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NUMERICAL MODELLING OF BEHAVIOUR OF CARBON NANOTUBE-REINFORCED COMPOSITES

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1 INTRODUCTION

Since their discovery by Lijima in 1991[1], carbon nanotubes (CNTs), are considered a new generation of reinforcement [2]. Their "nano" size structure makes them potentially free of defects, which provides them with excellent physical properties [3,4]. There are two main nanotube types: single wall nanotubes (SWNT) and multi wall nanotubes (MWNT). These last ones consist in several concentric walls, one inside the other.

In a composite, one the most important factors that condition their mechanical performance is the interfacial tension between matrix and reinforcement. In general, the loads in a composite structure are introduced to the matrix and then are transferred to the reinforcement through the interface [5]. Therefore, the interface can be defined as the region, surrounding the reinforcement, where this stress transfer takes place. The properties of the composite depend on the properties of this region and its ability to transfer the load efficiently.

This work proposes a new formulation to predict the mechanical properties and mechanical behaviour of nanotube-reinforced composites. The formulation is based on the mixing theory [6]. It obtains the behaviour of the composite from the mechanical performance of its constitutive materials: matrix, carbon-nanotube and the interface that bonds both of them.

2 DESCRIPTION OF CONSTITUTIVE MODEL

The theory presented in this work obtains the mechanical performance of the composite from the behaviour of the composite constituents, each one simulated with its own constitutive equation [7]. As it is written, the theory can be understood as a constitutive equation manager. This approach increases the versatility and simulation capability of the formulation.

The model assumes that the composite is the combination of three different materials: matrix, CNTs and interface zone [8]. The interface corresponds to the matrix surrounding the CNTs. It is considered an independent component, with its own constitutive law. The function of the interface material in the model is to define the capacity of the matrix to transfer the loads to the reinforcement.

Although the phenomenological performance of the composite completely justifies the definition of an interface material, its existence also justified by measurements performed on

CNTs reinforced composites. Differential Scanning Calorimetry (DSC) measurements, carried out in composites with semi-crystalline polymer as matrix material, show a linear increase of crystalline matrix as the nanotube volume fraction increases. This result suggests that each nanotube has a crystalline coating [9]. This phenomenon can be also seen in Scanning Electron Microscope (SEM) images such the ones shown in Figure 1. Such images revealed that the structures protruding from the fracture surface seemed to have larger diameters than the original MWCNTs used in the sample preparation [10].

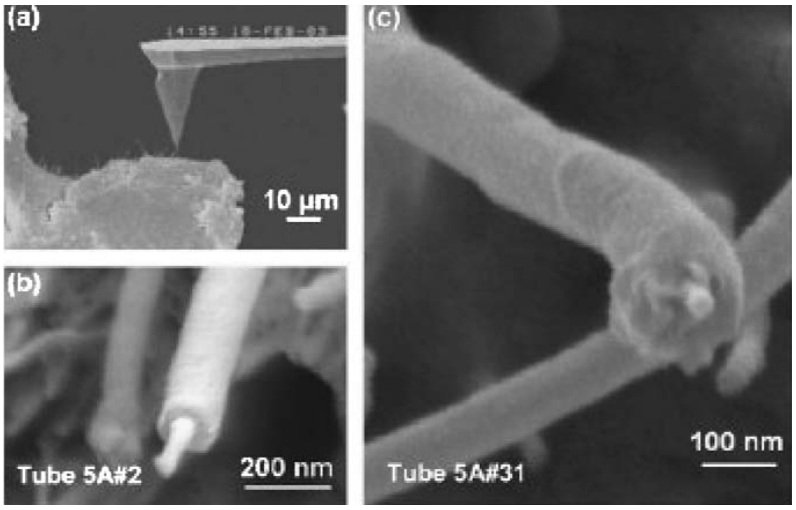

Figure 1: SEM image of nanomanipulation and fracture surface of composites [10].

