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Multiscale Modeling of Multifunctional Nanocomposites: Opportunities and Challenges

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ABSTRACT : In this lecture, I shall present multiscale modeling techniques that have successfully been developed in my laboratory to study multifunctional polymeric nanocomposite. Mechanical, interfacial, electrical, and piezoresistive properties of carbon nanotube (CNT)-reinforced polymer composites were investigated using molecular dynamics (MD), micromechanics, and coupled electromechanical modeling techniques. Experimentally, scanning electron microscopy and atomic force microscopy were used to determine the morphology and dispersion states of a typical CNT-epoxy composite. Based on these measurements, realistic nanocomposite structures were modeled using representative volume elements (RVEs) reinforced by CNTs with different aspect ratios, curvatures, orientations, alignment angles, and bundle size. The obtained atomistic mechanical properties of the composite constituents were then scaled up using Mori-Tanaka micromechanical scheme.

Additionally, Monte Carlo simulations were conducted to determine the percolation and electrical conductivity of RVEs containing randomly dispersed CNTs. An advanced search algorithm was developed to identify percolating CNT networks and transform them into an equivalent electrical circuit formed from intrinsic and tunneling resistances. A solver based on the modified nodal analysis technique was then developed to calculate the effective conductivity of the RVE. Finally, the electrical model was coupled with a three-dimensional finite element model of the RVE to determine the coupled electromechanical behavior of the composite under tensile, compressive, and shear loads from the resistance-strain relationship.

Keywords : Multiscale, Multifunctional, Nanocomposites, CNTs, Electromechanical

Biographical sketch: Prof. Shaker Meguid is an internationally renowned scholar with significant contributions in computational and experimental mechanics at varied length scales. He is the Founding Editor-in-Chief of Int. J. of Mechanics and Materials in Design, former Technical Associate Editor of ASME J. of Engineering Materials and Technology (for two consecutive terms), former Associate Editor of IMechE Journal of Mechanical Process Engineering, Guest Editor to a number of Journals. He is also the Founding Head of the Aerospace Engineering Division of Nanyang Technological University, Singapore. He is an Engineering Consultant to the United Nations, a lifetime senior member of AIAA, member of the American Academy of Mechanics, Professional Engineer in the Province of Ontario (PEng), Chartered Engineer in Great Britain (CEng), Fellow of ASME, Fellow of IMechE and Fellow of the Engineering Institute of Canada. He works closely with the aerospace and automotive industries and is regularly approached by members of the media for clarification of engineering issues and accidents. Prof. Meguid and his research team won numerous awards, with the most recent honor being the nomination by his department for the gold medal by the Governor General of Canada, holder of the Robert Hooke Award bestowed by the European Society for Experimental Mechanics, Engineering Award-Research and Development by the Professional Engineers of Ontario for his significant contribution to research and development in Canada.

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