THE EFFECT OF CARBON NANOTUBES ON STRESS REDISTRIBUTION AROUND THE FIBRE BREAK

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Abstract

This work is a numerical study to evaluate the influence of carbon nanotubes (CNTs) on the stress build-up in and around a broken fibre in a single carbon fibre/epoxy composite. The study is performed with the help of a two-scale 3D finite element model based on the embedded region technique. The advantage of this model is that microscopic fibres and nanotubes are simulated together and with their actual dimensions. The studied modifications on the fibre surface are CNT growth with aligned or randomly oriented morphologies and fibre sizing with different CNT concentrations and orientations. The predictions show that the stress build-up in the broken fibre is not significantly affected by grown CNTs. The most significant effect is found for the densest CNT-reinforced sizing in which CNTs are aligned in the fibre direction. The layer of the aligned CNTs restrains the crack opening displacement by 15%. The ineffective length of the coated fibre decreased by 28%, thus the stress in the broken fibre returned faster to its nominal value.

1. Introduction

Failure of fibre-reinforced composites is a topic of a great interest. Many efforts are devoted to the understanding of failure mechanisms and developing strategies to control them [1-4]. Nowadays, high-performing nanoscale reinforcements such as carbon nanotubes (CNTs) are often added to structural composites to improve their toughness and/or to add functionalities [5-7]. CNTs influence failure at the submicron-level by introducing additional energy dissipating mechanisms like crack bridging, CNT pull-out and crack deflection [8].

The longitudinal failure of a composite is accompanied by fibre breaking. When a fibre breaks, in the proximity to the break it loses its capacity to carry the load. Instead the surrounding matrix and neighbouring fibres take the arisen stress on themselves, which increases the chance of their failure [2]. If the stress concentration around the break can be redistributed and partially suppressed, the strength of the composite can be increased. This concept is commonly applied in hybrid composites (containing two fibre types) [9]. Composites with the CNT-modified fibre-matrix interface are a

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special case of hybrid materials where the diameter of two fibre types (CNTs and the fibres themselves) differs by almost three orders of magnitude.

Recent modelling studies showed that CNTs can drastically affect stress distribution in the composite [10-12]. Depending on the morphology of CNT assemblies the stress can be magnified or suppressed [10]. This was demonstrated for unidirectional composites loaded in the transverse direction. In the present work we investigate the effect of CNTs on the stress distribution around the fibre break under longitudinal loading.

2. Modelling approach

The current study is performed using a 3D finite element (FE) model containing a single microscopic carbon fibre in an epoxy matrix. Six modifications near the fibre-matrix interface are considered as depicted in Fig. 1. They include CNTs which are grown on the fibre ("forest") with a different degree of the CNT alignment ("aligned" and "curly" CNTs) and CNTs which are deposited on the fibre as sizing or coating. Some of these configurations (C1-C4), nowadays, are fabricated in nano-engineered composites. In addition to those, sizing with CNTs aligned along the fibre (C5-C6) is also studied here as it may be beneficial in the case of the longitudinal loading.

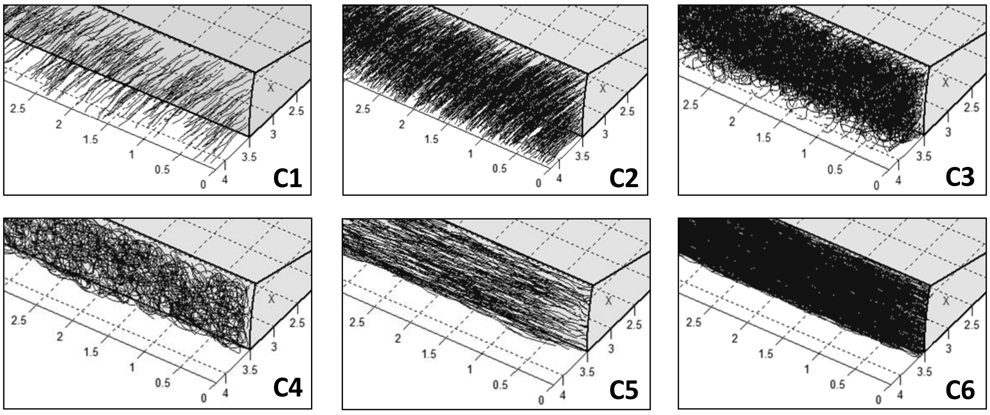

Figure 1. A sector of the fibre and modelled CNT configurations: **C1** – aligned forest with density of 90 CNTs/µm^2, **C2** – aligned forest with density of 450 CNTs/µm^2, **C3** – "curly" forest with density of 450 CNTs/µm^2, **C4** – randomly oriented CNTs in the sizing with density of 630 CNTs/µm^3, **C5** – aligned CNTs along the fibre in the sizing with density of 630 CNTs/µm^3, **C6** – CNTs aligned along the fibre with density of 3200 CNTs/µm^3.