A general description of the proposed procedure to simulate CNTs reinforced composites is shown in Figure 2. This figure shows that the composite is divided in several layers, each one containing nanotubes with a different orientation. All layers are coupled together using the parallel mixing theory. This division into layers allows taking into account the different orientations that may have the nanotubes in the composite. And, eventually, allows defining a composite with different materials in each layer (i.e. a foam core in a sandwich laminate).

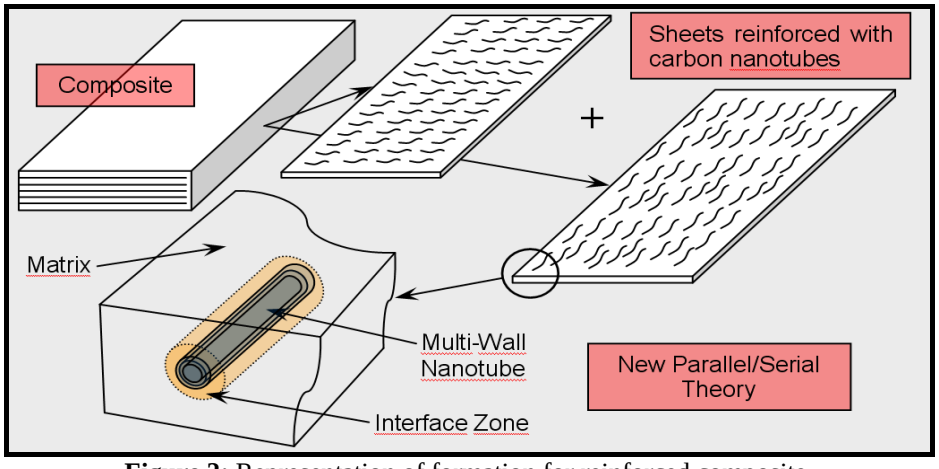

Figure 2: Representation of formation for reinforced composite.

Each layer is defined by the volume content of matrix, interface and carbon nanotubes. The mechanical performance of each layer is obtained with a new mixing theory formulation, which consists in combining the mechanical performance of the three co-existing materials.

First, the layer is split into matrix and a new material result of coupling the CNTs with the interface. The relation between the matrix and the CNTs-interface is established in terms of the parallel mixing theory; this is, they are assumed to have an iso-strain behaviour. On the other hand, CNTs and the interface zone are bonded together with a combination of parallel and serial mixing theories. The serial mixing theory states that all composite constituents have the same stresses.

The formulation used to characterize the CNTs-interface material is based in the short fibre model developed by Car [12]. Figure 3 shows the scheme used to obtain the performance of the CNTs-interface material. According to this model, the load transfer from the interface to the nanotube is produced at both the ends of the reinforcement, through shear stresses. At the centre of the reinforcement there is no load transfer and, therefore, shear stresses are null. A simplified model can be defined in which the CNT-interface performance is defined with a serial mixing theory at the ends of the reinforcement (iso-stress behaviour) and with a parallel mixing theory at the centre of it (iso-strain behaviour).

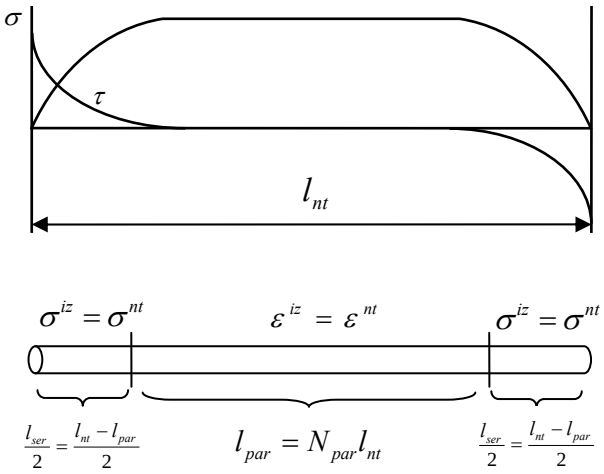

Figure 3: Different regions in the new material CNTs-interface.

