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Effect of transverse strains and angular distortions on the nanoscale elastic behavior of platelet nanocomposites

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ABSTRACT

In order to correctly predict the macroscale elastic behavior of nanocomposite macroscale structures, an accurate nanoscale model must be available for subsequent homogenization. In this work, we demonstrate that the accuracy of that nanoscale model greatly depends on the consideration of transverse strains and angular distortions, which are not frequently taken into account, but have a significant influence on the cohesive mechanisms at the nanofiller-matrix interface. We use a nanoscale cohesive model to qualitatively and quantitatively analyze the effect of transverse shear and angular distortion on the interfacial stress transfer mechanisms. While the effect of the transverse strain is less significant, results show that angular distortion greatly affects the interfacial damage pattern. It appears to shift the interfacial shear stress distribution to one of the interface ends, which consequently also modifies the interfacial longitudinal stress distribution and its mean value, resulting in reduced nanocomposite stiffnesses. The effect should be taken into account as shear and transverse strains may be present at the macroscale if, for instance, nanofiller misalignment or stress concentrators exist. We also provide design maps representing damage onset for different 2D multiaxial strain states in graphene-epoxy nanocomposites, so that the strain state limit can be inferred for the given nanocomposite properties. A substantial reduction in the allowable strains can be observed.

1. Introduction

Due to the impressive properties of carbon and other 1D and 2D nanoparticles, considerable enhancements are to be expected when small amounts of these materials are added to different matrices [1-4]. Interesting improvements in mechanical properties have been achieved for nanofiller weight fractions as small as 0.5% [5-8]. In order to allow for the design of complex structures and geometries based on nanocomposites, constitutive equations must be available that take into account these effects, along with those appearing at the meso or macroscale as filler misalignment or suboptimal filler dispersion, so that they can be introduced in the analysis codes used by mechanical designers.

Different material models have been developed that predict nanocomposite stiffness, with some based on molecular dynamics [9-11], and others using inclusion methods such as Eshelby's tensor [12] or multiscale modelling [13,14] At the nanoscale level, multiple papers have pointed to debonding as the main failure mechanism [15,16]. Due to its fundamental influence on nanocomposite mechanical properties [17-20], constitutive models must consider the interfacial stress transfer mechanisms at the filler/matrix interface. Firstly, given that the nanofiller-matrix interface has a finite stiffness, the nanofiller strain will be smaller than that theoretically obtainable with a perfectly rigid interface. Secondly, since interfacial strength is finite, excessive interfacial separation may lead to interfacial damage. Both of these issues can lead to a decrease in interfacial stress transfer capacity and the nanocomposite properties will diverge from those obtainable if the interface had infinite stiffness and strength. This can result in mechanical properties that are frequently below those that are theoretically achievable [5,21] .

Cylindrical carbon nanofiller-epoxy interfaces are studied in Ramdoum et al. [17] by means of a cohesive model to model the interfacial stiffness and damage. The stress transfer mechanisms at work in the elastic, debondable filler-matrix are also well explained in platelets composites by Heidarhaei et al. [18], Gong and Guo [19,20] or Ang et al. [22]. Those models demonstrate that when a strain is applied to the matrix parallel to the nanoparticle longitudinal axis, the nanoparticle is also strained by the shear created at the nanoparticle-matrix interfaces due to the difference in stiffness. Rahman et al. [23] studied the interfacial properties and the effect of nanofiller dispersion using

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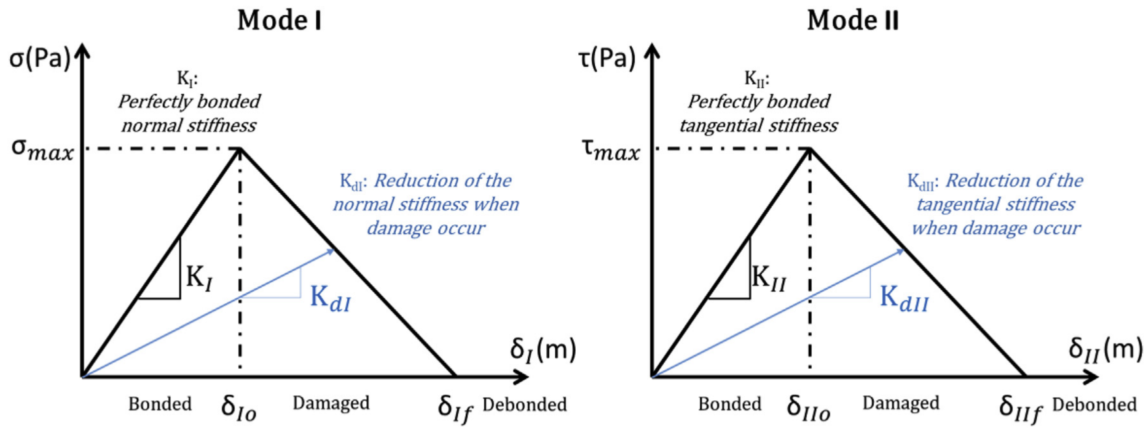

Fig. 1. Cohesive Zone Models (CZM) associated to frature mode I (left) and fracture mode II (right).

molecular dynamics. Similarly, Chen and Yan [24] proposed an analytical fiber pull-out model based on a shear lag model with cohesive interfaces.

