(\varepsilon_e^p), \quad \sigma_{Y_S}^* = h_S(\varepsilon_e^p) \quad (9)$$

where the superscript $*$ is used to indicate that these yield strengths are calculated for reference values of strain-rate and temperature. The equivalent plastic strain ε_e^p is defined as:

$$\varepsilon_e^p = \sqrt{\frac{1}{1 + 2\nu_p^2} \varepsilon^p : \varepsilon^p} \quad (10)$$

Having the hardening behavior defined for the reference conditions, the following phenomenological scaling laws are proposed to account for the influence of temperature and strain-rate on the material response:

$$\sigma_{Y_n} = \sigma_{Y_n}^* \left(1 + \alpha_n \log \frac{\dot{\varepsilon}_e^p}{\dot{\varepsilon}_e^{p*}} \right) \left(1 + \beta_n \log \frac{T}{T^*} \right) \quad (11)$$

where σ_{Y_n} are the predicted yield stresses at the desired temperature T and strain-rate $\dot{\varepsilon}_e^p$, and $\sigma_{Y_n}^*$ are the above mentioned yield stresses at the reference temperature T^* and strain-rate $\dot{\varepsilon}_e^{p*}$. The material constants α_n and β_n are determined experimentally by scaling back to the reference state each stress-strain curve that is obtained for the different strain-rates and temperatures. Note that the subscript $n = (C, T, S)$ is used to refer to the compressive, tensile and shear tests, respectively – see Eq. (9). The above phenomenological laws are proposed for uniaxial experiments to account for the strain-rate dependency [33] and to account for the temperature dependency [34]. Here, these laws are used to scale all three yield strengths independently so that accurate predictions for general stress states could be obtained.

3. Matrix model validation and predictions

The constitutive model for the polymeric matrix is used to predict the visco-thermo-mechanical response of two different epoxy matrices: Epoxy 3501-6 (I)

and Epon 862 (II). The input parameters are presented in Table 1 (The unit for E and σ_{Y_x} are MPa). The results presented herein are obtained by implementing a user material (UMAT) subroutine in a commercial finite element software ABAQUS according to the algorithm summarized in Table 2.

Table 1: Input parameters for the Epoxy 3501-6 and Epon 862 matrix constitutive model. Ref.[1, 35]

	E	ν	σ_{Y_T}	σ_{Y_C}	σ_{Y_S}	α_C	α_T	α_S	β_C	β_T
I	4600	0.34	44.4	112.7	30.3	0.042	0.0	0.0	-	-
II	2600	0.4	69.0	80.0	-	0.035	0.035	-	0.42	0.42

3.1. Results for Epoxy 3501-6

Fig.2 shows the results of the model after calibration for the three experimental tests. The improvement obtained for the description of the shear test using the proposed modification to the paraboloidal criterion is shown in Fig.2(a). The difference between the present model and the classical model is enlarged with the increase of strain.

Fig.2(a) also reveals that the tensile and shear test for this polymer has an almost linear behavior and, as pointed out by Werner and Daniel [1], is independent of the strain-rate for this epoxy; therefore, the rate dependence parameter α_T and α_S are considered to be zero.

Fig.2(b) demonstrates the response for the pure compressive case as well as the accuracy of the strain-rate dependence law. Note that the compressive yield strength is determined only for the reference strain-rate, here assumed to be the quasi-static test with strain-rate 10^{-4}s^{-1} , and then the compressive rate dependence parameter α_C is obtained from the experimental curves at different strain-rates such that all the curves collapse in a master curve.

Fig.3 shows the improvement of the model predictive capabilities by comparing the predictions obtained for a multi-axial load condition. An accurate

Table 2: Summary of the implementation algorithm for the polymer constitutive model.

