The Impact of Embeded Nanoinclusion in Nanofiber Reinforced Composite

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ABSTRACT

Studying the influence of a nanoinclusion embedded in nanofiber reinforced composite alongside a nanofiber is the objective of the present investigation. The analysis is done based on 2D, linear elastic finite element through using finite element package ANSYS/Mechanical to explore the impact of the nanoinclusion on the mechanical behavior of the nanocomposite. Mainly, two scenarios are the major outlines of the study, first whenever the presence of the nanoinclusion is located at the longitudinal side of the nanofiber, whereas in the second case, the nanoinclusion is proposed to be along the transverse side of the nanofiber. The levels of the interfacial stresses, normal and shear along the nanofiber's sides are estimated and discussed. The mechanical properties of the matrix and the nanofiber of the nanocomposite are considered be similar to the traditional well known materials, while for the modeling purposes of the stiffness of the nanoinclusion, is taken as 1/100 of the matrix stiffness. The nanocomposite is subjected to uniaxial tensile stress which is the main stress applied. The implications of the existence of the nanoinclusion on the failure of the nanocomposite due to increases of the interfacial stresses in the nanofiber/matrix line are discussed as well. It is shown through the analysis that the nanoinclusion has a great influence on the increase of the interfacial stresses along the sides of the nanofiber in a nanocomposite in different level and conditions according to the location of the nanoinclusion, and this essentially is considered as one of the main reasons of the anticipated nanocomposite failure.

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

1. INTRODUCTION

Nanocomposites are a novel class of composite materials where one of the constituents has dimensions in the range 1–100 nm [1,2]. Because of their potential applications in nano-scale polymer reinforcement, nanofibers and nanotubes have drawn vast attention from scientists and engineers worldwide over the past decades 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 [3,4], mainly due to their superior stiffness, strength, electrical as well as thermal conductivity. Researches have been shown that carbon nanotubes exhibit extraordinary mechanical properties [5], although there have been some variations in the reported levels for the carbon nanotubes mechanical properties, i.e., stiffness, which has been shown to be greater than 1 TPa and the tensile strength exceeds that of steel by over an order of magnitude [6]. The tremendous mechanical

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properties of carbon nanotubes and other nano-reinforcements can be realized only if efficient load transfer exists between the matrix and the reinforcement [7-10]. 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 [11-14]. 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 [1].

