Case study

Characterization of Nanoinclusion in Nanocomposite

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ABSTRACT

Studying the influence of nanoinclusion embedded in nanocomposite alongside a nanofiber is the objective of the present investigation. The analysis is done based on 2D, linear elastic finite element using ANSYS/Mechanical package to explore the impact of the nanoinclusion. Mainly, two assumptions are the major outlines, first whenever the presence of the nanoinclusion is at the longitudinal direction along the side of the nanofiber, whereas the second one is based of being along the transverse direction. The levels of the interfacial normal and shear stresses along the nanofiber are examined. The mechanical properties of the matrix and the nanofiber of the nanocomposite are considered as traditionally well known, while for the nanoinclusion stiffness is takes as 1/100 of the matrix stiffness. Uniaxial tensile stress is the principal stress that applied on the nanocomposite is in the longitudinal direction. Besides the implications of the nanoinclusion on the failure of the nanocomposite are studied as well. It is shown through the analysis that nanoinclusion has a great influence on the increase in the levels of the interfacial contact stresses along the sides of nanofiber in nanocomposite, which is considered as one of the main reasons of the nanocomposite failure.

Keywords: FEA, Failure, Interfacial, Nanocompoiste, Nanoinclusion, Stresses.

1. INTRODUCTION

Because of their potential applications in nano-scale polymer reinforcement, nanofibers and nanotubes have drawn vast attention from scientists and engineers worldwide in the past years and still being. In particular, the attention on the nanofiber reinforced composite, especially the nanofiber reinforced composite using CNF, has resulted in increasing focus to this newly promising material due to its amazing mechanical and electrical properties [1,2], mainly due to their superior stiffness, strength, stiffness, electrical as well as thermal conductivity. Carbon nanotubes have been shown by researches that exhibit extraordinary mechanical properties [3]. Although there has been some variation in the reported levels for the carbon nanotubes mechanical properties, i.e., stiffness, has been shown to be greater than 1 TPa, and the tensile strength exceeds that of steel by over an order of magnitude [4]. The tremendous mechanical properties of carbon nanotubes and other nano reinforcements can be realized only if efficient load transfer exists between the matrix and the reinforcement [5-8]. In some cases the load transfer between nanotubes and the surrounding matrix can be increased by introducing non-bonded interfacial compounds or chemical crosslinks between nanotubes and the matrix [9-12]. The stiffness properties of nanocomposites are always higher than those of the pure matrix; however, the final strength of the nanocomposite may or may not exceed the strength of the pure matrix if discontinuous nanofibers/nanotubes (even if they were aligned) are used in nanocomposites [13].

Many problems and challenges remain barriers to the development and applications of nanomaterials including the development of techniques to produce nano-scale particles of high quality in sufficient quantities and at a low cost; the

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upgrade of the low fracture toughness and poor ductility of nanoscale materials, the assembly of nanocomponents into devices and the improvement of the thermal stability of nanostructures[14].

Using nanoparticles of different properties can be used to enhance the properties of the strengthening of a fibre-matrix interface [15], but studying this impact will be helpful using FEA to minimize time and cost. The peeling as well as the shear mode failure of the nanofiber/matrix interface is considered one of the problematic issues due to the presence of the nanovoids and the nanoinclusions during the preparation stages. A uniform dispersion and good wetting of the nanofibers within the matrix of the nanocomposite must be implemented [16] to achieve the desired maximum utilization of the properties of nanofibers.

In general, the local levels of the interfacial stress in nanocomposites would be much higher than that in traditional composites due to well-known high property mismatch between the nanoscale reinforcement and the matrix, since high interfacial stress may lead to interfacial debonding and the final failure of nanocomposites, and this would be contributed to the low failure strains observed in nanocomposites [16,17]. Moreover, the main advantage of using small diameters of nanofibers or nanotubes is an increased interfacial contact area with the matrix, while its shortcoming is a high possibility of initial interfacial defects, which can lead to low failure strain of nanocomposites.

