Int. J. Nanoparticles, Vol. X, No. Y, xxxx

Nanocomposites damage characterisation using finite element analysis

M. Bourchak*, B. Kada, M. Alharbi and
K. Aljuhany

Department of Aeronautical Engineering, Faculty of Engineering,
King Abdulaziz University, Jeddah 21589, KSA
E-mail: mbourchak@kau.edu.sa
E-mail: belkacemkad@hotmail.com
E-mail: meshary2000@yahoo.com
E-mail: chairman-aero@kau.edu.sa
*Corresponding author

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 behaviour of nanofibres is characterised by finite element analysis (FEA). In particular, the stiffness mismatch of the nanofibres 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 optimised 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.

Keywords: nanocomposites; nanofibres; finite element analysis; FEA; failure analysis; damage initiation; static loading; von mises; damage characterisation; nanoparticles.

Reference to this paper should be made as follows: Bourchak, M., Kada, B., Alharbi, M. and Aljuhany, K. (xxxx) ‘Nanocomposites damage characterisation using finite element analysis’, *Int. J. Nanoparticles*, Vol. X, No. Y, pp.000–000.

Biographical notes: Mostefa Bourchak is Assistant Professor in the Department of Aeronautical Engineering at King Abdulaziz University, KSA.

Belkacem Kada is Assistant Professor in the Department of Aeronautical Engineering at King Abdulaziz University, KSA.

Mohamed Alharbi is Lecturer in the Department of Aeronautical Engineering at King Abdulaziz University, KSA.

Khalid Aljuhany is Assistant Professor and Head of Department in the Department of Aeronautical Engineering at King Abdulaziz University, KSA.

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 a reinforcement (e.g., nanofibres or nanotubes) in a matrix such as a polymer one (Ajayan et al., 2003) 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 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 (Njuguna and Pielichowski, 2004).

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 optimise their design.

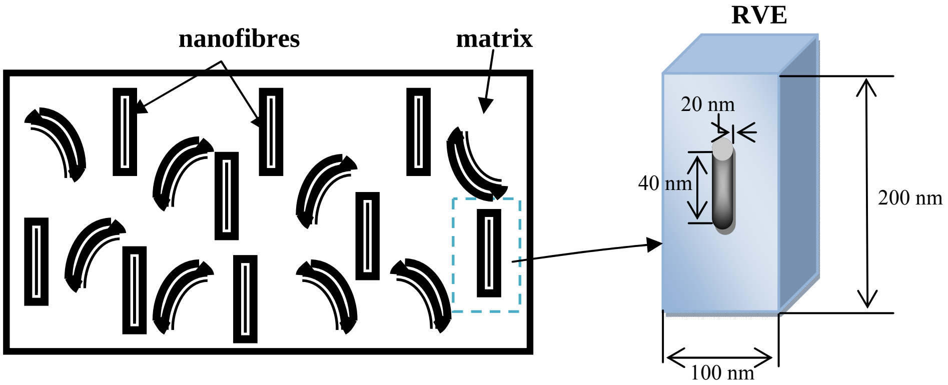
The matrix interface with the nanofibres and stress transfer are the two main sources behind a mechanically strong or weak nanocomposite material. All efforts are initially made to make this interaction strong. Under mechanical loading, stress concentrations will occur at the matrix/nanofibre interface which will eventually lead to damage nucleation, initiation, growth and final non-tolerated failure. There are two likely sources of damage nucleation in nanocomposites; poor wetting of the nanofibres by the polymer and the aggregation of the nanofibres (Xu et al., 2004). Both cases produce polymer rich nanocomposite portions that are likely to experience low stress to failure.

Xu and Sengupta (2005) 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.

2 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.

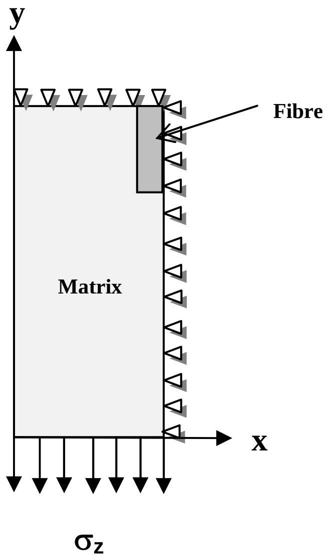
Figure 1 An illustration of a typical nanocomposite entity and an RVE (see online version for colours)



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 ($E_f = 600$ GPa, $E_m = 2.6$ GPa and $\nu_f = \nu_m = 0.3$) have been obtained from the literature (Xu and Sengupta, 2005).

