FAILURE OF PRE-CRACKED NANO-COMPOSITE

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Received 26 July 2012; accepted 16 October 2012

Abstract
The objective of this study is to investigate numerically using FEM the interfacial stresses and defects between the nanofibre and the matrix of nanocomposite. Because of complexity of the problem, 2D finite element analysis is carried out to simulate the cracked nanofibre composite, and 8-node quadrilateral element is utilized in the investigation. ANSYS software is used to explore Stress Intensity Factor (SIF) and the interfacial stresses of the matrix/nanofibre interface. The interfacial defect is simulated as a sharp crack to predict the SIF at the defect tip. The level of the local interfacial stresses arises at the defected spot is inspected as well. The defected nanocomposite is studied under simulated static loading conditions for both uniaxial and biaxial tensile stress. In addition, the defect size and the modulus of elasticity of various types of nanofibre are considered as parameters in the work. Consequently, it is shown that the interfacial stresses increase as the defect length increases. Furthermore, the stress level approaches fourteen times the applied stresses as the defect length come close to the fibre length. Whereas it is observed that the nanofibre restrain the SIF, but insignificant percentage of reduction in SIF is observed due to increase nanofibre modulus of elasticity.

1. Introduction
The fast progress in nanocomposites is one of the growing areas of nanotechnology, since carbon nanotubes have impressive mechanical properties and is intensively used as reinforcements in polymers and other matrices to form what is nowadays is called “Nanocomposite materials” [1-5]. Nanocomposites are a novel class of composite materials where one of the constituents has dimensions in the range 1–100 nm [6]. They can be produced by embedding reinforcement in the form of nanofibres or nanotubes in a matrix such as a polymer one in a similar manner to conventional composite materials [7].

In particular, nanocomposite fascinating for the fact that it is a bottom-up process, unlike the traditional method of producing engineering components from raw materials [8]. Industries, even aerospace has already benefited from the introduction of conventional composite materials with high strength reinforcements such as carbon fibres. The use of nanofibres particularly nanotubes which can be 50-100 times stronger than steel and six times lighter make nanocomposites a key candidate for aerospace applications [9]. Besides, it was shown that nanotubes increase composite strength by as much as 25% [10,11]. Reinforcement materials for nanocomposites may include nanofibres, nanoplatelets and nanoclay. These reinforcements are functionalized with additives, by this means resulting in a strong interfacial bond with the matrix [6].

In general, the main three mechanisms of interfacial load transfer are the weak van der Waals force between the matrix and the reinforcement, chemical bonding, and micromechanical interlocking [12]. Mainly, there are two causes behind a mechanically strong or weak nanocomposite material, the matrix interface with the nanofibres and the stress transfer. Therefore, efforts are done to make this interaction strong [8]. As the nanocomposite subjected to mechanical loading, stress concentrations will take place at the matrix/nanofibre interface which will eventually lead to damage nucleation, initiation, growth and final non-tolerated failure [8]. There are two probable sources of damage nucleation in nanocomposites; poor wetting of the nanofibres by the polymer and the aggregation of the nanofibres [13]. Both cases produce polymer rich nanocomposite portions that are likely to experience low stress to failure. Researchers [14] have observed that one of the reasons that nanocomposites may have a low strain to failure is the high interfacial stress that can lead to nanofibre/matrix debonding. In addition, the stress transfer from the matrix to the reinforcement is the main factor that will dictate the final nanocomposite material strength. It is reported that load transfer through a shear stress mechanism was observed at
the molecular level [6]. So far, it has been difficult to quantify the improved interfacial bonding between the matrix and the nanofibres accurately, either by direct measurement at the nanoscale [6]. Up to now, it has been quite complicated to evaluate the improved interfacial bonding between the matrix and the nanofibres accurately at the nanoscale level by direct measurement techniques, but it is quite easy to estimate the mechanical properties of the final macroscale nanocomposite materials with different types of standard tests for engineering materials [6]. A uniform dispersion and good wetting of the nanofibres within the matrix must be guaranteed in order to get the maximum utilization of the properties of nanofibres [6]. Moreover, local interfacial properties affect the macrolevel material behaviour, like reduction in flexural strength in nanotube/epoxy composite beams due to weakly bonded interfaces [15], as well the reduction in composite stiffness which was attributed to local nanofibres/nanotube waviness [16,17]. It was reported that local interfacial stress level in nanocomposites would be much higher than that in traditional composites because of high property mismatch between the nanoscale reinforcement and the matrix.

