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DESIGN AND ANALYSIS OF NANOCOMPOSITE CHARACTERIZATION USING FINITE ELEMENT METHOD

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ABSTRACT:

Nanocomposites are novel materials that are receiving great attention from the aerospace community because of the inherent high strength and stiffness of the nanotubes/nanofibres embedded in the Nanocomposite matrix. These features are particularly appealing to aircraft designers who strive to produce long lasting and safe components that can perform at the highest and extreme levels. However, the mechanical properties, damage initiation and propagation are yet to be fully comprehended. Consequently, in this work, the mechanical behavior of nanofibres is characterized by finite element analysis (FEA). In particular, the stiffness mismatch of the nano-fibres and the matrix are studied under simulated static loading conditions. A comparison of the formation of singular interfacial stress zones (stress concentrations) in various forms of nanofibre is then presented. It is shown that an optimized nanofibre composite design is not only influenced by the nanofibre stiffness but also by the nanofibre length and nanofibre shape. Finally, recommendations are made on producing Nanocomposites with high failure strength.

Key words: *Nanocomposites; Mechanical properties; Finite element analysis (FEA).*

1. INTRODUCTION :

The development of Nanocomposites is one of the rapidly evolving areas of nanotechnology. Nanocomposites are nano-crystalline materials with grains on the order of 1–100 nm (10^{-9} of a metre). They are produced by embedding reinforcement (e.g., nanofibres or nanotubes) in a matrix such as a polymer one in a similar manner to conventional composite materials. It is particularly fascinating for the fact that it is a bottom-up process, unlike the traditional method of producing engineering components from raw materials. The aerospace industry has already benefited from the introduction of conventional composite materials with high strength reinforcements such as carbon fibers. 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.

In aircraft design, fatigue strength is one of the key properties required of the aircraft components. However, because the fatigue strength decreases with the component undergoing cyclic loading, the aircraft components need to be made out of stronger materials. If the latter is achieved than the life of the aircraft is greatly increased. A reduction in the grain size of the material is known to lead to an increase in the fatigue strength. Conveniently, it is known that nanomaterials provide such a significant reduction in the grain size over conventional materials which give them the potential to significantly increase the fatigue life. However, understanding the behaviour of these materials under mechanical loading remains a vital task in order to have more confidence in their application and optimize their design.

1.1 Metal Matrix Composites:

These are composites with matrix constituent being metal, while the other can be another metal or a ceramic or organic compound. Metal Matrix Composites are superior to monolithic metals due to their high specific strength, can operate in wide range of temperatures, better electrical and thermal conductivity, higher specific modulus, low co-efficient of thermal expansion and do not display out gassing. Due to these attributes, metal matrix composites are considered for various applications viz. carbide drills, tank armours, modern high-performance sports car, radio frequency quadrupoles (RFQs) etc. A typical example is the titanium carbide cermet which constituting 30% nickel matrix reinforced with 70% TiC particles demonstrates high specific strength and stiffness at higher temperatures.

1.2 Literature Review :

Wang and Pyrz et al. [1] presented the theory and formulas for the prediction of overall moduli of layered silicate-reinforced polymeric nanocomposites. Formulas for the moduli of composite materials reinforced with transversely isotropic spheroids, were derived from the M-T method. The predictions were compared to approximate formulas found in the literature for isotropic thin oblate spheroids.

Sheng et al. [2] applied a multiscale modelling strategy, taking into account the hierarchical morphology of the polymer/clay nanocomposites, to the prediction of homogenized properties of the materials. The clay particles can have the form of exfoliated clay sheets, of nanometer level thickness or stacks of parallel clay sheets separated from one another by interlayer galleries of nanometer level height. It was shown that in the latter case the stacks could be represented by effective particles.

Hbaieb et al. [3] analyzed 2-D (plane stress) and 3-D FEM models of the polymer/clay nanocomposites with aligned and randomly oriented particles. They calculated the effective Young’s modulus in the axial direction, and Young’s modulus of the isotropic effective medium, according to the analysed case. The results were compared to the M-T model.

Figiel and Buckley et al. [4] calculated elastic constants for the layered-silicate/polymer nanocomposite with intercalated morphology by using the effective particle concept. Two methods were applied: plane strain FEM analysis and the M-T method.