As illustrated in Figure 2, 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.

Figure 2 A view of a 1/4 of RVE subjected to 10 MPa tensile load



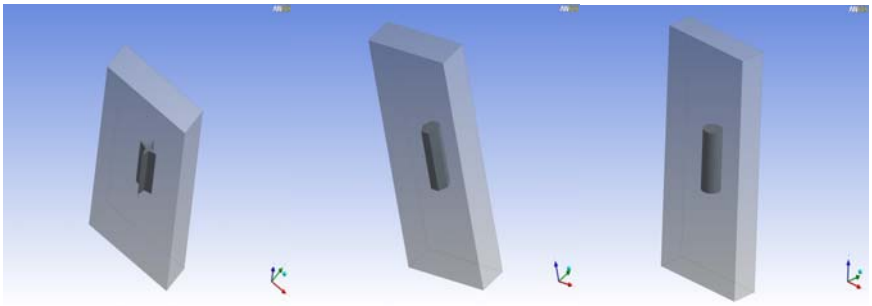
Maximum principal stresses, von mises stress and normal stresses were analysed along the nanofibre short interface (x direction in this study) and along the nanofibre cross section (e.g., in a rounded nanofibre, stresses were obtained along the circumference) as well as at the highest stress points on 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 Figure 3.

Figure 3 Three different cross shaped nanofibres were investigated (see online version for colours)



3 Results and discussions

3.1 Nanofibre length and volume fraction effect

Figure 4 shows 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 (2005) 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, 2005; Thostenson et al., 2005; Liu and Chen, 2002). 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.

Figure 4 FEA stress field on ¼ of RVE under 10 MPa tensile load (see online version for colours)

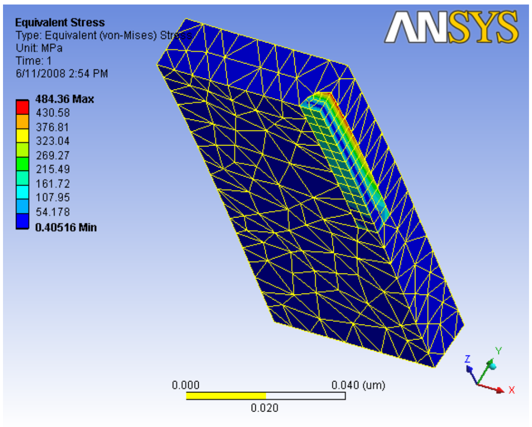


Figure 5 Nanofibre length effect on stresses along nanofibre circumference (see online version for colours)