Many problems and challenges are still barriers to the development and applications of the nanomaterials, including the development of techniques to produce nano-scale particles of high quality in massive quantities and at low cost; the 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[15]. Using nanoparticles of different properties can be used to enhance the properties of the strengthening of a fibre-matrix interface [16], 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 [17] 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 [17,18]. 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 stresses and stress singularities arising at the interfacial ends of a discontinuous nanofibers embedded in a matrix subjected to different loading conditions, the effects of Young's modulus and nanofiber volume fraction on the interfacial stresses distribution were investigated using FEA [1], proposing round-ended nanofibers to remove the interfacial singular stresses, which were 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 [1]. Computational modeling techniques for the determination of mechanical properties of nanocomposites have proven to be very effective [19-26]. 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 known 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 [27]. In particular, there are two reasons behind a mechanically strong or weak nanocomposite material, the matrix interface with the nanofibers and the stress transfer. Accordingly, efforts are done to make this interaction strong [28]. 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 [28]. There are two probable sources of damage nucleation in nanocomposites, poor wetting of the nanofibers by the polymer and the aggregation of the nanofibers [18]. Both cases produce polymer rich nanocomposite portions that are likely to experience low stress to failure. It has been observed by researchers [1] 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 [1]. 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 [1]. 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 [1]. 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 [18]. 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 [28,1]. Basically, one of the main engineering problems is how to predict the mechanical behavior of materials, but unfortunately voids, inclusions, defects, irregularities that cannot be avoided (i.e., there is no perfect material), therefore always it is tried to establish limits for the existence of such defects in the material. Many researchers have spent massive amount of effort for developing various analytical as well as numerical techniques for modeling and estimating the impact of the undesired inclusions in different types of materials. Since the presence of inclusions in materials affects their elastic field at the local and the global scale and thus greatly influences their mechanical and physical properties, so the significance of the inclusions to the development of advanced materials for aerospace, marine, automotive and many other applications were reviewed [35]. In some occasions, void or inclusion may be present in some region of the nanocomposite system. These void and inclusion may influence the distribution of interfacial stresses and hence increase the stresses at certain location and whenever exceed the of permissible stress levels, will lead to the initiation of cracks and hence lead to the failure of the nanocomposite. Thus, the influence of inclusions in the nanocomposite on interfacial stresses play a big role in failure mechanism of the nanocomposite due to its impact on the interfacial stresses along the nanofiber. Because the interfacial stresses occur at the interface nanofiber/matrix, it is important to understand that the direct measurement of the interfacial stresses which is almost impossible. Finite element method (FEM) is used to clarify the distribution of interfacial stresses and to give an clear estimation of the behavior of the nanocompsoite. In general, inclusions are not presented as isolated ones in the matrix material. On the one hand, inclusions frequently agglomerate into stringers or clusters as detrimental micro-defects during the material manufacturing process. Besides, inclusions are intentionally introduced into composite materials as reinforcing fibers or particles. These inclusions often cause stress concentration in their vicinities where cracks and dislocations may form. Thus, it is important to study multiple inclusions, dislocations and cracks and their interactions for optimal design of advanced materials and their performance improvement. A comprehensive survey of recent works on inclusion in an infinite space, a half-space under prescribed surface loading, a half-space under surface contact loading or a finite space besides to the impact of the presence of nano-sized cavity, nano-sized spheroidal inclusion, ellipsoidal nano-inclusion, nano-scale elliptical inclusions, nano-grained ceramics and nanoporous materials were provided. Moreover, the problems of a single inclusion, two inclusions, and multiple inclusions, dislocations and cracks as well as various methods used to address these problems were discussed. In addition, the review concluded with an outlook on future research directions.

The present analysis investigates through using finite element method the impact of a nano-inclusion 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 nanofiber and the matrix of the nanocomposite are the same well known traditional one. The stiffness of the nanoinclusion is proposed to be 1/100 the stiffness of the matrix, whereas the nanoinclusion is considered to have a circular shape of diameter equal to 1nm.

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 [1], 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 [1]. Although the applicability of continuum mechanics (including micro mechanics) to nanocomposites has been subjected to debate [35,36], many works directly applying continuum mechanics to nanostructures and nanomaterials have reported meaningful results and elucidated many issues [36-47], especially using FEA as a powerful tool to understand the behavior and the failure of the nanocomposites under different conditions. 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 and the properties used of the RVE are considered in this analysis similar to the Roy and Sengupta [1] to maintain consistency, which is represented by nanofiber volume fraction of 4%. Two dimensional case is considered using 4-node solid element (Plane 42). Figure 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 nanofiber and the matrix 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 0.3 Poisson's ratio. The modulus of elasticity of the nanoinclusion to the matrix stiffness(i.e., E_i/E_m) were investigated by many researchers for different range of values (i.e., $E_i/E_m=10^{-4}\sim10^{4}$) [48-51]. For the present study E_i/E_m is considered to be 1/100, while 0.3 is adopted for the Poisons' ratio. The nanoinclusion of 1nm diameter is proposed for the FE analysis.

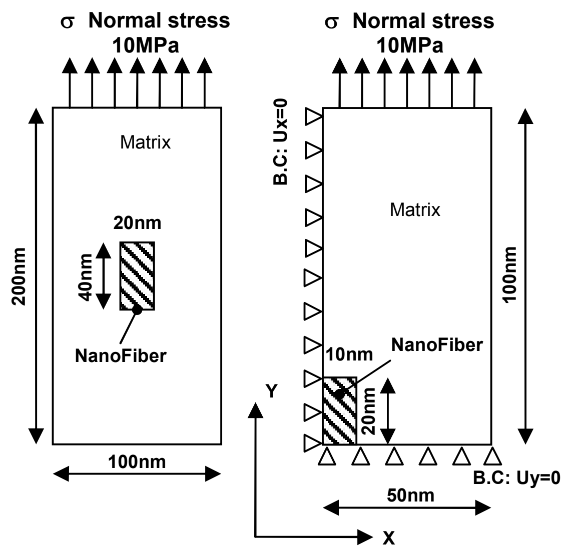


Fig. 1. Dimensions and boundary condition of the RVE used for FEA.