A parallel factor named N^{par} is defined to differentiate the two regions. This parameter, multiplied by the nanotube length, provides the length of the nanotube-interface element with a parallel behaviour. The length with a serial performance is defined by the complementary factor.

3 FORMULATION OF CONSTITUTIVE MODEL

The Helmholtz free energy [13] of a material point subjected to small deformations can be described with the following thermodynamic formulation [14, 15]:

$$\Psi = \Psi\left(\boldsymbol{\varepsilon};\theta,\boldsymbol{\alpha}\right) \tag{1}$$

where $\boldsymbol{\varepsilon}$ is the deformation tensor, θ the temperature and $\boldsymbol{\alpha} = \{\boldsymbol{\varepsilon}^p; d; \boldsymbol{s}\}$ a set of inner variables, for example: $\boldsymbol{\varepsilon}^p$ is the plastic deformation, d damage inner variable and $\boldsymbol{s}$ any other material internal variables.

The model proposed to simulate the composite material consists on a combination of the different components of the composite, using the parallel and the serial mixing theories, as has been described in previous section. The expression of the Helmholtz free energy for the composite material may be written as:

$$\Psi = k_m \Psi_m + \left(k_{nt} + k_{iz}\right)\left[\underbrace{N^{par}\left(\bar{k}_{nt}\Psi_{nt} + \bar{k}_{iz}\Psi_{iz}\right)}_{\tilde{\Psi}^{par}_{ntiz}} + \underbrace{\left(1 - N^{par}\right)\left(\bar{k}_{nt}\Psi_{nt} + \bar{k}_{iz}\Psi_{iz}\right)}_{\tilde{\Psi}^{ser}_{ntiz}}\right] \tag{2}$$

where Ψ_m, Ψ_{nt} and Ψ_{iz} are the specific Helmholtz free energy for the matrix, the nanotube and the interface components, respectively; $\tilde{\Psi}^{par}_{ntiz}$ and $\tilde{\Psi}^{ser}_{ntiz}$ states parallel and serial Helmholtz free energy of the news CNTs-interface material, k_m, k_{nt} and k_{iz} are the volume fraction of each component, and N^{par} is a parallel factor and:

$$\bar{k}_{nt} = \frac{k_{nt}}{k_{nt} + k_{iz}} \qquad \bar{k}_{iz} = \frac{k_{iz}}{k_{nt} + k_{iz}} \tag{3}$$

are the volume fractions of the composite components. These must verify:

$$k_m + k_{nt} + k_{iz} = 1 \qquad \bar{k}_{nt} + \bar{k}_{iz} = 1 \tag{4}$$

The relation among the strain tensors of the different components is:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_m = \boldsymbol{\varepsilon}^{par}_{ntiz} = \boldsymbol{\varepsilon}^{ser}_{ntiz} \tag{5}$$

where $\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}_{\mathrm{m}}$ are the composite and matrix deformations, respectively; $\boldsymbol{\varepsilon}^{par}_{ntiz}$ is the deformation of a new material, result of the combination of nanotubes with the interface, that has a parallel behaviour; and $\boldsymbol{\varepsilon}^{ser}_{ntiz}$ is deformation of a nanotube-interface material that has a serial behaviour.

The tangent constitutive tensor of the composite material may be derived from Eq. (2):

$$\boldsymbol{C} = \frac{\partial^2 \boldsymbol{\Psi}}{\partial \boldsymbol{\varepsilon} \otimes \partial \boldsymbol{\varepsilon}} = k_m \frac{\partial^2 \boldsymbol{\Psi}_m}{\partial \boldsymbol{\varepsilon}_m \otimes \partial \boldsymbol{\varepsilon}_m} + \frac{\partial^2 \tilde{\boldsymbol{\Psi}}^{par}_{ntiz}}{\partial \boldsymbol{\varepsilon}^{par}_{ntiz} \otimes \partial \boldsymbol{\varepsilon}^{par}_{ntiz}} + \frac{\partial^2 \tilde{\boldsymbol{\Psi}}^{ser}_{ntiz}}{\partial \boldsymbol{\varepsilon}^{ser}_{ntiz} \otimes \partial \boldsymbol{\varepsilon}^{ser}_{ntiz}} \tag{6}$$

