FINITE ELEMENT PREDICTION OF MECHANICAL PROPERTIES OF PLAIN WEAVE CARBON FABRIC AND CARBON NANOTUBES REINFORCED NANOCOMPOSITE

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Abstract
Modeling and analyzing a unit cell had been shown in this study as a successful technique for predicting mechanical properties for plain weave carbon fiber/carbon nanotube/phenolic resin composites. To simulate the effects of CNTs for the composites, Mori-Tanaka theory was used to calculate the mechanical properties of CNTs reinforced phenolic resin material. Then, these results were adopted for matrix of the unit cell model. This unit cell model was used to predict the tensile behavior of carbon fiber/carbon nanotube/phenolic resin composites. From the comparison between experimental and static analysis results, it may infer that when strain over 1%, the cracks will work for weaken the tensile strength of the composite. Moreover, due to the initial micro cracks and voids did not consider in this study, there is a difference between the results of experiments and simulations.

1 Introduction
Due to the high ratios of strength and stiffness to weight, high thermal and chemical resistance, and environmental resistance, these superior properties of composites that make them more specific than other materials. Most of composites, such as multiscale materials, are developed in order to improve the combination of mechanical characteristics of materials. Moreover, carbon fiber reinforced plastic (CFRP) materials are regarded as promising materials in many industry areas, especially for aerospace applications.

As known, nanostructured polymers, formed by addition of small amount of nanoparticles (e.g. carbon nanotubes (CNTs), carbon nanofibers (CNFs), and nano clay) have much better mechanical properties than the common polymers. Thus, by adding nano-scale particles, multiscale composites were developed based on CFRP materials [1]. Compared to unidirectional laminates, the mechanics of woven composites is more complex because of the curved shape of the reinforcing fibers. Thus, analytical and computational models can contribute to an enhanced understanding on damage evolution and laminate strength [2-4]. Many researchers also have devoted their efforts to the study of simulating mechanical properties of polymer composites with nano-scale reinforcement. The challenges were to simulate the mechanisms responsible for the strong effect of small amount of nanoreinforcement in composite and to generalize the micromechanical methods of modeling common micro-scale reinforced composites to the case of nano-scale reinforcement [1, 5].
However, modeling strength is particularly complex theoretically and accepted procedures have not yet been validated completely. In this study, a unit cell modeling was proposed to study the mechanical behavior of CFRP reinforced by CNTs. Firstly, Mori-Tanaka micro mechanics model [6] was employed to calculate the mechanical properties of CNTs reinforced phenolic resin material. Then, a unit cell modeling was used to predict the mechanical properties of the composite by using ANSYS Workbench 12.1v.

2 Numerical modeling

2.1 Mori-Tanaka theory

The theoretical approach used in this paper is based on the classical continuum mechanics of composites. The Young’s modulus, shear modulus and Poisson’s ratio of the CNTs reinforced phenolic resin material are obtained as a function of nanotube orientation, distribution, aspect ratio and volume fraction by using the Mori-Tanaka theory. When considered the orientation of CNTs, it was assumed that CNTs are rigid rods. In case of random distribution, CNTs reinforced phenolic resin material could be treated as a homogenous material. The aspect ratio of CNTs is presented as \( s = \frac{L}{D} \) (\( L \), length of CNTs; \( D \), diameter of CNTs). With these assumptions, the elastic constants can be calculated using the following expression [6]:

\[
C^e = C^M + V_f \left( (C^M - C^e) A^N \right) \left( 1 - V_f \right) f + V_f A^N
\]

where \( C^C \), \( C^M \) and \( C^cnt \) are the stiffness tensors of the composite, matrix and CNT, respectively, \( V_f \) is the volume fraction of CNTs, \( I \) is the identity tensor. The dilute mechanical strain concentration tensor, \( A^N \), is given by:

\[
A^N = \left[ I + S \left( C^M \right) \left( C^M - C^e \right) \right]^3
\]

where \( S \) is the Eshelby tensor, which is function of the aspect ratio of CNT and the Poisson’s ratio of matrix.