Two pairs of identical nanoinclusions located symmetrically around the nanofiber in addition to a nanoinclusion at the corner of the nanofiber are shown in Fig 2. A tensile stress of 10 MPa (i.e., 0.01 nN/nm^2) 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. The estimated normal stresses σ_y and σ_x of the non-inclusion case (i.e., intact) are estimated and compared with Roy et al. [1] with a max error of 3%, which are shown in Figs. 3 and 5. This validates the FE model used in the analysis.

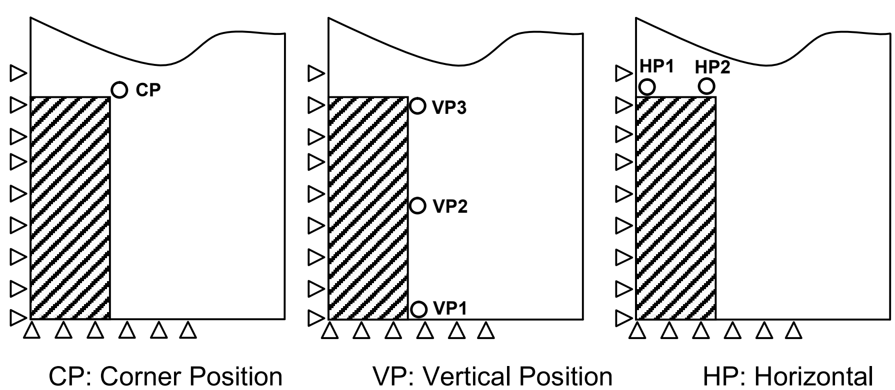


Fig. 2. Corner (left), longitudinal (mid) and transverse inclusion (right).

3. RESULTS AND DISCUSSION

Finite element analysis is used to study a RVE of a nanocomposite which is proposed to contain a nanoinclusion. Two scenarios are adopted in the analysis according to the location of the nanoinclusion with respect to the nanofiber sides. The nanoinclusion is assumed to exist along the side of the nanofibe (i.e., longitudinal direction) one time, whereas to be along the nanofiber's diameter (i.e., transverse direction) in the second time. The impact of the nanoinclusion's location on the normal and the shear stresses along the longitudinal and the transvers sides of the nanofiber are investigated. The results can be summarized as:

3.1 Corner Nanoinclusion (CP)

In the first case, the stresses are estimated whenever the nanoinclusion is located at the corner of the nanofiber (i.e., CP). An obvious increases of 80% in the normal (σ_y) along the transverse side of the nanofiber in comparison with the normal stresses of the non-inclusion case as illustrated in Fig. 3. In the other hand, a similar increase in the normal stress (σ_y) along transverse direction(i.e., 80%) is observed due to presence of the nanoinclusion at the corner position (CP) along the longitudinal direction, as depicted in Fig. 4. An observed increases of 183% in the transvers normal stresses (σ_x) along the longitudinal edge side of the nanofiber with respect to the intact case as the nanoinclusion location approaches the corner of the nanofiber (i.e., CP) through the short and long side of the nanofiber, as shown in Figs. 5 and 6. This tremendous increase can cause pealing failure between the nanofiber/matrix interface and eventually causes the loss of the stiffness.

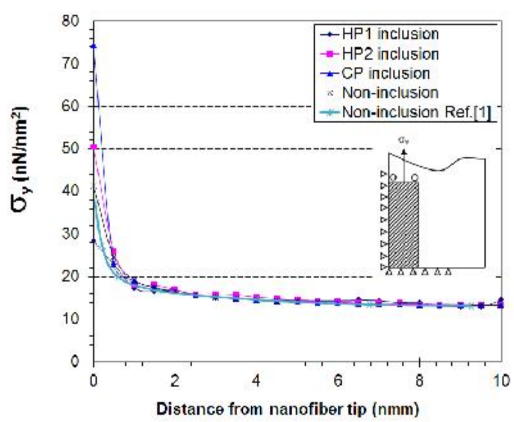


Fig. 3. Normal stress σ_y along the short side of the nanofiber due to horizontal inclusion.