Since high interfacial stress may lead to interfacial debonding and then final failure of nanocomposites, this may contribute to the low failure strains in nanocomposites seen in many experiments [18]. In general, the benefit of small diameters of nanofibres or nanotubes is an increased interfacial contact area with the matrix, while its shortcoming is a high possibility of initial interfacial defects, which may lead to low failure strain of nanocomposites [6]. Consequently, a theoretical analysis of interfacial stress transfer mismatch between the nanoscale reinforcement and the matrix will be highly required before designing and producing nanocomposite materials [6,8].

In this context, the present paper discuss through using the finite element technique the consequences of the mismatch between the nanofibre and the matrix. As a matter of fact, the current mismatch is treated for the first time as crack between the nanofibre and the matrix. Therefore, the impact of this crack will be studied and discussed in term of the fracture mechanics. Linear elastic fracture mechanic was chosen as the basis for the present analysis using finite element analysis. Both uniaxial and biaxial load cases were proposed to study the case, where three types of the stiffness of the reinforcement were used to simulate the nanofibre properties. Each case were investigated individually through using traditional software ANSYS to predict SIF at the interface between the matrix and the nanofibre. Representative volume element (RVE) was proposed to simulate the case, and two dimensional analysis was implemented to model the nanocomposite because of the complexity of the problem.

2. Stress Intensity Factor (SIF)

The finite element method is an appropriate technique to calculate the stress intensity factors for fracture mechanics problems. There are several formulas in the literature for calculating the stress intensity factors for cracks at the interface between two materials. Displacement correlation and stress extrapolation methods have been suggested by many authors to determine stress intensity factors from numerical methods [19,20]. For an interface crack with the length 2a and between two dissimilar materials subjected to a uniform tension loading, an analytical expression for the stress intensity factors K1 and K2 is given in the following complex form [21]:

$$K_1 + iK_2 = \sigma_0 (1 + 2i\varepsilon)(2a)^{-1}(\pi a)^{0.5}$$

(1)

Where,

$$\varepsilon = \frac{1}{2\pi} \ln \gamma$$

(2)

$$\gamma = \frac{G_1 + k_1 G_2}{G_2 + k_2 G_1}$$

(3)

and k1 for plane strain condition

$$k_j = 3 - 4v_j$$

(4)

$$\varepsilon$$ is the biomaterial constant, Gj, v_j are shear modulus and Poisson’s ratios of the jth material, respectively. Let Ej denotes Young’s modulus of the jth material. The corresponding shear modulus, G_j, is obtained through

$$G_j = \frac{E_j}{2(1+v_j)}$$

(5)

The mixed-mode crack propagation scheme can be implemented into the finite element analysis. The advantage of such a numerical method is that the calculations of the stress intensity factors are more accurate in terms of near crack tip nodal displacements [22]. This technique is called Displacement Correlation Method. In this study, Displacement Correlation method is used to calculate the stress intensity factors. The definitions are given in Fig. 1. In Fig. 1a, the interface crack, crack deviation angle (h) and crack tip coordinate system are shown. It is considered that
two isotropic elastic solids joined along the y-axis as shown in Fig. 1a. After obtaining finite element solutions for cracked structure, nodal displacement values of nodes a, b, c, d and e (Fig. 1b) were used to calculate the stress intensity factors. Opening mode $K_1$ and shear mode $K_2$ are defined as [20]:

$$K_1 = \frac{\pi E_j}{L} \left[ D_1[-v^c + 4v^d - 3v^a] - D_2[-v^c + 4v^b - 3v^a] \right]$$

$$K_2 = \frac{\pi E_j}{L} \left[ D_1[-u^c + 4u^d - 3u^a] - D_2[-u^c + 4u^b - 3u^a] \right]$$

