Experimentally Characterized 3D Maps of Carbon Nanotube Distributions: TestBeds for Accurate Electromagnetic Modeling of Nanocomposites

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Modeling the electromagnetic properties of carbon nanotube (CNT) composites has been a large research topic in recent years. In most of the reported modeling approaches, the exact three-dimensional (3D) shape and distribution of the CNTs in the composite was unknown. Therefore, simplifying assumptions were made regarding the CNT distributions. For example, all CNTs in the composite were assumed to be perfectly straight and aligned. To the best of our knowledge, the effect of these assumptions on the electromagnetic response of CNT composites has not been quantified. Recently, X-ray tomography techniques have advanced such that they are capable of generating sub-nanometer 3D maps of Multi-Walled Carbon Nanotubes (MWCNTs) distributions. The goal of this work is to calculate the full-wave electromagnetic response of these experimentally characterized MWCNT distributions for a better understanding of the interaction of electromagnetic radiation with nanocomposites. Multiple 3D CNT distributions are experimentally extracted from samples with four volume fractions: 1%, 3%, 4%, and 7%. A wide range of permittivity is assigned to these MWCNTs to cover the variations reported in the literature. Each MWCNT has five walls, on average, and different permutations of which walls are conducting versus semi-conducting were tested. The full-wave response of these nanostructures was then calculated and compared to the response calculated using the dilute limit effective medium approximation that does not account for the interactions between the CNTs. The results show that the electromagnetic response calculated using the dilute limit effective medium approximation differs significantly from the full-wave simulations especially at higher THz frequencies. However, good agreement between the two techniques exists at low frequencies, below a certain threshold that decreases with the increase in volume fraction or MWCNT conductivity. Moreover, the results show that these experimentally characterized 3D MWCNT maps act as useful testbeds for understanding the electromagnetic response of nanocomposites.