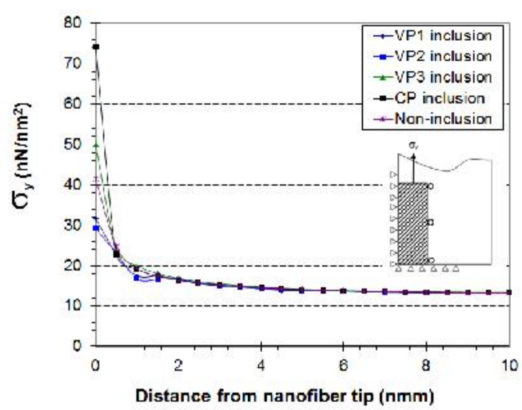
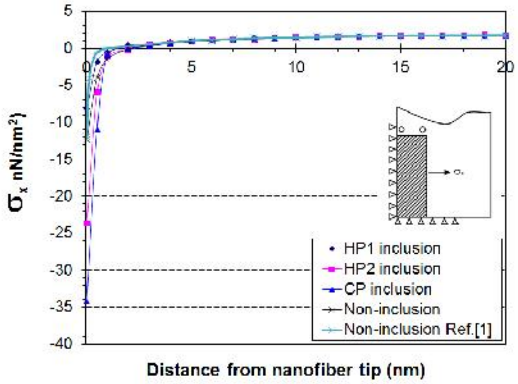


Fig. 4. Normal stress σ_y along the short side of the nanofiber due to vertical inclusion.



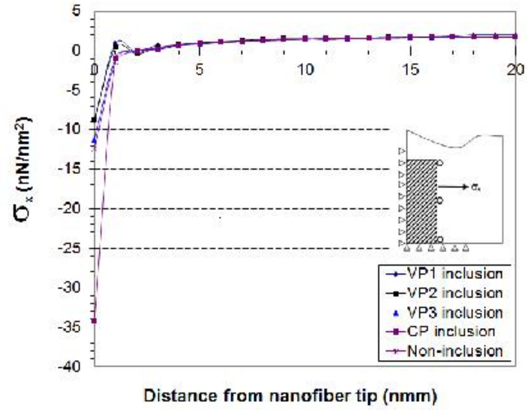
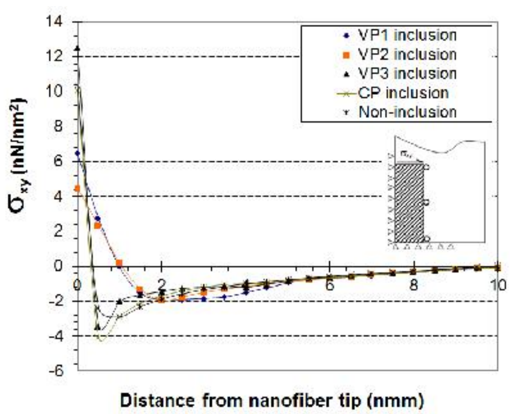


Fig. 5. Normal stress σ_x along the long side of the nanofiber due to horizontal inclusion.

Fig. 6. Normal stress σ_x along the long side of the nanofiber due to vertical inclusion.

3.2 Vertical Nanoinclusion (VP)

It is evidence that the vertical position of the nanoinclusion close the tip of the nanofiber (i.e., VP3), results increases of the shear stress (σ_{xy}) up to 20% of the shear stresses with respect to the shear stress for the non-inclusion case for both transverse and longitudinal sides of the nanofiber respectively, as shown in Figs. 7 and 8. This rise in the shears stresses can lead to the debonding between nanofiber/matrix interface, which eventually may lead to the degradation and hence failure of the nanocomposite.



