

Electromagnetic Analysis of Composites with Realistic Carbon Nanotube Distributions as Determined by 3D Quantitative Electron Tomography

Spencer On⁽¹⁾, Marjorie Castro⁽¹⁾, Douglas Heller⁽¹⁾, Ahmed M. Hassan*⁽¹⁾, Bharath Natarajan⁽²⁾, Itai Y. Stein⁽³⁾, Estelle Cohen⁽³⁾, Brian L. Wardle⁽³⁾, Renu Sharma⁽³⁾, J Alexander Liddle⁽⁴⁾, and Edward J. Garboczi⁽⁵⁾

(1) Materials and Structural Systems Division, National Institute of Standards and Technology, Gaithersburg, MD 20899

(2) Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD 20899

(3) Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139

(4) Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899

(5) Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO 80305

The electromagnetic scattering characteristics of straight carbon nanotubes (CNT) has been exhaustively quantified using multiple techniques. However, in composites CNTs are not perfectly straight and they acquire highly complex distributions that vary with their volume fraction, even in composites where the CNTs are thought to be aligned. In this work, Multiple Walled Carbon Nanotube (MWCNT) composites with volume fractions that vary from one to seven percent were fabricated. A detailed three-dimensional (3D) map of the MWCNTs was then generated using quantitative electron tomography. The MWCNT map provided an accurate description of the shape and location of each MWCNT in the sample. Using this detailed map, we calculated the electromagnetic response from composites with different volume fractions. We also generated numerical distributions with perfectly straight and aligned CNTs with the same length distributions and volume fractions as our experimental samples. The full-wave electromagnetic responses of the realistic experimentally-determined versus the simplified MWCNT distributions are then contrasted to quantify the frequency regions and polarizations where it is important to explicitly model the realistic shapes and orientations of the MWCNTs in a composite.

Moreover, we calculated the effective complex relative dielectric permittivity of each composite using full-wave simulations. The full-wave simulations were performed using an in-house developed MOM code as well as using multiple commercial solvers to validate the simulations. The effective complex relative dielectric permittivities are then compared to various effective medium approximations like the Maxwell Garnett and Bruggeman formalisms. Again the volume fraction and the frequencies where different effective medium approximations break down will be identified. The importance of this work is to use precise experimentally characterized CNT distributions to determine the limitations of the assumptions and approximations that are typically employed in estimating the electromagnetic characteristics of CNT composites. This analysis will lead to a better understanding of the electromagnetic responses of CNT composites, which will facilitate the accurate nondestructive electromagnetic evaluation of the CNT distributions that control the overall mechanical, thermal and electrical properties of the composite.