A parallel behaviour means that all composite constituents have the same value for this strain component and therefore:

$$\varepsilon^{par}_{ntiz} = \varepsilon_{nt} = \varepsilon_{iz} \quad \Rightarrow \quad \frac{\partial^2 \tilde{\boldsymbol{\Psi}}^{par}_{ntiz}}{\partial \boldsymbol{\varepsilon}^{par}_{ntiz} \otimes \partial \boldsymbol{\varepsilon}^{par}_{ntiz}} = N^{par}\left[\bar{k}_{nt}\boldsymbol{C}_{nt} + \bar{k}_{iz}\boldsymbol{C}_{iz}\right] = N^{par}\boldsymbol{C}^{par}_{ntiz} \tag{7}$$

A serial behaviour means that all composite constituents have the same value for this stress

component and therefore:

$$\sigma_{ntiz}^{ser} = \sigma_{nt} = \sigma_{iz} \quad \Rightarrow \quad \varepsilon_{nt} = \mathbf{C}_{nt}^{-1} : \mathbf{C}_{ntiz}^{ser} : \varepsilon_{ntiz}^{ser} \quad ; \quad \varepsilon_{iz} = \mathbf{C}_{iz}^{-1} : \mathbf{C}_{ntiz}^{ser} : \varepsilon_{ntiz}^{ser} \tag{8}$$

$$\frac{\partial^2 \widetilde{\Psi}_{ntiz}^{ser}}{\partial \varepsilon_{ntiz}^{ser} \otimes \partial \varepsilon_{ntiz}^{ser}} = \left(1 - N^{par}\right)\left[\bar{k}_{nt}\mathbf{C}_{nt}^{-1} + \bar{k}_{iz}\mathbf{C}_{iz}^{-1}\right]^{-1} = \left(1 - N^{par}\right)\mathbf{C}_{ntiz}^{ser} \tag{9}$$

Replacing Eq. (7) and Eq (9) in Eq (6) it is possible to obtain a simplified expression of the tangent constitutive tensor:

$$\mathbf{C} = k_m \mathbf{C}_m + \left(k_{nt} + k_{iz}\right)\left[N^{par}\mathbf{C}_{ntiz}^{par} + \left(1 - N^{par}\right)\mathbf{C}_{ntiz}^{ser}\right] \tag{10}$$

3.1 Definition of the parallel factor N^{par}

The parallel factor is defined as:

$$N^{par} := \frac{l_{par}}{l_{nt}} \qquad , \quad 0 \le N^{par} \le 1 \tag{11}$$

where l_{nt} is the length of the nanotube and l_{par} is function of geometry and mechanical properties of the nanotube and the interface.

Based on the short fiber formulation defined in [5], the equation of tension distribution in a reinforcement considering perfect bond with the matrix is:

$$\sigma_{nt}(x) = E_{nt}\left[1 - \frac{\cosh\left(\beta\left(l_{nt} - 2x\right)\right)}{\cosh\left(\beta l_{nt}\right)}\right]\varepsilon_m \qquad \beta = \sqrt{\frac{2G_{iz}}{E_{nt}\, d_{nt}^2 \ln\left(1 + b/r_{nt}\right)}} \tag{12}$$

where x represents the longitudinal positions in the reinforcement, the subscript "nt" and "iz" refers to the properties of nanotube and interface zone, respectively, and b is the thickness of interface.