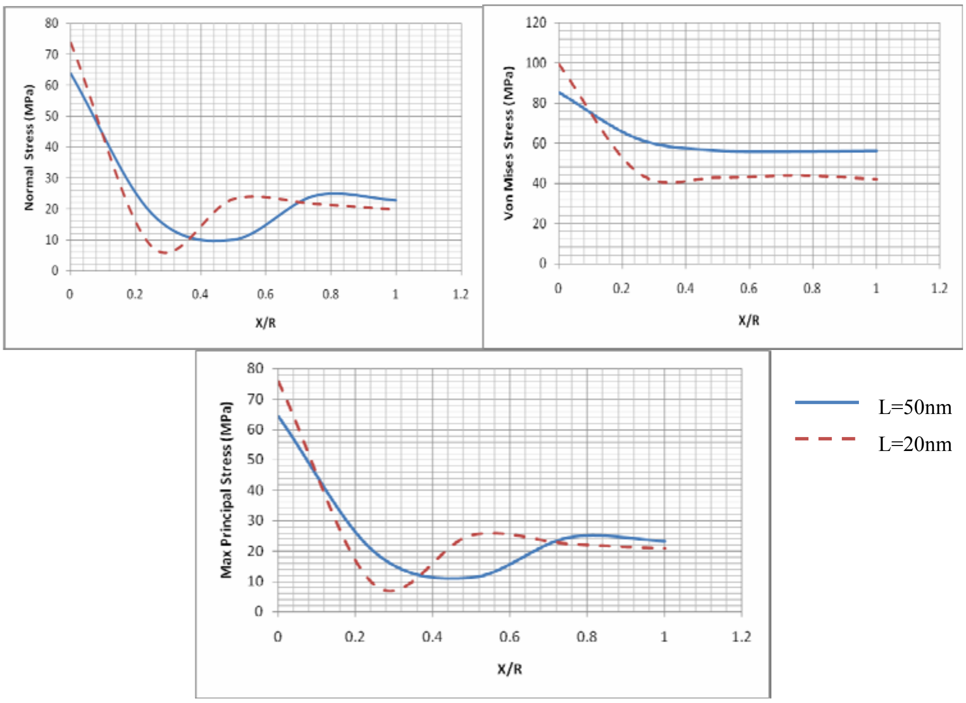
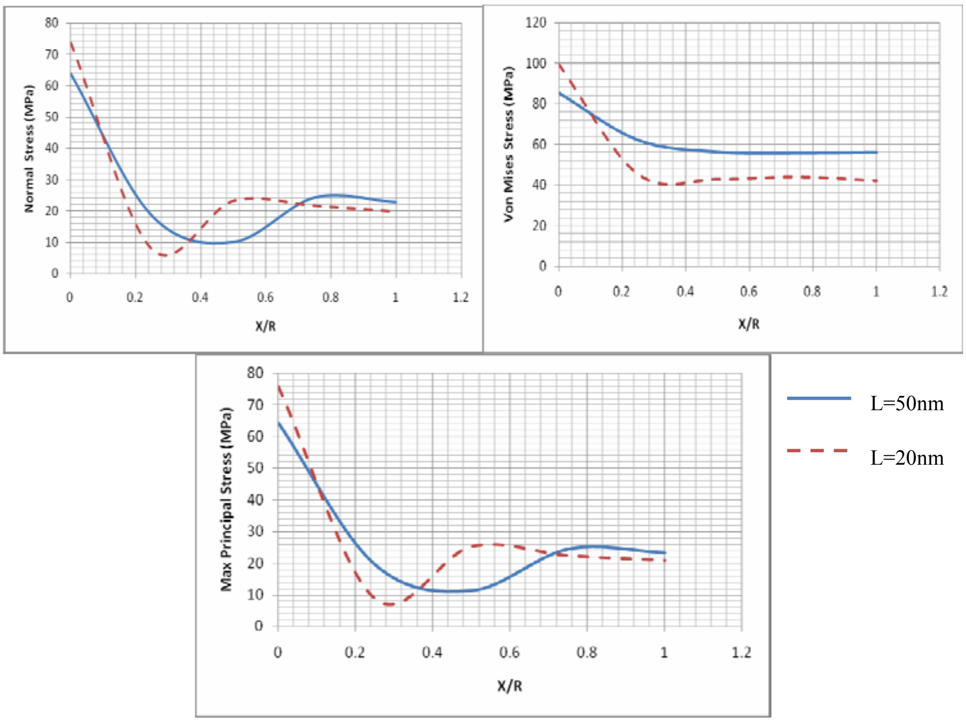


Figure 6 Nanofibre length effect on stresses along nanofibre radius (see online version for colours)



3.2 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 7 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, as those investigated by Xu and Sengupta (2005) are not conclusive indicators. 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 7 Nanofibre stiffness effect on stresses along nanofibre circumference (see online version for colours)