(1)	Elastic predictor
	$\boldsymbol{\sigma}_{n+1}^{tr} = \boldsymbol{\sigma}_n + \mathbf{D}^e : \Delta \boldsymbol{\varepsilon}$
	$\mathbf{S}_{n+1}^{tr} = \mathbf{S}_n + 2G\Delta \boldsymbol{\varepsilon}_d, p_{n+1}^{tr} = p_n + K\Delta \varepsilon_v$
(2)	Check strain-rate and temperature
	IF $\dot{\varepsilon}_e^p \neq \dot{\varepsilon}_e^{p*}$ OR $T \neq T^*$ THEN
	Scale yield strength and hardening law, Eq. (11):
	$\sigma_{Y_n} = \sigma_{Y_n}^* \left(1 + \alpha_n \log \frac{\dot{\varepsilon}_e^p}{\dot{\varepsilon}_e^{p*}} \right) \left(1 + \beta_n \log \frac{T}{T^*} \right)$
(3)	Check yield criterion via Eq. (2):
	IF $f(\boldsymbol{\sigma}, \sigma_{Y_C}, \sigma_{Y_T}, \sigma_{Y_S}) \leq 0$ THEN
	$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{tr}$
(4)	Return mapping algorithm
	Calculate plastic multiplier $\Delta \lambda$
(5)	Update stress tensor
	$\mathbf{S}_{n+1} = \frac{\mathbf{S}_{n+1}^{tr}}{1+6G\Delta \lambda}, p_{n+1} = \frac{p_{n+1}^{tr}}{1+2K\alpha\Delta \lambda}$
	$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{tr} - 6G\Delta \lambda \mathbf{S}_{n+1} - \frac{2}{3}K\alpha\Delta \lambda p_{n+1} \mathbf{I}$
(6)	EXIT

description of the matrix behavior under non-trivial stress states is a key factor in order to obtain satisfactory predictions for the response of the composite material. Therefore, the developed matrix constitutive model is validated by considering the experimental results obtained for a combined load case of compression and torsion. In the figure it is clear the improvement of the predictions of the proposed model when compared to the paraboloidal yield model.

3.2. Results for Epon 862

The modified constitutive model is also applied to the Epon 862 epoxy. Poulain et al. [35] conducted experiments for both strain-rate and temperature

dependence of this material. Fig.4 shows the predictions for different temperatures and strain rates for both tensile and compressive loads using the proposed constitutive model. Good agreement is observed for both the strain-rate and temperature dependence.

4. Composite material results and model validation

This section is focused on the prediction of the micro-scale behavior of unidirectional polymer matrix composites via an experimentally validated micro-scale analysis. For consistency, the experimental results [36] for the composite material considered in this section are obtained for an AS4-3501-6 composite, i.e. with the same matrix material (epoxy 3501-6) as the one considered in Section 3.1 to validate the proposed polymer constitutive model.

As described in the previous section, the matrix material properties and the inputs for the proposed polymer constitutive model can be found in Table 1. The transversely isotropic material properties for the AS4 carbon fibers are $E_1 = 225.0\text{GPa}$, $E_2 = 15.0\text{GPa}$, $\nu_{12} = 0.2$, $G_{12} = 15.0\text{GPa}$ and $G_{23} = 7.0\text{GPa}$, according to Ref.[37]. To investigate the influence of matrix nonlinear properties on composite effective property, the interfacial debonding between fiber and matrix is ignored. Comparison studies also show that the debonding had slight influence on effective property under compressive loading. [28]

Transverse compression tests and 45° off-axis compression tests at different strain rates are used to validate the proposed micro-scale model. For each simulation, several three-dimensional unit cells are generated using randomly distributed fibers [3] in the transverse section. It is well known that the size of the unit cells is an important parameter in predicting the response of the material [23, 28]. If the size of the unit cell is not large enough then the randomness of the fibers position significantly affects the response of the composite and the unit cells are called Statistical Volume Elements (SVEs). However, if a sufficiently large domain is considered, then the homogenized response is virtually independent of the randomization of the microstructure and the unit cell

is denominated as a Representative Volume Element (RVE). The finite element mesh of SVE and RVE are illustrated in Fig. 5.