Considering that $l_{par} = l_{nt} - 2x$ and finding the positions "x" which verifies that the effective modulus obtained of integrate the tension distributions is equal to:

$$\bar{E}_{nt} = \frac{l_{par}}{l_{nt}} E_{ntiz}^{par} + \left(1 - \frac{l_{par}}{l_{nt}}\right) E_{ntiz}^{ser} \tag{13}$$

The parallel longitudinal can be written as:

$$l_{par} = \frac{1}{\beta}\cosh^{-1}\left[\tfrac{1}{3}\cosh\left(\beta l_{nt}\right)\right] \tag{14}$$

4 CONSTITUTIVE MODEL FOR A SINGLE MATERIAL

All models used in the formulation depart from Eq. (1). Therefore it is possible to use any constitutive law to describe the behaviour of the constituent materials defined: matrix, interface and CNTs. However, for the sake of clarity, in the following are defined three

specific models that will be used afterwards.

4.1 Constitutive model for matrix material

Matrix material is defined with an elastoplastic law. Therefore, the specific Helmholtz free energy for this material, considering uncoupled elasticity is:

$$\Psi\left(\boldsymbol{\varepsilon}^e, \boldsymbol{p}\right)=\Psi^e\left(\boldsymbol{\varepsilon}^e\right)+\Psi^p\left(\boldsymbol{p}\right)=\frac{1}{2}\boldsymbol{\varepsilon}^e:\boldsymbol{C}:\boldsymbol{\varepsilon}^e+\Psi^p\left(\boldsymbol{p}\right) \tag{15}$$

where the total deformation of the material tensor is split into its elastic, $\boldsymbol{\varepsilon}^e$ and plastic, $\boldsymbol{\varepsilon}^p$ parts. This is:

$$\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}^e+\boldsymbol{\varepsilon}^p \tag{16}$$

The local form of the Clausius-Duhem inequality for this material can be expressed as:

$$\Xi=\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}-\eta\dot{\theta}-\dot{\Psi}-\frac{1}{\dot{\theta}}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}}\geq 0 \tag{17}$$

$$\boldsymbol{\sigma}:\left(\dot{\boldsymbol{\varepsilon}}^e+\dot{\boldsymbol{\varepsilon}}^p\right)-\eta\dot{\theta}-\left[\frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}^e}:\dot{\boldsymbol{\varepsilon}}^e+\frac{\partial\Psi^p}{\partial\boldsymbol{p}}.\dot{\boldsymbol{p}}+\frac{\partial\Psi}{\partial\theta}:\dot{\theta}\right]-\frac{1}{\dot{\theta}}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}}\geq 0 \tag{18}$$

$$\left(\boldsymbol{\sigma}-\frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}^e}\right):\dot{\boldsymbol{\varepsilon}}^e-\left(\eta+\frac{\partial\Psi}{\partial\boldsymbol{\theta}}\right)\dot{\theta}+\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}^p-\frac{\partial\Psi^p}{\partial\boldsymbol{p}}.\dot{\boldsymbol{p}}-\frac{1}{\dot{\theta}}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}}\geq 0 \tag{19}$$

where $\boldsymbol{\sigma}$ is the stress tensor, η the entropy, and $\boldsymbol{q}$ the vector field of heat flow.

To ensure compliance with the second thermodynamic law it must be defined:

$$\boldsymbol{\sigma}:=\frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}^e}\qquad\eta:=-\frac{\partial\Psi}{\partial\boldsymbol{\theta}}\qquad\boldsymbol{P}:=-\frac{\partial\Psi^p}{\partial\boldsymbol{p}} \tag{20}$$

where $\boldsymbol{P}$ is the thermodynamic tensor associated with the internal variable tensor $\boldsymbol{p}$.

Finally, the mechanical dissipation for a material point is:

$$\Xi_m=\Xi_p=\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}^p+\boldsymbol{P}.\dot{\boldsymbol{p}}\geq 0 \tag{21}$$

4.2 Constitutive model for interface material

The interface region will be simulated with a damage material. In this case, the expression of the Helmholtz free energy is:

$$\Psi\left(\boldsymbol{\varepsilon}^e,d\right)=\Psi^e\left(\boldsymbol{\varepsilon}^e,d\right)=\left(1-d\right)\Psi_o^e\left(\boldsymbol{\varepsilon}^e\right)=\left(1-d\right)\frac{1}{2}\boldsymbol{\varepsilon}^e:\boldsymbol{C}:\boldsymbol{\varepsilon}^e \tag{22}$$