The interfacial stress transfer and possible stress singularities, arising at the interfacial ends of discontinuous nanofibers embedded in a matrix subjected to different loading conditions, the effects of Young's modulus and volume fractions on interfacial stress distributions were investigated using FEA [13] proposing round-ended nanofibers to remove the interfacial singular stresses, which were the caused by highly stiffness mismatch of the nanoscale reinforcement and the matrix. The normal stress induced in the nanofiber through interfacial stress transfer was still less than two times that in the matrix itself, this stress value is far below the high strength of the nanofiber. Therefore, the load transfer efficiency of discontinuous nanofibers or nanotube composites is very low [13].

Computational modeling techniques for the determination of mechanical properties of nanocomposites have proven to be very effective [18-25]. Computational modeling of polymer nanocomposite mechanical properties renders the flexibility of efficient parametric study of nanocomposites to facilitate the design and development of nanocomposite structures for engineering applications.

As a matter of fact, it has been know that mainly there are three mechanisms of interfacial load transfer, which are: chemical bonding, the weak van der Waals force between the matrix and the reinforcement and the micromechanical interlocking [26]. In particular, there are two reasons behind a mechanically strong or weak nanocomposite material, the matrix interface with the nanofibres and the stress transfer. Accordingly, efforts are done to make this interaction strong [27]. Since the nanocomposite is exposed to mechanical loading in general, the stress concentrations will take place at the interface matrix/nanofiber which will eventually lead to damage nucleation, initiation, growth and final nontolerated failure [27]. There are two probable sources of damage nucleation in nanocomposites, poor wetting of the nanofibres by the polymer and the aggregation of the nanofibres [17]. Both cases produce polymer rich nanocomposite portions that are likely to experience low stress to failure. It has been observed by researchers [28] that one of the most reasons that nanocomposites can have a low strain to failure is the high interfacial stress which may lead to nanofibre/matrix debonding. Moreover, 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 levels [29]. So far, it has been difficult to quantify the improved interfacial bonding between the matrix and the nanofibers accurately, either by direct measurement at the nanoscale [28]. Up to now, it has been quite complicated to evaluate the improved interfacial bonding between the matrix and the nanofibers 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 [28]. A uniform dispersion and good wetting of the nanofibers within the matrix must be guaranteed in order to get the maximum utilization of the properties of nanofibers [28]. Moreover, local interfacial properties affect the macrolevel material behavior, like reduction in flexural strength in nanotube/epoxy composite beams due to weakly bonded interfaces [29], as well the reduction in composite stiffness which was attributed to local nanofibers waviness [30,31]. 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 [17]. Moreover, finite element analysis in particular was used to study the influence of the nanoholes [32], flexural loading [33] as well as the interlaminar crack [34] on the failure of the nanocomposite. In general, the benefit of small diameters of 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 [28]. 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 [27,28].

The present analysis investigate through using finite element method the impact of the inclusions embedded in nanocomposite and exist in two main directions, through the transverse and the longitudinal direction of the nanofiber of the nanocomposite. Linear elastic analysis is used in the analysis, whereas the system of the nanocomposite analyzed is considered through representative volume element (RVE). Two dimensional RVE is adopted through the study to simplify the analysis, whereas the mechanical properties used for the nanofibe and the matrix of the nanocomposite are the same well know traditional one, except for the nanoinclusion where proposed to be 1/100 the stiffness of the matrix.

2. MODELING OF NANOCOMPOSITE

Mainly, finite element analysis (FEA) is adopted as the primary tool for the present analysis instead of using molecular dynamics simulations, since the latter could only deal with physical phenomena at the level of a few nanometers [30], whereas the size of a representative volume of a nanocomposite material ranges from 10 nm to several hundreds of nanometers which is within the range of continuum mechanics.

It was reported that mostly the smallest dimension of the nanofiber under investigation of the researchers lies in the range 20-50 nm [28], 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 Fisher et al. [30] 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 doable interphase [28].

Although the applicability of continuum mechanics (including micro mechanics) to nanocomposites has been subjected to debate [32,35], many works directly applying continuum mechanics to nanostructures and nanomaterials have reported meaningful results and elucidated many issues [35-44].

In this study, finite element analysis was used to investigate the influence of inclusions on the interfacial stresses in the RVE and the structural performance by utilizing (ANSYS11/Mechanical) finite element package. ANSYS/Mechanical software is utilized to predict the interfacial stresses of RVE along the nanofiber sides. The dimensions used of the RVE are considered in this analysis similar to the Roy and Sengupta [13] to maintain consistency, which is represented by nanofiber volume fraction of 4%.