2.1. Generation of CNTs configurations

Six CNT configurations (Fig. 1) were generated in MATLAB using the algorithm described in detail in [11]. If geometrical dimensions of CNTs (length and waviness), their concentration and positioning to the fibre (forest or sizing) are defined, the program simulates a CNT configuration by creating CNTs independently one by one. For each CNT it randomly draws six points which are approximated with a 3D spline. The latter is considered as a CNT central axis. For configurations C4-C6 sizing thickness was taken equal to 0.2 µm.

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2.2. Finite element model

For the analysis of the stress distribution around a fibre break, a two-scale FE model was developed and implemented in ABAQUS. A single carbon fibre with the diameter of 7 µm was embedded in an epoxy matrix. For the sake of simplicity, representative volume element (RVE) was defined in the cylindrical coordinate system and had the geometry shown in Fig. 2. The RVE radius was taken large enough to avoid influence of the free surface and was equal to 64 µm. The RVE length was 200 µm, which is the minimal ineffective length of a broken carbon fibre. This value was obtained from the analytical solutions of the shear-lag model [13]. Due to a large size of the model, the axial symmetry of the cylindrical RVE was exploited. The RVE was reduced to a sector of 15°.

The CNT configurations generated in MATLAB (Fig. 1) were imported into the ABAQUS model using a Python script. CNTs were modelled as wavy cylindrical objects of 700 nm long and with diameter of 9 nm. They were placed along the length of 5 µm starting at the fibre break plane (Fig. 2, *right*). Due to a large size of the obtained model and, consequently, long computational time, the rest of the matrix with CNT modification (195 µm in length) was replaced with a homogeneous layer. The layer received homogenised elastic properties of the particular CNT configuration embedded in the epoxy matrix, which were calculated using the Mori-Tanaka approach [14]. Such a simplification was found to be acceptable as the stress-concentration decayed sufficiently fast as a function of the distance from the crack plane. Material properties used as input data to the model are summarised in Table 1.

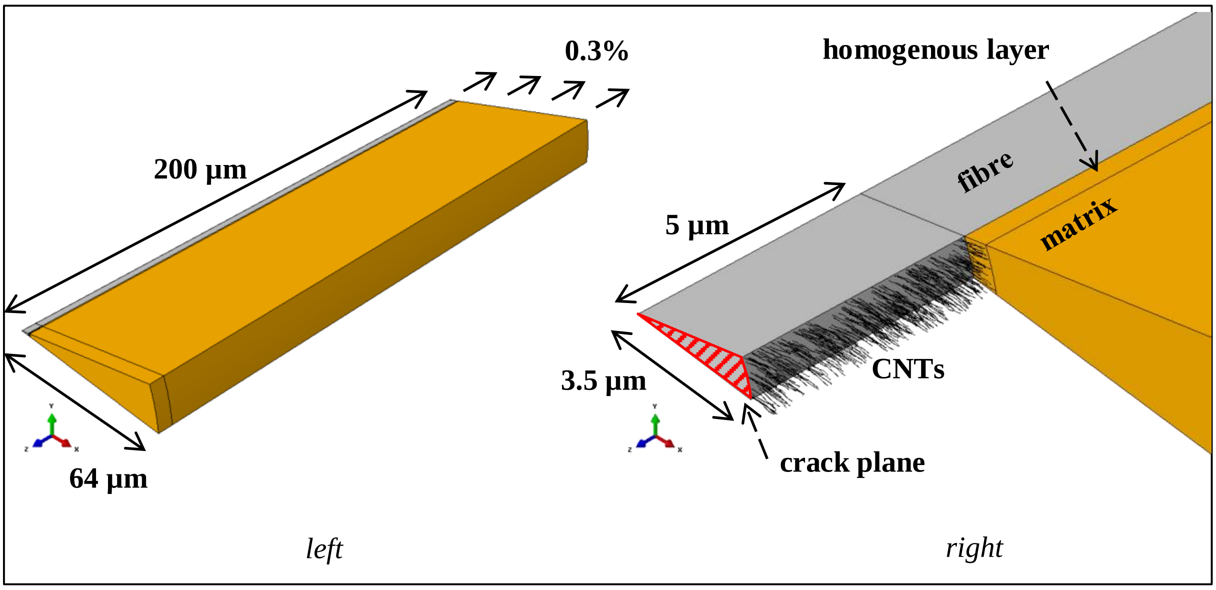

Figure 2. Representative volume element: its dimensions (*left*), a zoom-in view at the crack plane (*right*). A part of the matrix material was cut out to show CNTs (configuration C1).

The RVE was loaded under the axial tension. The average strain in the axial direction was set to 0.3%. On the opposite side, axial symmetry boundary conditions in the cylindrical coordinate system were introduced on the matrix. The plane of the fibre was left free of tractions mimicking the fibre break (Fig. 2, *right*). Angular symmetry boundary conditions in the cylindrical coordinate system were introduced at the side surfaces of the sector.