Gorski and Fedelinski et al. [5] modelled 2-D RVEs of the nanocomposites by using coupled boundary and finite element methods (BEM/FEM). The matrix was modelled by the BEM, and the reinforcement by beam finite elements. The authors considered both the aligned and randomly distributed particles. It was shown that the proposed method was more effective than the FEM, in terms of the number of degrees of freedom of the numerical model.

In the recent paper by Fedelinski et al. [6], different formulations of the BEM were presented, for the analysis of composites containing rigid or deformable stiffeners and inclusions. The developed computer codes were used to compute effective elastic or piezoelectric material properties by the analysis of 2-D RVEs or unit cells. One of the analysed materials was a polymer/clay nanocomposite reinforced with stacks of clay sheets.

2. DESIGN AND FINITE ELEMENT MODELING OF NANOCOMPOSITE :

2.1 Finite element analysis of matrix/nanofibre property mismatch:

When combining highly stiff nanofibres with a matrix, it is expected that the final nanocomposite material should have higher strength than the resin otherwise it would not be much of an improvement. The aim of the finite element analysis (FEA) is to investigate the stresses at both the matrix and most importantly the reinforcement. The FEA modelling was carried out using ANSYS software to derive various stresses at the matrix/nanofibre interfaces.

The proposed FEA investigation is based on a representative volume element (RVE) of a nanocomposite material as shown in Figure 1. Constituents properties of the reinforcement and the matrix (Ef = 600 GPa, Em = 2.6 GPa and νf = νm = 0.3) have been obtained from the literature. As illustrated in Figure, the behaviour of the RVE under tensile stresses was investigated by loading various forms of the RVE to 10 MPa. These forms are characterised by the nanofibre shape and length. A constant required by ANSYS FEA software for matrix/nanofibre contact was chosen to be 0.028 nm. However, altering it had no significant effects on the resulting stresses. Maximum principal stresses, von mises stress and normal stresses were analysed along the nanofibre short interface (x direction in this study) and along the nanofibre cross section (e.g., in a rounded nanofibre, stresses were obtained along the circumference) as well as at the highest stress points on the nanofibre. Three different scenarios were investigated.

1. long and short nanofibres (50 nm and 20 nm respectively)
2. high modulus and low modulus nanofibres (600 GPa and 50 GPa respectively)
3. Shaped nanofibres (rounded, star and hexagonal cross section shapes) as illustrated in Fig 1