The local form of the Clausius-Duhem inequality for this material can be expressed as:

$$\Xi = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \eta\dot{\theta} - \dot{\Psi} - \frac{1}{\theta}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}} \geq 0 \tag{23}$$

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \eta\dot{\theta} - \left[\frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \frac{\partial\Psi^e}{\partial d} : \dot{d}\right] - \frac{1}{\theta}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}} \geq 0 \tag{24}$$

$$\left(\boldsymbol{\sigma} - \frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} - \left(\eta + \frac{\partial\Psi}{\partial\boldsymbol{\theta}}\right)\dot{\theta} - \frac{\partial\Psi^e}{\partial d}\dot{d} - \frac{1}{\theta}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}} \geq 0 \tag{25}$$

To ensure compliance with the second thermodynamic law it must be defined:

$$\boldsymbol{\sigma} := \frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}} \qquad \eta := -\frac{\partial\Psi}{\partial\boldsymbol{\theta}} \qquad D := \frac{\partial\Psi^e}{\partial d} \tag{26}$$

where D is the thermodynamic scalar associated with the internal scalar variable d.

And, the mechanical dissipation for a material point is:

$$\Xi_m = \Xi_d = D\,\dot{d} \geq 0 \tag{27}$$

4.3 Constitutive model for nanotubes

Nanotubes are considered elastic, therefore the Helmholtz free energy is:

$$\Psi\left(\boldsymbol{\varepsilon}^e\right) = \Psi^e\left(\boldsymbol{\varepsilon}^e\right) = \frac{1}{2}\boldsymbol{\varepsilon}^e : \boldsymbol{C} : \boldsymbol{\varepsilon}^e \tag{28}$$

And the local form of the Clausius-Duhem inequality can be expressed as:

$$\Xi = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \eta\dot{\theta} - \dot{\Psi} - \frac{1}{\theta}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}} \geq 0 \tag{29}$$

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \eta\dot{\theta} - \frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\theta}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}} \geq 0 \tag{30}$$

$$\left(\boldsymbol{\sigma} - \frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} - \left(\eta + \frac{\partial\Psi}{\partial\boldsymbol{\theta}}\right)\dot{\theta} - \frac{1}{\theta}\boldsymbol{q}.\frac{\partial\theta}{\partial\boldsymbol{x}} \geq 0 \tag{31}$$

To ensure compliance with the second thermodynamic, $\boldsymbol{\sigma}$ and η are defined as:

$$\boldsymbol{\sigma} := \frac{\partial\Psi^e}{\partial\boldsymbol{\varepsilon}} \qquad \eta := -\frac{\partial\Psi}{\partial\boldsymbol{\theta}} \tag{32}$$

5 NON-LINEARITY OF THE PROPOSED MODEL

In the proposed model, the composite performance is obtained from the mechanical

performance of its constituent materials. Therefore, if a constituent (i.e. the interface) is simulated with a non-linear law and the strains applied to it lead to a non-linear state, the whole composite will become non-linear.

However, beyond the non-linear performance provided by the constitutive law used to simulate each constituent, the load transfer capacity in the interface region is also affected if the interface is damaged. This effect must be included in the formulation.

According to Figure 3, the load transfer from the interface to the reinforcement is produced at the ends of the reinforcement. Therefore, initial interface damage will occur at the ends of the reinforcement, where there is larger stress concentrations, reducing the effective length of the nanotube. In other words, the parallel length of the nanotube is reduced based on the damage of the interface material. The new parallel length can be computed as:

$$l_{par} = l^{o}_{par}\left(1 - d\right) \tag{33}$$

where l^{o}_{par} is the initial length of the nanotube working in parallel and d is the interface damage.

The addition of this new length, depending on the non-linear performance of the interface material, provides a non-linear response of the composite (see equation 10), even when matrix and the carbon nantotube reinforcement are in their linear range.