Different sizes are considered in order to study if we are in the presence of an SVE or an RVE. The diameter of the fiber is considered constant and equal to $6 \mu m$. The SVE's length is $24 \mu m$ (approximately 270,000 elements), while the RVE's length is $58 \mu m$ (approximately 4,800,000 elements). A larger RVE is considered and the homogenized response is the same for the load conditions considered herein. Periodic boundary conditions(PBC) are applied to the RVEs [38]. The derivation of the PBC for 45° off-axis compression can be found in APPENDIX B. The reader is reminded that results in this section for the composite did not require any calibration. The only calibration process conducted is at the level of the constituents, as discussed in Section 3.

4.1. Transverse compression

The results obtained for transverse compression, i.e. with the fibers aligned out of the plane and the loading direction being perpendicular to their alignment direction, are presented in Fig.6. This figure illustrates that a significant portion of the equivalent plastic strain of the resin in Fig.6(b) is due to the in-plane shear stress component as seen in Fig.6(a).

The comparison of the average stress-strain curves obtained using the new constitutive model for the matrix and the classical paraboloidal model are shown in Fig.7 (a). The significant improvement of the predictions from the micro-scale analysis of the composite can be explained by the importance of the shear behavior of the resin, since it is found to be a key factor in the yielding process of the composite in transverse compression. In addition, the composite response under higher strain-rates is also predicted as shown in Fig.7 (b). Once again, good agreement is observed between the micro-scale analysis and the experiments.

4.2. 45° off-axial compression

For the 45° off-axial compression test the influence of the shear stresses is evidently even more important. Fig.8 presents the distribution of the shear

stress (a) and equivalent plastic strain (b) for the simulations of this test. In the figure the influence of the shear on the plastic localization is observed clearly. The comparison of the average stress-strain curves between the presented model and the classical paraboloidal model is shown in Fig.9. The classical model will yield later at around 200 MPa and reach a higher plateau than the experiment, while the modified paraboloidal model shows good agreement on both the yield point and the plateau value.

These results, as well as the previously presented results for transverse compression, demonstrate the importance of having an accurate plasticity model for the matrix material that accounts for tri-axial stress states. In particular, the contribution of the shear behavior for the plastic deformation of the matrix is important. We also note that for the model presented herein, the improvements of the predictions come from the changes in the growth of the yield surface that are controlled by the inter-play between the tensile, compressive and shear stresses.

5. Longitudinal compression with the formation of a kink band

Carbon fiber reinforced composite plies subjected to compressive loads aligned with the fibers direction fail by generating a kink band, i.e. fibers break at two points and create a kink band inclined at an angle, $\beta \approx 15^\circ$ with the transverse direction [39–43]. The fibers within the band rotate by an approximate angle $\phi \approx 30^\circ$ from the initial fiber direction, and the kink width $w = 50 - 60 \mu\text{m}$ is approximately equal to 10 fiber diameters [39, 40, 44]. This failure mode is explained by different authors [41, 45, 46] as a combination between fiber microbuckling and the transferred shear stresses by the interface between matrix and fiber. Therefore, due to the fact that the formation of a kink band involves an unstable behavior of a group of fibers (microbuckling) over a large width (for a micro-scale model) driven by the shear stresses transferred by the matrix, this failure mode is particularly challenging to model.

A unit cell with the size $53 \times 53 \times 162 (\mu\text{m})$ containing approximately 34,000,000

elements is used for the kink band simulation. Since the authors did not have access to detailed longitudinal microstructural information (fiber waviness and fiber misalignment) and the matrix-fiber interface property, the presented prediction for the compressive strength of the composite is higher than one would get in the actual experiments for this load case. Here, the intention is to demonstrate a study with the presented micro-scale model that is able to predict the details in the formation of a kink band. Fig.10 shows that the initiation and rapid propagation of the kink band is captured by the presented model, including the approximate width of the kink band.