Where, $L$ is the distance between nodes of a–c or a–e (see Fig. 1b). To get better results, singular element size is kept at 10% of the crack length, $v_j$ is the displacements of nodes a, b, c, d, e along y-axis and $u_j$ is the displacement of nodes a, b, c, d, e along x-axis. The displacement values obtained from the numerical solution have been multiplied by $D_1$ and $D_2$ coefficients as the mechanical properties of the material on the left crack surfaces differ from those at the right surface (see Fig. 1). $D_1$ and $D_2$ coefficients can be expressed as:

$$D_1 = \frac{(1+\nu)\lambda_0}{\cosh(\pi \nu)} \frac{G_1}{k_1 e^{\pi \nu} + y e^{-\pi \nu}}$$

$$D_2 = \frac{(1+\nu)\lambda_0}{\cosh(\pi \nu)} \frac{G_2}{k_2 e^{\pi \nu} + y e^{-\pi \nu}}$$

Where

$$\lambda_0 = \left(\frac{1}{4} + \nu^2\right)^{1/2}$$

![Fig. 1: Crack mouth](image)

The prediction of the crack growth direction is conducted at the initial crack tip in both mode one and mixed mode loading crack growth analysis. Because of the restrictions of ANSYS, crack growth analysis was not accomplished. For that basis, this paper is based on the calculation of the stress intensity factors.

3. Finite element simulation

Many studies and researches have used the finite element analysis (FEA) as the primary tool to investigate the interfacial stresses and the failure strains of the nanocomposites instead of molecular dynamic simulation [6], since the latter can only deal with physical phenomena at the level of a few nanometres at the present stage, whereas the size of a representative volume of a nanocomposite material ranges from 10 nm upward to several hundreds of nanometres [23]. It was reported that mostly the smallest dimension of the nanofibre under investigation of the researchers lies in the range 20–50 nm [6], therefore continuum mechanics assumptions, like the one used in the finite element analysis are still valid at such length scales. Analogous finite element analyses have been reported by [16,23] with a focus on stiffness analysis incorporating micromechanics theory. In fact, these finite element analyses simplified the complex interaction among the nanoscale reinforcement, matrix and the double interface [6]. Ahmed et al. [24-26] investigated the impact of the embedded nano-inclusion, interfacial debonding as well as the mismatch on the mechanical properties and the stresses of the nanocomposite.

In this paper, the objective of the finite element analysis (FEA) is to investigate the proposed mismatch between the matrix the reinforcement by estimating the SIF using LEFM. The FEA modelling was carried out using ANSYS software. In order to simplify the simulation of the study, two dimension analyses was conducted by FEA which is mainly based on the representative volume element (RVE) of the nanocomposites material as shown in Fig. 2. Besides, constituents properties of the nano-reinforcement and the matrix have been obtained used similar to the previous investigators [6].

Due to complexity of the problem, 2D finite element analysis is carried out to simulate the cracked nanofibre composite, and 8-node quadrilateral element is utilized in the investigation. ANSYS software is used to determine (SIF) and the interfacial stresses of the matrix/nanofibre interface. The interfacial defect is simulated as a sharp crack to predict the SIF at the defect tip. A dense mesh in and around the nanofibre-matrix interface to a relatively coarser mesh utilized for the rest of the RVE Fig. 2. The material properties used in the baseline RVE were epoxy matrix, $E_m = 2.6$ GPa, $\nu_m = 0.3$. Similar to other finite element analyses [6], these nanofibres were considered as transversely isotropic materials [14,16]. The elastic modulus of the nanofibre was varied with the three well known reinforcement types were considered: $E_f = 200, 600$ and 1000 GPa for carbon fibres, graphite nanofibres and carbon nanotubes respectively. A tensile stress of
0.01 nN/nm² was applied along the long edge of the nanocomposite. LEFM was used and a linear, elastic analysis was executed to determine the SIF and the interfacial stresses.