6 NUMERICAL IMPLEMENTATION

The proposed model has been implemented in PLCd [16] a finite element code that works with 3D solid geometries. The algorithm developed has been implemented as a new composite equation manager in the FEM code [17]. PLCd has already implemented the constitutive laws that will be used to predict the performance of the composite components (elastoplastic, damage and elastic). The formulation proposed has been written so that the constitutive laws of the constituents are seen as “black boxes”, that will compute the material stresses for a given strain.

7 RESULTS

The elastic performance of the model presented in this work has been already validated, proving that it provides good results. The validation performed consisted in comparing the prediction made by the model, of different elastic parameters (Young modulus and shear modulus) for several CNTs reinforced polymers, with the data existing in literature for these same composites. A detailed description of this comparison is reported in [18].

The non-linear behaviour of the numerical model is validated hereafter, comparing the results provided by the model with experimental data obtained from M-Rect project (see acknowledgements). The matrix used is PEEK; Young’s modulus and shear modulus were measured: *3.9* [GPa] and *1.9* [GPa], respectively. The composite has a 3% weight of MWNT (Baytubes® C 70 P). However, measurements with X-ray showed an apparent 5% weight, this means that the nanotubes have a higher apparent diameter than the pristine one. Therefore, the b/r_{nt} is calculated assuming that 2% weight extra is the coating polymer around the nanotubes. The Young’s modulus of the interface zone was estimated using the procedure proposed by Coleman et al. [19]. The data used for the estimation of the modulus is the one

defined by Díez-Pascual et al. [20,21], obtaining a final value of *5* [GPa].

The properties used in the model for the CNTs were obtained considering them as solid cylinders with the same external diameter. To do so it is necessary to reduce their elastic modulus in order to have an equivalent material. The values used as effective Young's modulus and effective shear modulus are $E_{nt} = 4.t/d_{nt}.E_g$ and $G_{nt} = [1- (1-2.t/d_{nt})4].G_g$, respectively [22]. The value of the properties used to get the effective properties were $E_g = 1$ [TPa], $G_g = 0.44$ [TPa] (the Young' modulus and the shear modulus of graphite sheet), its thickness was considered to be $t = 0.34$ [nm].

Table 1: Project data for implementation of numerical model

Type	d_{nt} [nm]	l_{nt} [μm]	l_{nt}/d_{nt}	b/r_{nt}	E_{nt} [GPa]	G_{nt} [GPa]	N^{par}
MWNT	13	1	44	0.3	105	85	0.97

The composite is defined with different layers in order to assign different CNTs orientations. Each layer contains a volume fraction of CNTs with a specific orientation. The constitutive model used for PEEK material is an elasto-plastic model, for the interface zone is an explicit scalar elasto-damage, and for the nanotube is an elastic model. The parameters that control the no-lineal behaviour on the interface zone were calibrated with the experimental data of project.

Figure 4 shows the mechanical performance of the model when the composite is loaded with a shear load. The simulation has been performed applying a controlled displacement load. The figure shows the strain-stress graph obtained for the composite (red line) and these same graphs for the interface material of the different layers in which the composite is divided. These last graphs show that the maximum stress in all interface materials do not exceed the defined threshold value of 15 MPa.