Two dimensional case is considered using 4-node solid element (Plane 42). Fig.1 shows the dimension and the boundary conditions of the modeled RVE. It was attempted to maintain the same degree of refinement for all models to obtain consistent results .The mechanical properties of the a are considered to be isotropic. Matrix properties for Young's modulus and Poisson's ratio are 2.6 GPa and 0.3 respectively. For the nanofiber, the properties that are used 200 GPa for Young's modulus and and 0.3 Poisson's ratio. The modulus of elasticity of the nanoinclusion considered as 1/100 of the matrix while 0.3 is adopted for the Poisons' ratio.

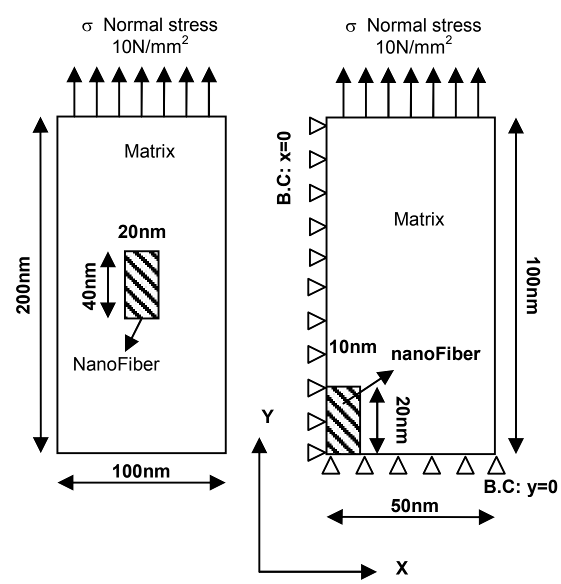

Figure (1) The dimensions and boundary condition of the RVE used for FEM

Two pairs of identical nanoinclusions located symmetrically around the fiber in addition to a nanoiclusion at the corner of the nanofiber are shown in Fig 2. A tensile load of 10 MPa is applied at the longitudinal direction of the RVE, whereas no lateral load is applied. Interfacial stresses through the short and long side of the specimen are estimated.

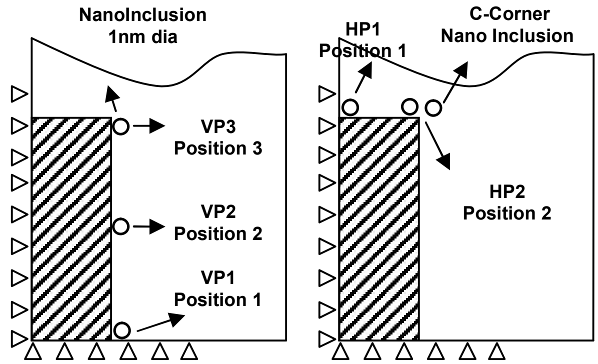

Figure (2) NanoInclusion at the longitudinal (left), and transverse (right) edge of the nanofiber.

3. RESULTS AND DISCUSSION

The FE analysis of the RVE which contains nanonclusion along the longitudinal and the transverse sides of the nanofiber, the impact of the location of the nanonclusion along the fiber side on the interfacial stresses is studied, i.e., the traverse and the longitudinal sides of the nanofiber. The results can be summarized as:

1. The first case studies ia whenever nanoinclusion located at the corner of the nanofiber. An obvious increases of 80% in the normal (σy) along the transverse side of the nanofiber in comparison with the normal stresses of the non-inclusion case (N). In the other hand, an observed increases of 183% in the transvers normal stresses (σx) along the longitudinal edge side of the nanofiber with respect to the intact case (N) as the nanoinclusion location approaches the corner of the nanofiber, as shown in Figures (3) and (4). This tremendous increase can cause pealing failure between the nanofibe/matrix interface and causes the loss of the stiffness.