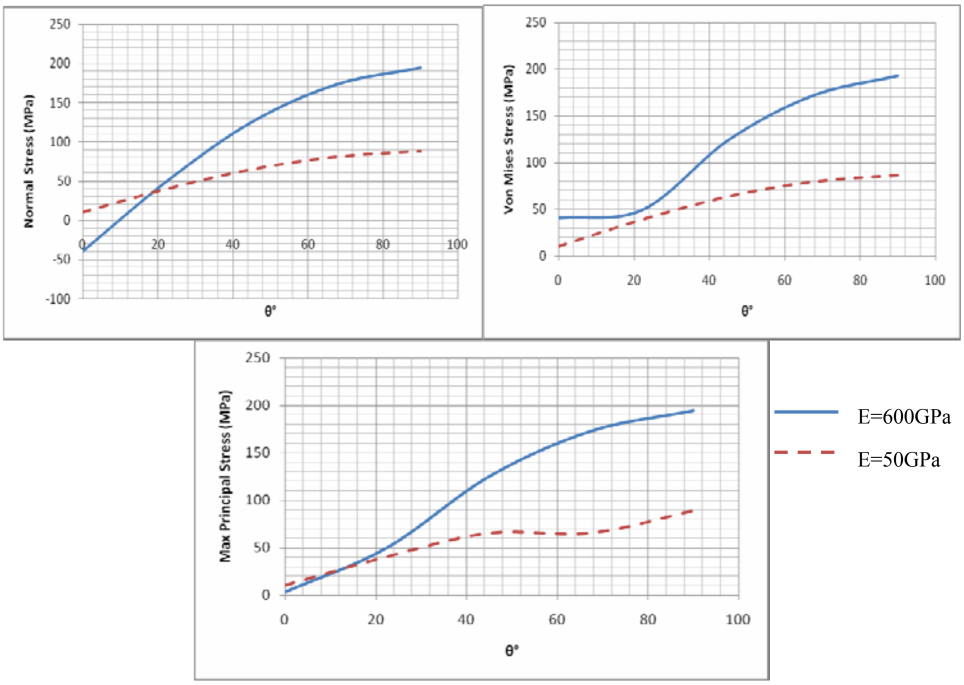
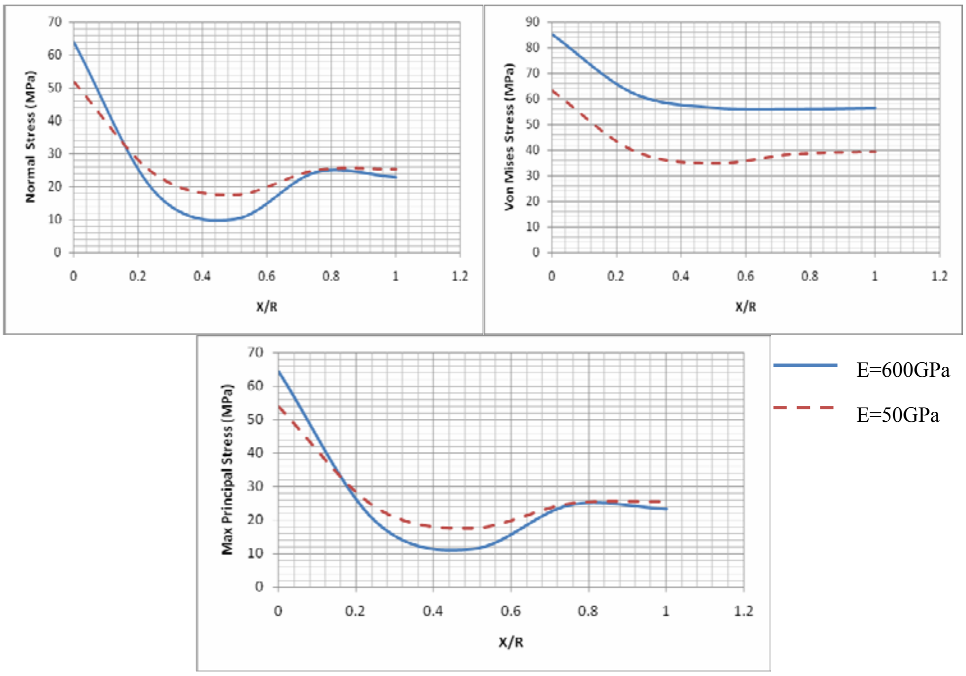


Figure 8 Nanofibre stiffness effect on stresses along nanofibre radius (see online version for colours)

