This is the published version:


Available from Deakin Research Online:

http://hdl.handle.net/10536/DRO/DU:30057802

Every reasonable effort has been made to ensure that permission has been obtained for items included in Deakin Research Online. If you believe that your rights have been infringed by this repository, please contact drosupport@deakin.edu.au

Copyright : 2013, Fragrance Journals
Bending Behavior of Step-wise Graded Carbon Nanofiber/Polymer Nanocomposites

Ehsan Bafekrpour¹, ³, Chunhui Yang², Bronwyn L. Fox³
¹Department of Materials Engineering, Monash University, Clayton, Melbourne, Victoria 3800, Australia
²School of Computing, Engineering and Mathematics, University of Western Sydney, Locked Bay 1797 Penrith, New South Wales 2751, Australia
³Institute for Frontier Materials, Deakin University, Locked Bag 20000 Geelong, Victoria 3220, Australia
¹ehsan.bafekrpour@monash.edu, e.bafekrpour@gmail.com

Abstract - In this study, a finite element-based model was developed to investigate the mechanical behavior of step-wise graded carbon nanofibre/phenolic nanocomposites. Four step-wise graded nanocomposites (FGNs), a non-graded nanocomposite (NGN), and a pure phenolic with the same geometry and total carbon nanofiber content were designed, fabricated and analyzed. Flexural tests were conducted to validate the finite element model. Close agreement was obtained between experimental results and numerical predictions. The results showed that flexural modulus was highly influenced by the compositional gradients.

Keywords - Finite element modeling; nanocomposites; carbon nanofiber; phenolic

1 INTRODUCTION

Functionally graded materials (FGMs) are advanced composite materials consisted of two constituents with a controlled compositional gradient in one or two directions of the structure (Jin and Paulino 2001). The idea of FGMs enables tailoring the mechanical, thermal, and chemical properties of materials by comprising different properties. A common example of FGMs is step-wise graded ceramic-metal composites which are based on the thermally insulating properties of ceramic component and the mechanical strength, thermal conductivity, and ductility of the metallic component (Praveen and Reddy 1998; Peng and Li 2010). One of the main applications of ceramic-metal FGMs is as thermal barrier coatings, allowing for a smooth transition from metal to ceramic in aerospace industry (Nemat-Alla, Ahmed et al. 2009). Nanocomposite materials are a relatively new class of materials with a reinforcing constituent in nano-scale level (Al-Saleh and Sundararaj 2011). They have generated much interests due to their superior thermal (Adhikari, Georgiev et al. 2012), mechanical (McCullen, Stevens et al. 2007), electrical (Liu, Wood et al. 2011), and physical (Ramaswamy, Clarke et al. 2011) properties, often for low concentrations of additives. The concept of FGMs has been recently applied to nanocomposites to optimize the nano-scale reinforcing constituent consumption and providing nanocomposites with different properties for multifunctional applications. We have recently reported the fabrication of functionally graded nanocomposites with a significant improvement in thermo-mechanical and viscoelastic properties (Bafekrpour, Kafi et al. 2012; Bafekrpour, Simon et al. 2012; Bafekrpour, Simon et al. 2012; Bafekrpour, Simon et al. 2013). We also showed that the temperature gradient field and transient time of functionally graded nanocomposites are highly influenced by the compositional gradients (Bafekrpour, Habsuda et al. 2011; Bafekrpour, Simon et al. 2012; Bafekrpour, Simon et al. 2013). Taeprasartsit (Taeprasartsit 2012) derived the exact displacement fields of a functionally graded column subjected to mechanical and thermal loads under the assumptions of the Timoshenko beam theory and von Karman strains. Shahjerdii et al. (Shahjerdii, Mustapha et al. 2011) employed Second-order shear deformation theory to analyze vibrations of temperature-dependent functionally graded plates. Bayat et al. (Bayat, Sahari et al. 2012) elastic solutions of a disk made of functionally graded material (FGM) with variable thickness subjected to rotating load and concluded that sigmoid functionally graded rotating functionally graded disk with metal–ceramic–metal combination can be more efficient than the one with ceramic–metal or metal–ceramic. Finite element method (FEM) had been extensively used to analyze mechanical behavior of FGMs (Boukhalfa, Hadjou et al. 2008; Taeprasartsit 2010). Hamza-cherif et al. analyzed transient temperature distribution in functionally graded materials using the h-p version of the FEM. Chen (Chen and Lin 2007) presented the crack problem in antiplane elasticity of FGMs using Fourier transform method. However, a systematic study on influence of compositional gradient on mechanical behavior of step-wise graded carbon nanofiber/phenolic nanocomposite beams has not been reported yet in literature, and thus further studies of such advanced nanocomposites are still required.