The average shear stress, axial stress and equivalent plastic strain along longitudinal axes are shown in Fig.11. This figure provides support to the hypothesis explored by different authors in their analytical models [41, 45] that attributed particular importance to the shear stresses as opposed to the early analytical studies [47] where pure microbuckling is considered to be the key mechanism. Recently, this reasoning is also applied to derive a three-dimensional failure criteria [48] and damage model [7] for composite plies. Note that stress σ_a, σ_s and strain ε are divided by the respective yield strength σ_{ay}, σ_{sy} and failure strain ε_f of the matrix in order to facilitate the identification of the contributing mechanisms. The longitudinal coordinate (position along the fibers direction) is also normalized by the fiber diameter ($d = 6\mu\text{m}$) so that a comparison with the reference value for the width of the kink band ($\approx 10d$) could be presented clearly.

Further evidence supporting the key role of shear stresses transferred by the matrix material can be obtained from Fig.12 that presents the global average stress-strain curve for the matrix material. As can be seen in the figure, at the beginning of deformation ($\varepsilon/\varepsilon_f < 0.4$) the matrix material does not exhibit plasticity until the compressive yield stress of the matrix is reached, points A and A'. Afterwards, both the normal and shear stresses show a nonlinear relation until the shear stress reaches a maximum value, point B. Mapping the trigger point B to Fig.11 (a), we can see the kinking band is formed by local shear stress reach the yield strength value ($\sigma_s/\sigma_{sy} = 1$). Shortly after the kink band is

formed, at point B', the normal stress also reaches its peak value and the kink band propagates unstably to failure.

6. Conclusions

This work presented an experimentally validated micro-scale analysis of fiber reinforced polymer composites under different load cases. In order to achieve an accurate prediction, a new constitutive model for the matrix is proposed based on modifying the paraboloidal yield criterion. A combination of three hardening laws is included in this new model to describe the hardening process under tri-axial stress states. This plasticity model is experimentally validated by considering two different epoxy resins, thermal and strain-rate effects are also considered.

By using this new constitutive model, the predictions of micro-scale analyses for composite is significantly improved under nontrivial tri-axial stress states. Furthermore, a more complicated longitudinal compression simulation is considered, and the result indicates that local plastic shear triggers the initiation of kinking band. This new evidence found at micro-scale is supporting the hypothesis that shear stresses transferred between fibers and matrix are particularly important in the formation of the kink band. The interplay between these shear stresses and microbuckling is then expected to be the correct explanation for this failure mode.

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APPENDIX 1: Determination of parameters in modified paraboloidal model

Two specific loading case are used to determine the parameters a and b in the proposed modified paraboloidal yield criterion.

$$f(\boldsymbol{\sigma}, \sigma_{Y_C}, \sigma_{Y_T}, \sigma_{Y_S}) = a(J_2^3 + bJ_3^2)^{1/3} + 2(\sigma_{Y_C} - \sigma_{Y_T})I_1 - 2\sigma_{Y_C}\sigma_{Y_T} \quad (12)$$

First, considering the yield point in uniaxial tension $\sigma_2 = \sigma_3 = 0$ and $\sigma_1 = \sigma'$ in Eq. (12), the following results are obtained:

$$I_1 = Tr(\sigma_{ij}) = \sigma' \quad (13)$$

$$J_2 = \frac{1}{2} s_{ij} s_{ij} = \frac{1}{3} \sigma'^2 \quad (14)$$

$$J_3 = \det(s_{ij}) = \frac{2}{27} \sigma'^3 \quad (15)$$

Then let

$$f(\sigma, \sigma_{Y_C}, \sigma_{Y_T}, \sigma_{Y_S}) = 0 \quad (16)$$

The relationship between a and b can then be written as

$$a = 6 \left(\frac{27}{4b + 27} \right)^{1/3} \quad (17)$$

Similarly, considering the pure shear yielding $\sigma_1 = -\sigma_2 = \sigma'$ and $\sigma_3 = 0$, in Eq.(12), the following results is obtained:

$$I_1 = 0 \quad (18)$$

$$J_2 = \frac{1}{2} s_{ij} s_{ij} = \frac{2}{3} \sigma'^2 \quad (19)$$

$$J_3 = \det(s_{ij}) = 0 \quad (20)$$

Then the parameter b can be obtained as:

$$b = \frac{1}{4} \left(\frac{(3\sigma_{Y_S})^6}{(\sigma_{Y_C} \sigma_{Y_T})^3} - 27 \right) \quad (21)$$

related uniquely to parameter a via Eq. 17.

APPENDIX 2: A note on the boundary conditions for the 45° off-axis compression test

For the 45° off-axis compression test it is concluded that modeling the orientation of the fibers directly would lead to a poor finite element discretization since it would require a significantly larger number of elements, or the use of tetrahedral elements that have (in general) worst performance than hexahedral ones. Instead, an equivalent response for the unit cells can be obtained by considering adequate boundary conditions that lead to the same state of stress. The stress tensor in the original coordinate system σ is rotated to σ' in the unit cell coordinate system by

$$\sigma'_{kl} = q_{ki} q_{lj} \sigma_{ij} \quad (22)$$

where $q_{ij} = \cos(x'_i, x_j)$.

Then the strain boundary can be calculate by

$$\varepsilon'_{ij} = S_{ijkl} \sigma'_{kl} \quad (23)$$

where S_{ijkl} is the transverse isotropic compliance matrix.

For the 45° off-axis compression, the boundary conditions are

$$\varepsilon'_{11} = \frac{(1 - \nu)}{2E_1} \sigma \quad (24)$$

$$\varepsilon'_{22} = \frac{1}{2} \left(\frac{1}{E_2} - \frac{\nu_{12}}{E_1} \right) \sigma \quad (25)$$

$$\varepsilon'_{33} = -\frac{1}{2} \left(\frac{\nu_{12}}{E_1} + \frac{\nu_{23}}{E_2} \right) \sigma \quad (26)$$

$$\varepsilon'_{12} = \frac{1}{4G_{12}} \sigma \quad (27)$$

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Figure 1: Effect of the parameter b on the yield surface of the matrix constitutive model in principal stress space with $\sigma_3 = 0$.

(a) Uniaxial tension and shear test.

(b) Uniaxial compression test.

Figure 2: Calibration of the polymeric matrix constitutive model for Epoxy 3501-6. Experimental results from Ref.[1].

Figure 3: Matrix constitutive model prediction for Epoxy 3501-6 under a combined load of compression and torsion. Experimental results from Ref.[1].

(a) Tension under different strain-rates

(b) Tension at different temperatures

(c) Compression under different strain-rates

(d) Compression at different temperatures

Figure 4: Calibration of the polymeric matrix constitutive model for the Epon 862 epoxy. Experimental results from Ref.[35].

Figure 5: Finite element mesh for SVE and RVE

Figure 6: Relationship between shear stress and equivalent plastic strain under transverse compression

Figure 7: Comparison of experiment and present model for transverse compression.

Figure 8: Relationship between shear stress and equivalent plastic strain under 45° off-axial compression

Figure 9: Comparison of experiment and present model for out-of-plane shear.(Strain rate: $1e-4/s$)

(a) Initiation of the kink band.

(b) Kink band formed at the peak load.

Figure 10: The equivalent plastic strain evolution during the kinking band formation.

Figure 11: The evolution of axial stress, shear stress, equivalent plastic strain during the kinking band formation.

Figure 12: The global average axial stress, shear stress, equivalent plastic strain during the kinking band formation.