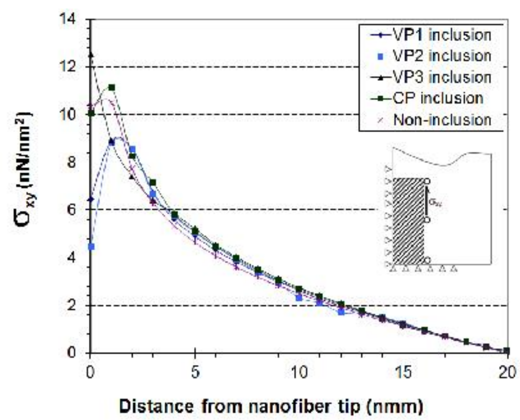


Fig. 7. Shear stress σ_{xy} along the short side of the nanofiber due to vertical inclusion.

Fig. 8. Shear stress σ_{xy} along the long side of the nanofiber due to vertical inclusion.

3.3 Horizontal Nanoinclusion (HP)

Regarding the shear stress (σ_{xy}) along the short and the long side of the nanofiber due to the presence of the nanoinclusion close to the nanofiber tip along the short side (i.e., HP2), insignificant change in the stress levels of the shear stress in both sides with respect to the non-inclusion case. This is illustrated in Figs. 9 and 10.

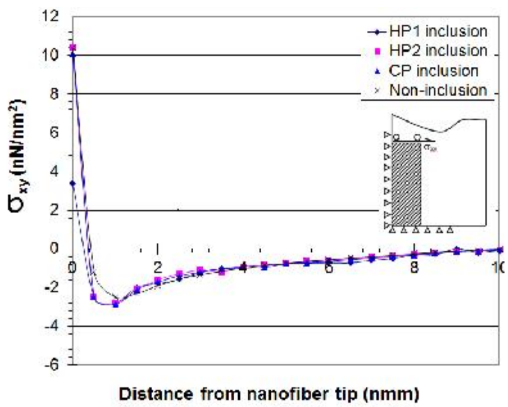


Fig. 9. Shear stress σ_{xy} along the short side of the nanofiber due to horizontal inclusion.

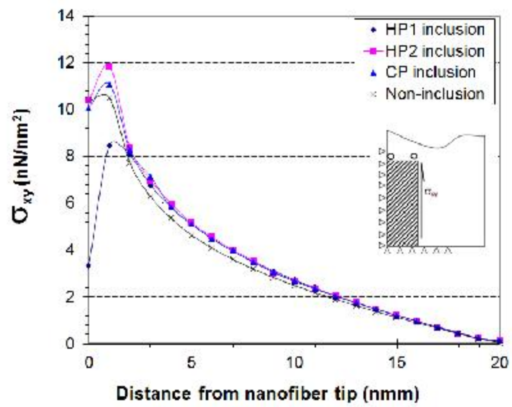


Fig. 10. Shear stress σ_{xy} along the long side of the nanofiber due to horizontal inclusion.

4. CONCLUSION

Nanofiber reinforced composite with embedded nanoinclusion produces increase in the interfacial stresses along the nofiber/matrix line. However, it is estimated that corner nanoinclusion located at the nanofiber's tip (i.e., CP) shows hike in the normal stresses (σ_y) along the short side as well as normal stress (σ_x) at the long side of the nanofiber. In the other hand, a nanoinclusion which is located close to the nanofiber's tip, along the short side (HP2), shows increase in the shear stress (σ_{xy}) along the longitudinal direction as well as the shear stress (σ_{xy}) along the transverse side of the nanofiber. An obvious escalating in the shear stress (σ_{xy}) along both short and long side of the nanofiber are observed whenever the nanoinclusion being at the longitudinal side of the nanofiber and approaches the nanofiber's tip (i.e., VP3). Insignificant change in the shear stress (σ_{xy}) along the short and long side of the nanofiber due to existence of the nanoinclusion close to the nanofiber's tip along the short side (i.e., HP2). The present analysis emphasis on the significance of the nanoinclusion impact on the increases of the interfacial stresses along the nanofiber/matrix, therefore the analysis in the present investigation can be used to draw the attention of the nanocomposites analysts to consider it in the assessment of the effectiveness of the nanofiber reinforced composite with inclusions as well as for failure prediction.

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