The model used in this study is shown in Fig. 3. The crack length of a = 5 mm, 10 mm, 15 mm and 20 mm were studied. These values are corresponding to crack length to the half nanofibre length ratio a/L of 0.25, 0.5, 0.75 and 1 respectively is assumed to be at the interface between the nanofibre and the matrix. The nanofibre and the matrix in the model are assumed to be bonded perfectly with the exception of the crack faces. Frictionless sliding behaviour is assumed between the crack faces.

The level of the local interfacial stresses arises at the defected spot is inspected as well. The defected nanocomposite is investigated under simulated static loading conditions for both uniaxial and biaxial tensile stress. In addition, the defect size and the modulus of elasticity of various types of nanofibre are considered as parameters in the work. Moreover, mode II SIF is estimated as well for both uniaxial and biaxial load cases.

![Typical nanocomposite and RVE](image.png)

**Fig. 2: Typical nanocomposite and RVE**

**Fig. 3: Quarter 2D of RVE with crack**

### 4. Results and discussions

Figure 4 shows the normal stress $\sigma_y$ along the crack face with crack depth $a = 5$ mm for both uniaxial stress and biaxial stress cases. The results represent the stress distribution with respect three types of nanofibres, carbon, graphite and nanotube of different stiffness besides where the whole RVE has a matrix properties only without reinforcement and this variation of the reinforcement stiffness is applied for the whole cases studied in the present paper to examine the effect of the stiffness on the stresses and hence the SIF. It is observed that there is a significant increase in the $\sigma_y$ as approaching toward the crack tip, and this can be about 6.1 times the applied stress for the uniaxial stress Fig. 4.a, whereas little bit more than this value (6.7) for the biaxial stress Fig. 4.b. Besides, it is noted that the stresses will be reduced again behind the crack tip. It is essential to mention that the increase in the $\sigma_y$ at the crack tip is almost the same regardless the nanofibre properties, and this is generally true for the subsequent results. For crack $a = 10$ mm, as the crack length increased the normal stress $\sigma_y$ increased slightly more than the previous case especially for the biaxial stress. It is clear in Fig. 5a and Fig. 5b the this increase can be as 6.1 time the applied stress for the uniaxial stress case, while approaching 7 time for the biaxial stress. Moreover it is observed an increase in the $\sigma_y$ behind the crack tip toward the end of the nanofibre, and this can be estimated to be 2.8 and 2 times the applied stress for both uniaxial and the biaxial load cases respectively. With increase of the crack depth to $a = 15$ mm, it is observed that there is minor raise in $\sigma_y$ for both uniaxial and biaxial load cases, and this is expressed as 6.7 and 7.7 times the applied stresses respectively. Besides, there is significant increases in $\sigma_y$ behind the crack tip more the previous cases, which can be as 5 times and 2.8 times the applied stress exactly at the end length of the nanofibre element. As the crack length becomes as the nanofibre length, major amplify in the $\sigma_y$ is observed t the crack tip, which is the biggest even one notice through the present analysis, and definitely this occurred at the crack tip which is 15.3 and 14.6 times the applied stress for the studied load cases (uniaxial and biaxial). Consequently, a summary of the percentage increase of the normal stress $\sigma_y$ at the crack tip with respect to the applied load at the RVE, this relation can be express as shown in Fig. 8, which is mainly represents both uniaxial and biaxial load cases. Stress intensity factor is estimated at the crack tip, normalized SIF was adopted to represent the variation of SIF at the crack tip with respect to the case where there was no nanofibre used in the RVE, (ie. no reinforcement) means just matrix without any nanofibres. In this regard, both mode-I SIF and mode-II were calculated at two different load applications, uniaxial and biaxial loading case. Figure 9 represents the increase of the normalized SIF of mode-I as the crack depth to half of the nanofibre length increases. The ratio varies from 0.5 at the 5 mm crack depth and approach 0.85 as the crack length coincided with the nanofibre length. This is for the uniaxial loading, whereas for the biaxial it is observed that the normal-
ized mode-I SIF increases from 0.55 at the smallest crack depth to 0.85 at the largest crack depth. The final stage of the present analysis was to estimate mode-II SIF at the crack tip for both uniaxial and biaxial load cases in parallel with the mode-I. Therefore, case by case mode-II SIF was calculated and normalized and expresses with respect to the crack depth. Accordingly, Fig. 10 represents the reduction of the normalized SIF as the crack depth approach the nanofibre length. It was observed that a reduction of the normalized SIF starts from 8.8 to 2.2 as the crack depth increases for the uniaxial stress, whereas a drop from 7.6 to 1.7 for the biaxial case at the maximum crack depth proposed.