The current 3D FE model is based on the embedded regions technique [10-12]. This technique helps to overcome the challenge related to the simultaneous modelling of the microscopic fibre and nanotubes,

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the objects which have a significant difference in dimensions. CNTs and fibre/matrix were meshed independently. Two meshes were linked such that a given CNT node was constrained by equations of equality of its interpolated displacements with the displacements of nodes of the closest matrix element [11]. In this way every CNT limited the displacement of the matrix elements and introduced its stiffness to the model.

In the previous work Romanov et al. [10] revealed that the results obtained with the embedded regions technique were sensitive to the ratio of sizes of the matrix and CNT elements. The authors recommended keeping the ratio between the interface elements in the matrix and the total number of CNTs in the model at least equal to 5:1. To overcome the mesh sensitivity, in this work mesh size of the matrix region was taken as a function of the CNT number. Thus, the ratio of 5:1 was fulfilled in the densest configuration C6. Then the mesh size was fixed in all the studied cases (C0-C5). The elements ratio was proportionally higher in the other configurations. The smallest matrix element size was equal to 20 nm.

Table 1. Material properties used in the model.

Type	Engineering constants
Epoxy matrix	*Isotropic material*: E = 3 GPa, ν = 0.4.
Carbon fibre	*Transversely isotropic material*: E_1 = 10.3 GPa, E_3 = 276 GPa, G_{12} = 3.8 GPa, G_{23} = 27.9 GPa, ν_{12} = 0.355, where “3” is the fibre direction.
CNTs*	*Isotropic material*: E = 475.3 GPa, ν = 0.4.

*A case study was also performed on transversally isotropic CNTs with the properties: E_1 = 10.3 GPa, E_3 = 475.3 GPa, G_{12} = 3.8 GPa, G_{23} = 27.9 GPa, ν_{12} = 0.355. For the configuration C3, it was shown that the maximum error of the crack opening was about 3%. At the same time, the assumption of the CNTs isotropy significantly helped to reduce computational time (by a factor of 9 for the studied configuration C3). Knowing the error introduced by this simplification, we considered CNTs to be isotropic in this work.

3. Results and conclusions

The modelling results showed that the stress build-up in the fibre was not significantly changed by the grown CNTs (see C1-C3 configurations, Fig. 1). The ineffective length of the broken “fuzzy” fibre, i.e. the length corresponding to less than 90% of the nominal stress bearing capacity of the fibre, remained within 12% range from the length of the unmodified fibre (Fig. 3). The stress transfer from the broken fibre still occurred mainly through the matrix, in-between the CNTs. In the vicinity of the crack (distance of tens of nanometers), a high stress was also generated in the matrix regions along the CNTs and was transferred along their length to the CNT tips. However, their influence was negligible. The crack opening displacement at the fibre break was also not affected much by the CNT forests. The crack opening in configurations C1-C3 was not larger than 7% in comparison with the unmodified fibre (data are not shown). Grown CNTs are widely used to improve functional properties and to suppress transverse cracking. This study shows that when this is done the effect on the longitudinal properties is negligible. Further research is needed to confirm this conclusion for the composites with multiple fibres.

On the other hand, a considerable effect on the stress build-up was found for the case of the high fraction of CNTs aligned with the fibre length and, consequently, in the direction of the loading (see C6 configuration, Fig. 1). The layer of the aligned CNTs constrained crack opening by 15% and redistributed stress at the interface. The ineffective length in this case decreased by 28%. The stress

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build-up occurred faster (red line in Fig. 3) and, thus, the stress transfer was improved. Shear stress at the fibre-matrix interface decreased by a factor of two in comparison with the CNT-free case (data are not shown). These findings can be beneficial for understanding the behaviour of CF-reinforced composites modified with nanotubes.

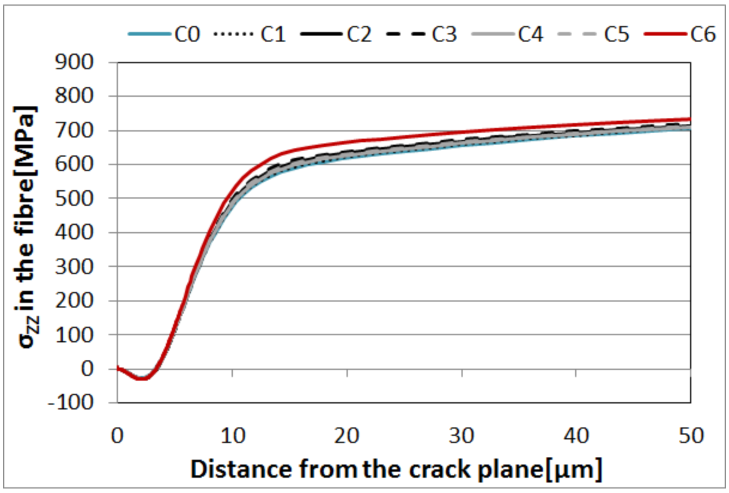

Figure 3. Stress build-up in the fibre. Z direction coincides with the fibre axis. C0 is a carbon fibre without CNTs. C1-C6 are fibres with the CNT configurations depicted in Fig. 1.

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