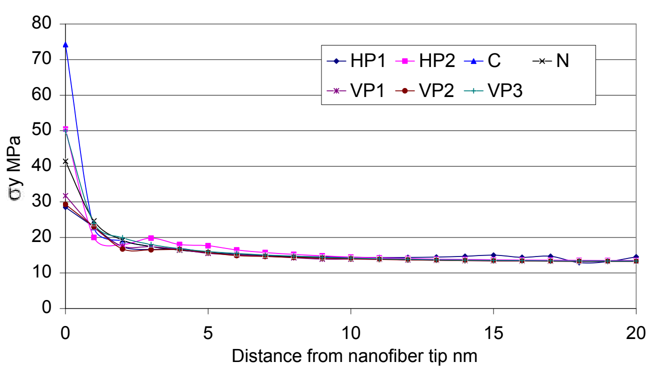

Figure (3) Stress (σy) Transverse Edge

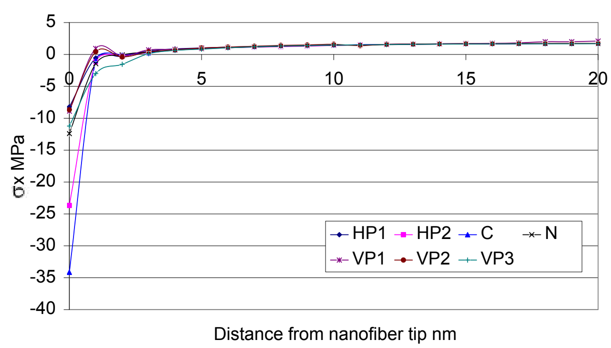

Figure (4) Stress (σx) at Longitudinal Edge

2. It is evidence that the vertical position 3 of the nanoinclusion near the tip of the longitudinal edge of the nanofiber results in the increase of the shear stress (σxy) up to 100% and 120% of the shear stresses of (σxy) for transverse and longitudinal sides of the nanofiber respectively, as shown in Figures(5) and (6). This rise in the shears stresses can lead to the debonding between nanofiber/matrix interface, which eventually lead to the degradation and hence failure of the nanocmposite.

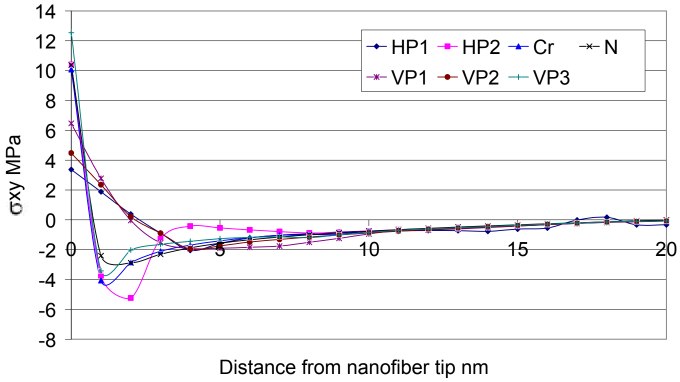

Figure (5) Stress (σxy) Transverse Edge

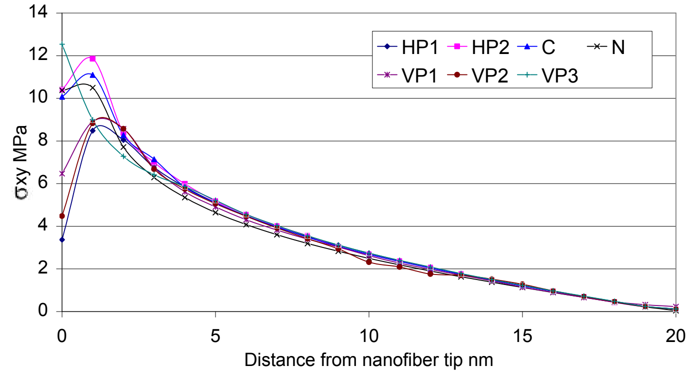

Figure (6) Stress (σxy) at Longitudinal Edge

4. CONCLUSION

It is shown in this FE study that the location of the nanoinclusions around the nanofiber composite affects the rise up of the interfacial stresses many time compared with the intact case, i.e., non-nanonclusion-case for both transverse and longitudinal location of the nanonclusions. The increase in the normal stresses for the both longitudinal and transverse sides of the nanofiber can causes in the pealing of the nanofunbe/matrix interface, whereas the rise in the shears stresses can result in the failure mode due slipping.

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