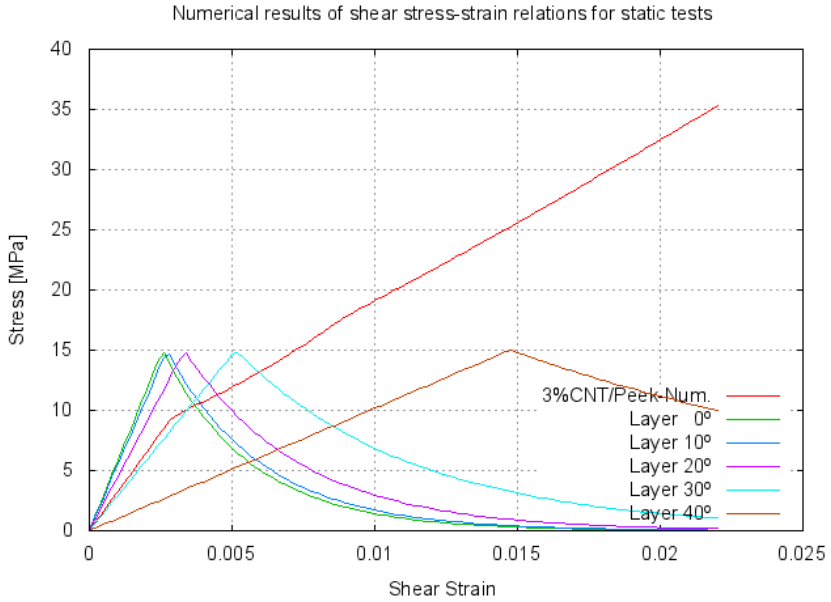

Figure 4: Numerical behaviour for the model proposed in shear load.

Figure 4 shows that once the first interface material reaches its threshold value, the composite modifies its mechanical performance reducing its stiffness. This occurs because the interface itself reduces its stiffness due to damage, but also because damage in the interface reduces the parallel fraction of the CNTs-interface material (equation 33); hence, the participation of the CNTs in the composite is less significant. When all interfaces (in all layers) are completely damaged, the CNTs contribution to the composite stiffness and strength becomes null and the composite behavior is such as having just matrix material with some voids in it.

The mechanical performance just described is better shown in figure 5, in which is represented the behaviour of the numerical model calibrated in a load-unload test. The PEEK curve shows the plastic behaviour of the numerical model. When it is unloaded, the composite curve shows not only plastic deformation, but also a variation in its stiffness produced by interface damage.

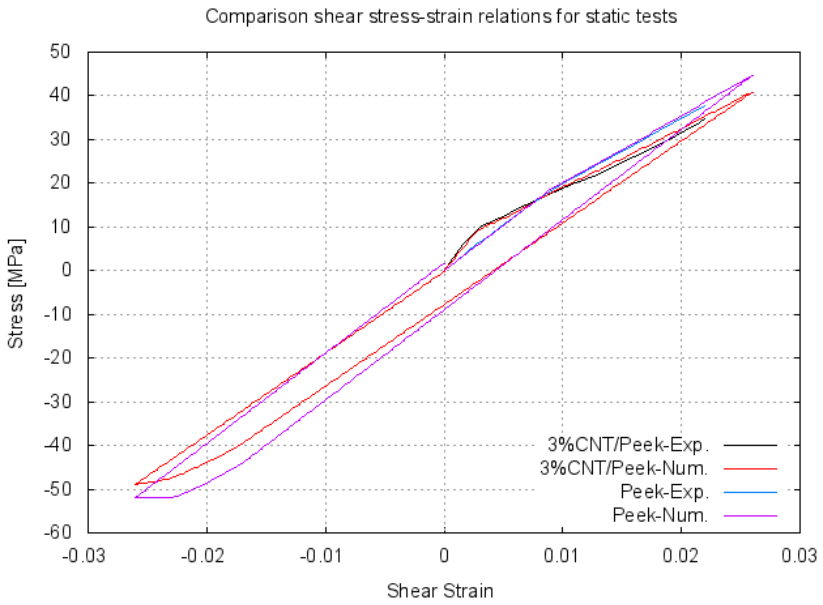

Figure 5: Comparison of numerical and experimental results, load and unload curves.

8 CONCLUSIONS

- A new formulation has been presented, which is based on the mixing theory, developed to predict the mechanical performance of composites reinforced with carbon nanotubes. The model presented has the advantage of relating the CNTs and the matrix with an interface material. This makes possible to simulate the composite material by using constitutive laws defined for each composite component and the interaction between them.
- The model was calibrate and compared with experimental data. The elastic properties predicted by the model, as well as the nonlinear behaviour estimated are in good agreement with experimental values.

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