11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

MULTISCALE MODELING OF COILED CARBON NANOTUBE/POLYMER NANOCOMPOSITES

Seyed Hadi Ghaderi[1] and Ehsan Hajiesmaili[2]

[1] Shahrood University of Technology, Shahrood 3619995161, I.R. Iran,
s.h.ghaderi@shahroodut.ac.ir
[2] Universitat Politecnica de Catalunya, CIMNE, Edifici C1, C/Gran Capitán, 08034 Barcelona, SPAIN, hajiesmaili@cimne.com

Key Words: *Nanocomposites, Coiled carbon nanotubes, CCNT, Multi-scale modelling, Molecular dynamics finite element method, MDFEM.*

The high stiffness and low density of carbon nanostructures suggest their use as reinforcement for nanocomposites. However, experimental observations indicate weak interfacial bonding between the carbon nanotubes (CNTs) and the matrix, stating that the performance of carbon nanocomposites is limited by the load transfer between the reinforcement and the matrix. Mechanical locking of the matrix and the reinforcement can improve the load transfer. From this point of view, helically coiled carbon nanotubes (CCNTs), which are CNTs with helical structure, may hold promise as reinforcement for nanocomposites. The helical shape of the CCNTs allow them to anchor in matrix and enhance the load transfer between the reinforcement and the matrix.

In this paper, mechanical properties of CCNT nanocomposites is studies and the effect of anchoring on their stiffness is investigated. For this purpose, two models are analysed. One model consists of a compact CCNT with small pitch where the matrix material cannot enter the space between the coils of the CCNT and thus no anchoring occurs, figure 1. The other model consists of a non-compact CCNT with large pitch where the matrix fills the space between the coils of the CCNT and thus the CCNTs are anchored in the matrix.

The CCNTs are modelled at the atomistic scale following the techniques presented in [1]. To model the bond stretching, bond bending and bond torsion the molecular dynamics finite element method (MDFEM) [2] and the DREIDING force-field are used. This model has been already verified in [3] and successfully used to predict the nonlinear mechanical properties of CCNTs. The matrix is modelled at the macroscopic scale using the continuum finite element method. For the compact CCNT model, the matrix is a hollow cylinder while for the non-compact CCNT model, the matrix looks like a nut into which the CCNT is screwed. The CCNT and the matrix are connected at the interface by van der Waals bonds. Two-node line elements and Lennard-Jones potential are used to model the van der Waals bonds at the interface.

Firstly, the two CCNTs are subjected to tensile axial forces at their ends to measure their spring constant. Figure 2 shows the tensile behaviour of the CCNTs normalized for one pitch. The spring constant for one pitch of the compact and the non-compact CCNTs are measured to be 4.08nN/nm and 4.04nN/nm respectively. To study the effect of anchoring on the stiffness of the nanocomposites, the CCNTs are selected such that their spring constant are almost equal.

The two CCNT composites are subjected to tensile force at their ends and the young's moduli of the CCNT composites are measured. The results reveal the effect of anchoring on the stiffness of the CCNT nanocomposites.

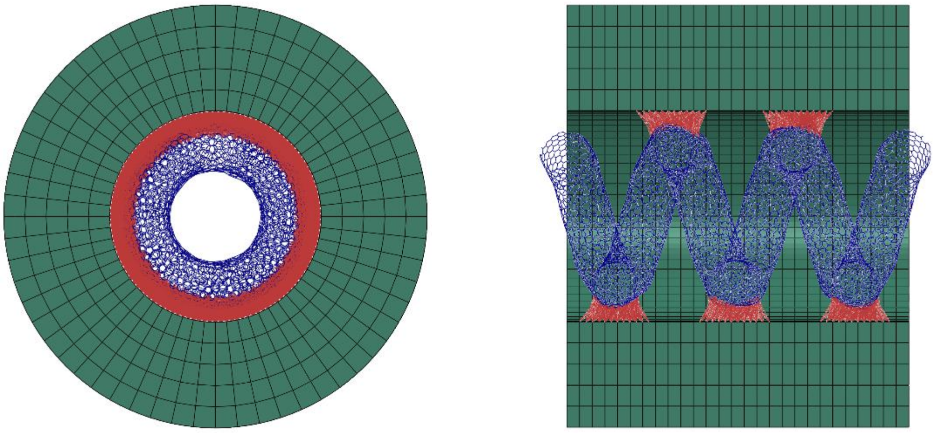

Figure 1. Multiscale model of the representative volume element of compact CCNT nanocomposite.

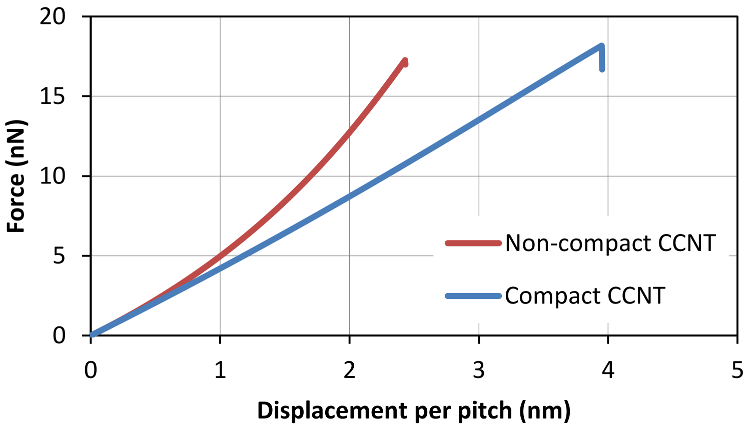

Figure 2. Nonlinear behaviour of compact and non-compact CCNTs under tensile force.

REFERENCES

[1] S. H. Ghaderi and E. Hajiesmaili, Molecular structural mechanics applied to coiled carbon nanotubes, *Computational Materials Science*, Vol. **55**, pp. 344-349, 2012.

[2] L. Nasdala and G. Ernst, Development of a 4-node finite element for the computation of nano-structured materials, *Computational Materials Science*, Vol. **33(4)**, pp. 443-458, 2005.

[3] S. H. Ghaderi and E. Hajiesmaili, Nonlinear analysis of coiled carbon nanotubes using the molecular dynamics finite element method, *Materials Science and Engineering: A*, Vol. **582**, pp. 225-234, 2013.