In present study, step-wise graded carbon nanofiber/phenolic nanocomposites were designed and fabricated and a finite element-based model was also employed to investigate the effect of gradient patterns on flexural properties. For validation and verification, flexural tests were conducted for all graded non-graded samples according to the ISO 178 the numerical results were compared with the experimental data.
Graphitized carbon nanofibers with diameters of 200-500 nm, 99% purity and density of 1.75 g/cm³ supplied by Nanostructured & Amorphous Materials, Inc., were used as nano-scale reinforcing constituents. A phenolic thermosetting resin with ~9% hexamethylenetetramine obtained from Hexion Specialty Chemicals Pty Ltd was used as the matrix material. Four different stepwise step-wise graded nanocomposites as well as non-graded nanocomposites with the same geometry and total CNF content (5.5 wt% CNF) were designed and prepared. In order to keep the total CNF content constant in all FGNs and NGN samples, the samples were divided to eight distinct layers across thickness and various compositions in these layers were purposely designed as shown in Fig. 1.

![Fig. 1. (a) Geometry of the beam; schematic representations of compositional gradient configurations across the thickness of the beam: (b) FGN-1, (c) FGN-2, (d) FGN-3, (e) FGN-4, and (f) NGN.](image)

The powder mixtures of CNFs and phenolic resin with 2, 4, 5.5, and 16 wt% CNF contents were ball milled for 3 minutes (8000M, Mixer/Mill, Maker, Spex, USA) to ensure homogeneous dispersion of CNF within the phenolic resin. A die with a rectangular cut-out of dimension 200 × 200 mm² and depth of 50 mm and a punch were designed. Premixed composite powders of certain CNF contents were settled in a die of a hot press in a desired sequence using a stacker device. The graded stacks of composite powders were heated up to 130°C for 10 minutes and subsequently hot pressed at 180°C and with a 4-tonne force for 10 minutes and finally cooled down. The square plate samples had the thickness of 5 mm (Bafekrpour, Simon et al. 2013; Bafekrpour, Simon et al. 2013).

### 3 TENSILE AND FLEXURAL TESTS

The Young's modulus of phenolic and its nanocomposites containing 2, 4, and 16 wt% CNF were measured especially for finite element analysis. They were obtained from the tensile test according to ISO 527-3 using a 30 kNInstron tensile tester with a video camera for recording displacement. All tests were conducted at a crosshead speed of 1 mm/min at room temperature. The tensile test samples were 50 × 10 × 1.5 mm³. Three measurements were taken for each individual nanocomposite layer.

The three-point bending test was performed on phenolic, FGNs, and NGN samples using a computer controlled LLOYD LR30K testing machine as shown in Fig. 2. The tests were conducted according to the ISO 178 at the crosshead speed of 1 mm/min. The beam samples for flexural tests were cut with 100 × 10 × 5 mm³, while the span length was 80 mm. FE predictions of deflection and flexural modulus of phenolic, FGNs, and NGN were verified by studying the load-deflection behavior of the samples. At least three identical samples were used for each sample condition to ensure the reproducibility in load-deflection results.
4 FINITE ELEMENT MODELING

Due to symmetry, a ½ 2-D finite element model was developed using a commercial finite element analysis package – Abaqus to simulate the flexural test (Hibbitt, Karlson et al. 2009). To be able to assign the stepwise variation in material properties of the experimentally produced step-wise graded nanocomposite, a beam with thickness of 5 mm, consisting of eight layers of the same thickness of 0.625 mm was developed. Fig. 3 shows the typical mesh of the proposed FE model.

Fig. 3. 2-D FE model of three-point bending test of the stepwise step-wise graded nanocomposite beams.