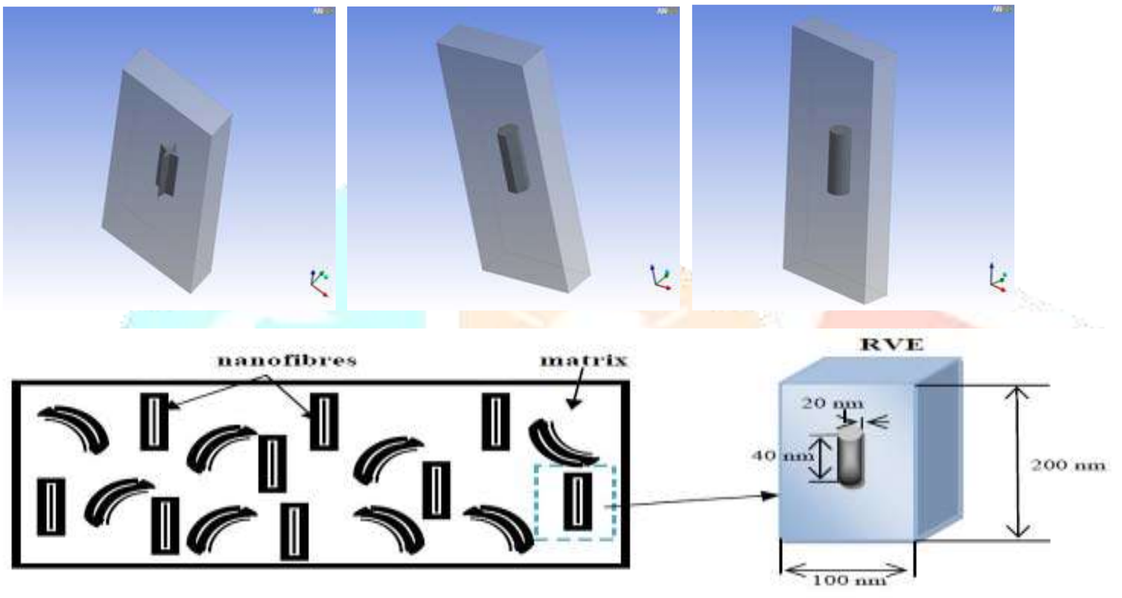

Figure 1 Three different cross shaped nanofibres were investigated.

3.ANALYSIS OF MODELED NANOCOMPOSITE USING FINITE ELEMENT METHOD:

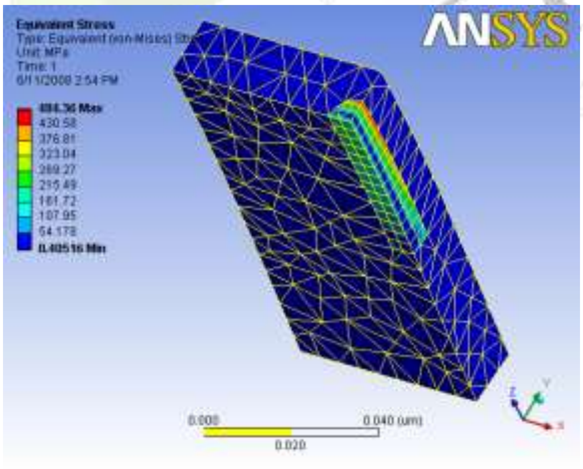

Figure 2 Nanofibre length effect on stresses along nanofibre circumference

3.1 Nanofibre stiffness effect:

In this analysis, an RVE with a nanofibre 50 nm in length and a stiffness E = 600 GPa was subjected to 10 MPa static tensile loading. The same analysis was repeated with a nanofibre having a stiffness E = 50 GPa. Similar to the length effect investigation, Figures 3 and 8 reveal high normal, principal and von mises stresses for the stiff nanofibre along the circumference but only an increase in the von mises stresses along the radius. The results show that stresses along the nanofibre radius. The reason is that there are potentials for higher stresses along the circumference. Again, although this shows that there can be high stress concentration zones that are considered bad for nanofibre/matrix interface they can also indicate a better stress transfer with a convenient matrix.