Fig. 4a: Normal stress at a=5 mm(Uniaxial)  
Fig. 4b: Normal stress at a=5 mm(Biaxial)  
Fig. 5a: Normal stress at a=10 mm(Uniaxial)  
Fig. 5b: Normal stress at a=10 mm(Biaxial)  
Fig. 6a: Normal stress at a=15 mm(Uniaxial)  
Fig. 6b: Normal stress at a=15 mm(Biaxial)
Fig. 7a: Normal stress at \( a = 20 \text{ mm}(\text{Uniaxial}) \)

Fig. 7b: Normal stress at \( a = 20 \text{ mm}(\text{Biaxial}) \)

Fig. 8a: Max. norm. stress at crack tip(\text{Uniaxial})

Fig. 8b: Max. norm. stress at crack tip(\text{Biaxial})

Fig. 9a: Normalized KI(\text{Uniaxial})

Fig. 9b: Normalized KI(\text{Biaxial})

Fig. 10a: Normalized KII(\text{Uniaxial})

Fig. 10b: Normalized KII(\text{Biaxial})
5. Conclusions
The mismatch between the nanofibre and matrix interface is modelled as crack for the first time to predict stresses levels and hence their impact on the SIF which can be a guide for the possible sources of the nanocomposite failure that could be a reference to the anticipate failure mode. The following points represent the conclusions predicted through the study:

1. It is observed the high normal stress at the crack tip which can be 6 times at the smallest crack size and as big as 16 times approaching the nanofibre length. This is for the uniaxial stress load, whereas for the biaxial stress, a slight increase is noticed with respect to the first case, and this is expected because of the crack. Whereas insignificant effect is observed by the variation of the reinforcement stiffness.

2. Significant increase in the normal stress at the end of the nanofibre as the crack depth increases that quarter the nanofibre length (a/L=0.25), and this definitely will cause increase stress levels and even stress concentration at the sharp corner between nanofibre and the matrix interface. In general this is obvious for both loading cases.

3. Increases in mode-I SIF and hence the normalize done as crack depth increases for both loading cases and this is true and this contributed to the increase in normal stresses at the crack tip. Almost no impact is observed on the estimated SIF caused by the stiffness variation.

4. A drop in the mode-II SIF as the crack depth increases especially at the a/L=0.25, and this approximately identical for the uniaxial and the biaxial loading cases and behind this point this reduction is quit constant.

Acknowledgments
Waleed K. Ahmed would like gratefully to express his acknowledges to the invaluable and endless support offered by both Dr.Kubilay (University of Afyon Kocatepe, Department of Manufacturing and Machining) and Dr.Yarub (Institute of Nano Electronic Engineering, University Malaysia Perlis) through their suggestion and recommendations.

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