Dimensions of the model were devised according to the ISO 178. layers were considered homogeneous and isotropic. Tie conditions were applied to the contact surface of the layers. The element CPS4R was selected to discretise the FGN beams, which is a 4-node bilinear plane stress quadrilateral element available in Abaqus element library. Mesh sensitivity and convergence of the model were checked by changing the number of elements. The load was converged using 600 (3×200) elements in each layer as shown in Fig. 4.
5 RESULTS AND DISCUSSION

The Young’s modulus of the pure phenolic was 2.63 GPa and continuously increased to 3.09, 3.55, 4.49 GPa by adding 2, 4, and 16wt% CNF, respectively. However, the increase of Young’s modulus was less significant beyond 16wt% CNF due to the non-uniform dispersion of CNFs within the matrix. This behavior has also been reported for other nanocomposites (Choi, Sugimoto et al. 2005). Therefore, an optimization in design of nanocomposite compositions is essential due to the limited reinforcing effects and fully take advantage of their mechanical properties. The effective flexural modulus of FGNs, NGN, and phenolic was calculated using the Euler–Bernoulli beam theory (classical beam theory) from the experimental and numerical mid-span deflection for the applied load of 100 N as below:

\[ E_{ex} = \frac{FL^3}{48Iw(f/j)} \]  

Where, \( F \), \( L \), \( I \), and \( w(f/j) \) denote the applied load, span length, moment of inertia, and the mid-span deflection of the beam, respectively. The FE predictions of mid-span deflection and effective flexural modulus of FGNs, NGN, and phenolic are presented in Table 1 and compared with the experimental results.

Table 1. Numerical and experimental values for mid-span deflection and effective flexural modulus for the total applied load of 100 N.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Mid-span deflection, ( w(f/j) ) (mm)</th>
<th>Error (%)</th>
<th>Flexural modulus, ( E_{ex} ) (GPa)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FEA</td>
<td>Experimental</td>
<td></td>
<td>FEA</td>
</tr>
<tr>
<td>FGN-1</td>
<td>2.58</td>
<td>2.76</td>
<td>6.52</td>
<td>3.97</td>
</tr>
<tr>
<td>FGN-2</td>
<td>3.57</td>
<td>3.84</td>
<td>7.03</td>
<td>2.86</td>
</tr>
<tr>
<td>FGN-3</td>
<td>3.05</td>
<td>3.42</td>
<td>10.8</td>
<td>3.35</td>
</tr>
<tr>
<td>FGN-4</td>
<td>3.05</td>
<td>3.48</td>
<td>12.35</td>
<td>3.35</td>
</tr>
<tr>
<td>NGN</td>
<td>2.90</td>
<td>3.15</td>
<td>7.93</td>
<td>3.53</td>
</tr>
<tr>
<td>Pure</td>
<td>3.91</td>
<td>4.19</td>
<td>6.68</td>
<td>2.62</td>
</tr>
</tbody>
</table>

The graded and non-graded incorporation of CNF into the phenolic resin can reinforce the flexural properties. However, this improvement in flexural modulus was strongly affected by the distribution pattern of CNF within the matrix. FGN-1 with the highest concentration of CNFs on the top and bottom layers and pure phenolic in the center showed the highest flexural modulus, whereas FGN-2 with a reverse compositional change had the lowest modulus. The NGN sample with a uniform distribution of CNFs had the second highest modulus after FGN-1. FGN-3’s modulus was slightly higher compared to FGN-4. Therefore, the flexural properties can be optimized in terms of CNF content.

It was observed that FE results have good agreement with the experimental values. However, the FE model predicted lower deflection and higher effective flexural modulus for all samples compared to experimental data. The highest errors in the predicted mid-span deflection were 10 and 12% related to FGN-3 and -4, respectively, while the lowest errors were 6 and 7% related to FGN-1 and -2, respectively, among all FGNs. This is mainly...
due to the imperfect bonding between adjacent layers, anisotropy within the layers, existence of porosity, and induced residual thermal stress during fabrication process of FGNs due to differences in coefficient of thermal expansion of layers (Patton, Pittman et al. 1999).

Moreover, as shown in Fig. 5, the layers below the neutral axis are under tension while the layers above this neutral axis are under compression in three-point bending test and their tensile module may be different from compressive module. However, only tensile modulus was used for all layers in FE models. This effect was also confirmed with the fact that FGN-3 and -4 exhibited the same mid-span deflection as well as the same flexural modulus according to models, while their experimental deflections as well as their module were different. The contours of stress distribution in phenolic, NGN, and FGNs are also shown in Fig. 5.

6 CONCLUSION

Bending behavior of step-wise graded and non-graded nanocomposites were experimentally and numerically investigated. The flexural properties of nanocomposites were highly influenced by the gradient patterns across the thickness. With the same geometry and total CNF content, the sample, FGN-1 showed the best bending behavior.

ACKNOWLEDGEMENT

The authors would like to acknowledge the financial support of Advanced Manufacturing Cooperative Research Centre (AMCRC), Australia. We also acknowledge Dr. Steven Agius for his helpful guidance.

References