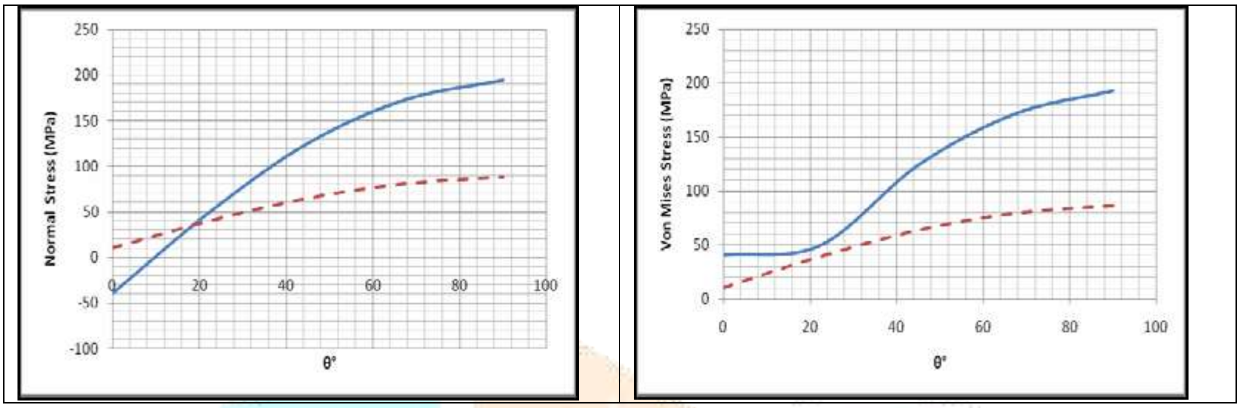

Figure 3 Nanofibre stiffness effect on stresses along nanofibre circumference

3.2 Nanofibre shape effect :

Micromechanical matrix/reinforcement interlocking, chemical bonding and the weak van der Waals force are three main mechanisms of interfacial load transfer hence, the use of shaped nanofibres. The latter are not new in conventional composite materials. Consequently, in this investigation, star-shaped and hexagonal-shaped nanofibres with the same volume were simulated under loading using FEA. The aim was to investigate their performance in improving matrix/reinforcement stress transfer compared to rounded cross section nanofibres. Figure 4 shows that star shaped nanofibres carry higher stresses than rounded and hexagonal shaped nanofibres even if the nanofibre length was increased. Hexagonal shaped nanofibres also performed better than rounded nanofibres with 20 nm to 50 nm long. It should also be noted that von mises minimum stresses are not appearing in the figure because they are close to 0. In summary, the results indicate that by maintaining a strong bond between the nanofibre and the matrix, star shaped fibres have a good potential in producing high strength nanocomposites. However, experimental investigations are required to confirm this study since researchers have reported some discrepancies between FEA studies and their equivalent experiments especially since it is known that inefficient shear stress transfer can lead to poor nanocomposites properties.

Length 10nm And Stiffness 50GPa

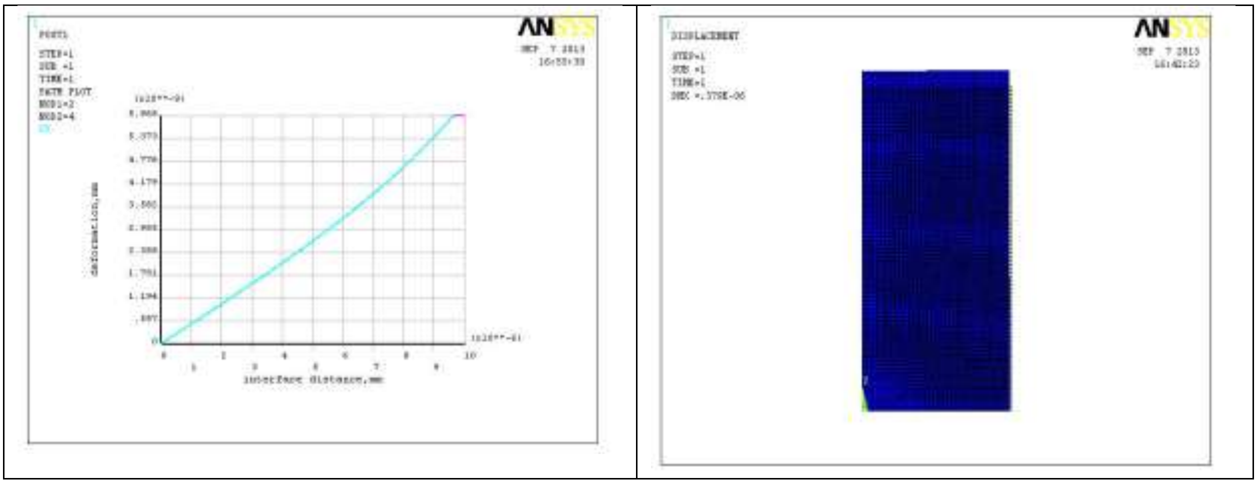

Figure 4: Deformation of Shape.