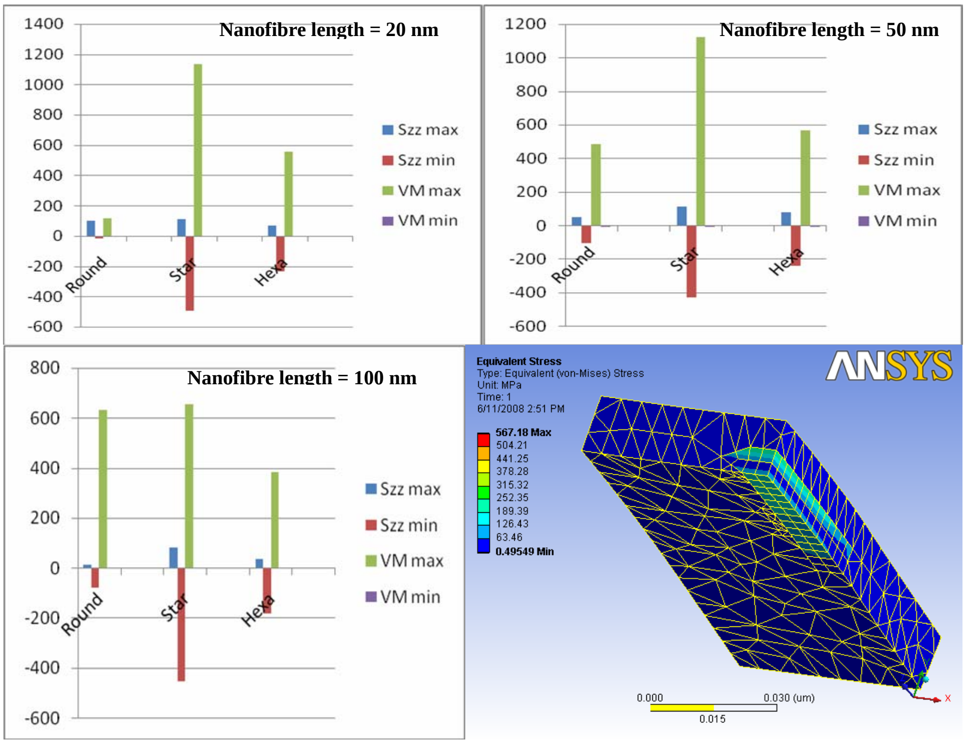


3.3 *Nanofibre shape effect*

Micromechanical matrix/reinforcement interlocking, chemical bonding and the weak van der Waals force are three main mechanisms of interfacial load transfer (Schadler, 1998) 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 9 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 (Spanos and Kontsos, 2008) especially since it is known that inefficient shear stress transfer can lead to poor nanocomposites properties (Xu et al., 2007).

Figure 9 Nanofibre shape and length effect (see online version for colours)



4 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.

References

Ajayan, P.M., Schadler, L.S. and Braun, P.V. (2003) *Nanocomposite Science and Technology*, p.77, Wiley-VCH Verlag GmbH Co. K GaA, Weinheim.

Liu, Y.J. and Chen, X.L. (2002) 'Evaluations of the effective material properties of carbon nanotube-based composites using a nanoscale representative volume element', *Mechanics of Materials*, Vol. 35, pp.69–81.

Njuguna, J. and Pielichowski, K. (2004) 'Polymer nanocomposites for aerospace applications: characterization', *Advanced Engineering Materials*, Vol. 6, No. 4, pp.204–210.

Schadler, L.S., Giannaris, S.C. and Ajayan, P.M. (1998) 'Load transfer in carbon nanotube epoxy composites', *Applied Physics Letters*, Vol. 73, pp.38–42.

Spanos, P.D. and Kontsos, A. (2008) 'A multiscale Monte Carlo finite element method for determining mechanical properties of polymer nanocomposites', *Probabilistic Engineering Mechanics*, article in press, corrected proof.

Thostenson, E.T., Li, C. and Chou, T. (2005) 'Review: nanocomoposites in context', *Composites Science and Technology*, Vol. 65, pp.491–516.

Xu, L.R. and Sengupta, S. (2005) 'Interfacial stress transfer and property mismatch in discontinuous nanofibre/nanotube composite materials', *Journal of Nanoscience and Nanotechnology*, Vol. 5, No. 4, pp.620–626(7).

Xu, L.R., Bhamidipati, V., Zhong, W., Li, J., Lukehart, C.M., Lara-Curzio, E., Liu, K.C. and Lance, M.J. (2004) 'Mechanical property characterization of a polymeric nanocomposite reinforced by graphitic nanofibres with reactive linkers', *Journal of Composite Materials*, Vol. 38, No. 18, pp.1563–1582.

Xu, L.R., Li, L., Lukehart, C.M. and Kuai, H. (2007) 'Mechanical characterization of nanofibre-reinforced composite adhesives', *Journal of Nanoscience and Nanotechnology*, Vol. 7, pp.1–3.