2.1 Unit cell model

Finite element method (FEM) is a numerical method of structural analysis. The basic idea of this method is a physical discretization of a continuum. Because plain weave fabrics are formed by interlacing or weaving two sets of orthogonal yarns in weft and warp directions, thus, plain weave fabric reinforced composite could be divided into numerous repeated unit cells consisting resin matrix, weft yarns, and warp yarns as shown in Fig. 1. In the unit cell, a global Cartesian coordinate system (\( x, y, z \)) is established. The unit cell was subject to a uniaxial tensile displacement loading along \( x \) or \( y \) axis direction (defined as Fig. 1a). FE model shown in Fig. 1b was modeled and meshed for the simulations by using ANSYS Workbench 12.1v. With a 0.002mm size of element, total nodes and elements of the model are 306739 and 157567, respectively. Moreover, the fiber volume fraction in the yarn \( V_f \) is necessary to calculate the yarn properties using micromechanics. Although the yarn volume fraction is very difficult to measure directly, it can be calculated from the overall volume fraction \( V_o \) and the calculated mesoscale volume fraction \( V_g \). It was easily to calculate the fiber volume fraction in this model is 50%.
3 Experimental details

3.1 Preparation of specimen

Multi-wall carbon nanotube (MWCNT, Hanwha Nanotech Corporation, Korea), plain weave carbon fabric (Mitsubishi TR30, 3K), and phenolic resin were used to prepare multiscale composites. To obtain a good dispersion of CNTs in phenolic resin, three-roller mill was used, then, resin films were produced having a 3 mm thickness. The weight fraction of CNTs was kept as 1 wt.% with respect to phenolic resin. After cured in the oven, resin films and carbon fabrics were stacked up one by one. Finally, the product was put into mold for hot-press processing.

3.2 Tensile test

The tensile tests were performed at room temperature and pressure using a universal tensile test machine (Instron, US) at Korean Institute of Materials Science (KIMS) as shown in Fig. 2. The crosshead speed for tests was set at 0.5 mm/min.

4 Results and discussion

Using the Mori-Tanaka theory, the Young’s modulus and shear modulus of CNTs reinforced phenolic resin material were calculated as a function of CNT volume fraction. The results were shown in Fig. 3.
The Young’s modulus in x-direction could be calculated by the loading a nonzero displacement on the face which is located at X=l_w. According to the periodic boundary condition, symmetrical boundary conditions were loaded on the faces which are located at X=0, Y=0 and Z=0.

The elasticity modulus in x-direction could be calculated by the following equation,

$$E_x = \frac{\sum F_x \times l_w}{l_z \times H_z \times \Delta x}$$

\hspace{1cm} (3)

Figure 4. Results of the equivalent stress: a) X=0.001 mm, b) X=0.003 mm, and c) X=0.005mm

For a static analysis, three different displacement loadings were given on the model. Results of the equivalent stress were shown in Fig. 4. The maximum stress was found at the yarns of warp direction. In case of X=0.001 mm, the maximum stress is around 270 MPa, it may cause the initial failure of the matrix in the composite. In case of X=0.003 mm, the maximum stress is over 1120 MPa, it indicates the failure of fibers and matrix had been generated. And in case of X=0.005 mm, the maximum stress is reach to 1869 MPa, the generated cracks would be propagated.

The results of total deformation distribution were shown in Fig. 5. The asymmetric distribution was caused of the different curve shapes of fiber yarns in warp and weft directions.

Compared to the experimental results of tensile strength, it is found that there is a good agreement of Young’s modulus as shown in Fig. 6. However, due to only static analysis was performed, the result of FEA increased linearly, which means failure of the experimental
tensile behavior could not be predicted. In other words, because the damage cannot be accumulated in static analysis, crack propagation and imperfect bonding conditions were not considered.

![Figure 5](image1)

(a) ![Figure 5](image2) (b) ![Figure 5](image3) (c) Figure 5. Results of the total deformation distribution: a) X=0.001 mm, b) X=0.003 mm, and c) X=0.005mm.

![Figure 6](image4)

Figure 6. Comparison between experimental result and FEA result of tensile behavior.

5 Conclusions
Based on Mori-Tanaka theory, the mechanical properties of CNTs reinforced phenolic resin material were calculated. Then, a unit cell model was developed to study the tensile behavior of carbon fiber/carbon nanotube/phenolic resin composite. From the comparison between experimental and static analysis results, it may infer that when strain over 1%, the cracks will work for weaken the tensile strength of the composite.

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