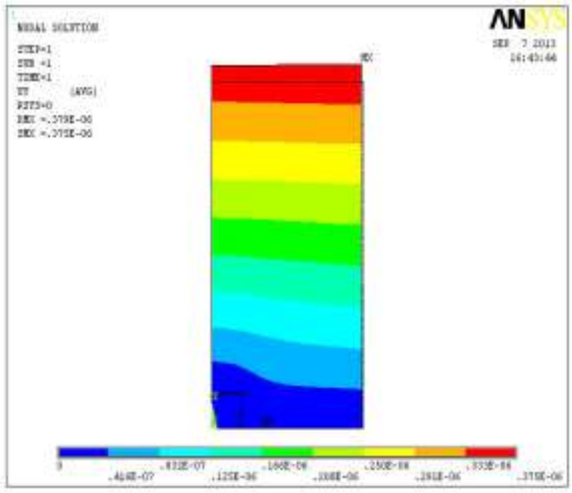

Figure 5: Deformed in Y Direction

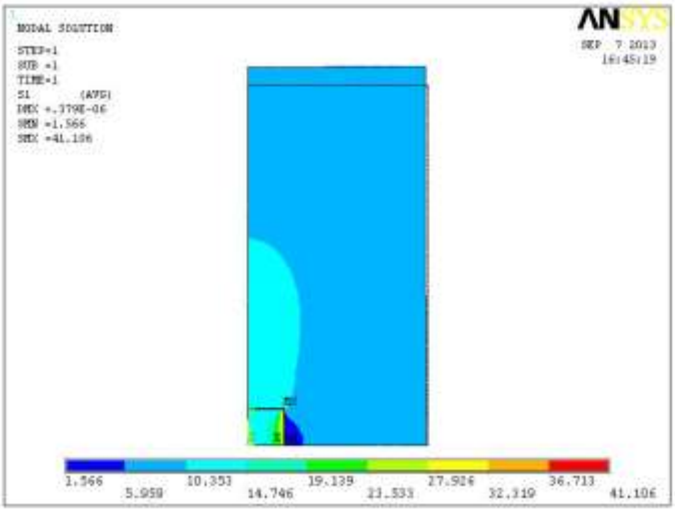

Figure 6: Principal Stress

4.RESULTS AND DISCUSSIONS :

The FEA equivalent (von mises) stress field as a result of applying a 10 MPa tensile stress on an RVE with a rounded nanofibre. It is clearly seen that the very high stresses are found at the nanofibre/interface which has the potential to initiate damage. Figures 5 and 6 show the effect of increasing a nanofibre length from 20 nm to 50 nm (with a stiffness E = 600 GPa for both nanofibres) under the 10 MPa static tensile load. It should be noted here that the increase in the nanofibre length was made while maintaining the volume of the matrix. Hence, this length increase implies a nanofibre volume fraction increase. Figure 5 shows how the normal, principal and von mises stresses increase along the cross section circumference where high stresses are registered at the nanofibre/matrix interface. It is found here that a long nanofibre results in more stresses being applied on it. This increase in stress is also expected to result in a stronger nanocompsoite as a result of the nanofibre length increase. In Figure 6, von mises stresses show that a longer nanofibre carries more stress along its radius, whereas the principal and normal stresses are not affected greatly. Another initial observation which was noticed throughout all of this investigation is the apparent high stress ratio between the nanofibre and the matrix. Unlike what Xu and Sengupta have noticed (a 1.6 stress ratio between nanofibre and the matrix), a stress ratio of over 100 times was observed in this investigation. In comparison to conventional composite materials, researchers have been proposing the use of continuous (long) fibres over the traditional discontinuous (short) fibres Xu and Sengupta, Thostenson et al., However, a manufacturing challenge still remains in using high nanofibre/nanoftube aspect ratios due the formation of bundles, agglomerates and clusters when mixing with the matrix.

CONCLUSIONS

Nanofibre/nanotube reinforced polymeric nanocomposites have the potential of widespread use in aerospace structures. However, to achieve highly tailored properties, the nanofibre/matrix interface properties need to be controlled. In this work, it has been demonstrated that understanding of the micromechanical interactions that take place between the reinforcement and the matrix is the first step into producing multi-functional nanocomposite components. In particular, the FEA of various forms of nanofibre shapes and volume fractions revealed, as expected, that interfacial debonding is the most likely source of damage nucleation and initiation. It is found that the nanofibre/matrix debonding can be attributed to the high stress concentrations at the nanofibre ends which can be made more severe with poor interfacial shear stress transfer. It is therefore recommended that to achieve high strength in aerospace components made of nanofibre reinforced polymeric nanocomposites and to reduce early damage initiation and propagation the following are necessary:

- The reinforcement: shaped nanofibres with an optimised length rather than the conventional rounded and short nanofibres/nanotubes.

- The matrix: as with conventional composites, the interface should not be too strong and not too weak to produce an optimised stress transfer. It is also argued that the formation of stress concentrations at the fibre/matrix interface can be regarded as an indication of good matrix to nanofibre stress transfer.

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