The above analytical considerations have all been experimentally validated. Jiang et al. [25] and Lee et al. [26], measured the strain field in a single graphene layer on the surface of an epoxy matrix; while the matrix was gradually strained they observed certain strain-dependent Raman band shifts. Cui et al. [27] also used Raman spectroscopy to measure strain in carbon nanotubes to infer the interfacial characteristics. Experimental results have a close correlation with the theoretical predictions for interfacial shear strengths of about 0.5 MPa and fracture energies of about 0.08 N/m.

However, all the aforementioned models and experiments are based on uniaxial strain states. This assumption, which can be experimentally reproduced and modelled at the nanoscale, has led to many useful and interesting results that have provided a better understanding of nanoscale mechanisms. However, at the macroscale, nanoparticles will be subjected to a multiaxial strain state if, for instance, they are not perfectly aligned with any of the principal strain fields or are close to stress concentrators. As shear and transverse strains may not be negligible in those situations, correct constitutive models should consider them at the nanoscale; they may have an influence on the interfacial mechanisms and consequently on the nanocomposite properties.

Few cohesive models have been found that are able to analyze the interfacial mechanisms for multiaxial strain states [28,29]. use an inverse analysis for their study and do not, therefore, focus on the interfacial stress state. Belabed et al. [30] introduce shear and normal deformation in functionally graded materials. Experimentally, the problem is even more complex due to the difficulty of isolating and applying multiaxial strains to a single particle which, additionally, must not be located on a matrix-free surface. This requirement also poses an important problem for the Raman measurement. At the macroscale level, Lee et al. [31] have studied biaxial behavior in a polymer-steel interface by means of a cohesive model. Data was obtained using a three point bending test. However, the results cannot be extrapolated at the nanoscale due to the reinforcement stiffness and aspect ratio difference.

In this work, we present a nanoscale cohesive model for platelet nanocomposites that considers a 2D multiaxial strain state, so that the influences of angular distortions and transverse strains can be studied. The goal is to provide the scientific community with design tools that can be useful to determine the needed nanocomposite properties for a given strain state.

In section 2 we describe the model developed. In section 3, we present a parametric study and qualitatively and quantitatively explain the effect of shear and transversal strains taking a graphene-epoxy nanocomposite as an example. In section 4, we provide some maps that can be useful to determine the feasibility of certain nanocomposite properties for a given strain state. Finally, the conclusions are presented in section 5.

2. Model description

Traditional cohesive models were used as the basis (1) [19,32,33]:

$$\sigma_x = f\,(\varepsilon_C,\ l_F,\ t_F,\ \upsilon_F,\ E_F,\ G_F,\ E_M,\ G_M,\ k_{II},\ \tau_a,\ G) \tag{1}$$

where σ_x is the longitudinal stress along the nanofiller length for a given uniaxial applied strain ε_C at the nanocomposite, l_F the nanofiller length, t_F the nanofiller thickness, υ_F the nanofiller volumetric fraction, E_F, E_M, G_F and G_M the nanofiller, matrix, Young's modulus and shear modulus, respectively; k_{II} the in-plane interfacial stiffness,τ_a the interfacial shear strength and G the interfacial fracture energy. We have introduced an applied angular distortion γ_{xy} and an applied transverse strain ε_y. These additional strains will produce additional shear stress at the interface, as well as a transverse stress σ_y, with the corresponding Poisson effect on the longitudinal axis. For the calculation of the transverse stress state, additional interfacial parameters must be considered: transverse interfacial stiffness k_I and transverse strength σ_a. The resulting model is described in eq. (2).

$$[\sigma_x,\ \sigma_y,\ \tau_{xy}] = f\,(\varepsilon_x,\ \varepsilon_y,\ \gamma_{xy},\ l_F,\ t_F,\ \upsilon_F,\ E_F,\ G_F,\ E_M,\ G_M,\ k_{II},\ \tau_a,\ k_I,\ \sigma_a,\ G) \tag{2}$$

For both in-plane and transversal directions, we use a bilinear interfacial stress-interfacial separation curve. Fig. 1 shows the bilinear constitutive laws for each fracture mode. K is the interface stiffness, δ is the actual matrix-nanofiller separation, δ_0 is the separation at the onset of interfacial damage, δ_f the separation needed to fully debond the filler-matrix interface, τ and σ the stresses appearing at the interface and G_c the area under the lines, which corresponds to the interfacial fracture energy. For any of the fracture modes taken individually, eqs. (3)–(6) apply.

$$\delta_{I0} = \frac{\sigma_{max}}{K_I} \quad \delta_{II0} = \frac{\tau_{max}}{K_{II}} \tag{3}$$

$$\delta_{If} = \frac{2{*}G_i}{\tau_{max}} \quad \delta_{IIf} = \frac{2{*}G_i}{\sigma_{max}} \tag{4}$$

$$Damage = \left(\frac{\delta_i - \delta_{i0}}{\delta_i}\right)\left(\frac{\delta_{if}}{\delta_{if} - \delta_{i0}}\right) \tag{5}$$

$$K_{i\ NEW} = K_i(1 - Damage) \tag{6}$$

As both in-plane and transverse interfacial separations may simultaneously exist, we use a fracture mode I and fracture mode II mixed-mode debonding method as suggested by Ref. [32,33]. This implies the use of eq. (9) for defining a unique, equivalent interfacial damage from two interfacial displacements [34], being δ_{mi} the mixed-