Electromagnetic Scattering Properties of Individual Carbon Nanotubes with Realistic Three Dimensional Shapes

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Carbon Nanotubes (CNT) in composites exhibit a wide variety of complex shapes and are rarely perfectly straight even when they are highly aligned. Moreover, fabrication capabilities have advanced enough to allow the synthesis of CNT with specific three-dimensional shapes, e.g. helixes, rings, and Y-shaped junctions. The shape of the CNT has a profound effect on the mechanical properties of the composites as predicted by numerous simulations and measurements. However, electromagnetic scattering from CNTs with realistic shapes has not yet been quantified.

In this work, electromagnetic scattering from individual CNTs with realistic three dimensional shapes was simulated using the Method of Moments (MOM) formulation for Arbitrary Thin Wires (ATW). The Drude model (G. Slepyan, S. Maksimenko, A. Lakhtakia, O. Yevtushenko, and A. V. Gusakov, Physical Review B 60, 17136, 1999) was used for the axial surface conductivity of the CNTs. CNT realistic shapes were generated using a coarse-grained molecular dynamics model, calibrated such that all the generated shapes had the average geometrical properties of commercial CNTs. The simulations show that certain CNT shapes and/or orientations can exhibit resonances which can be absent in other shapes and/or orientations. These resonances are explained using the Theory of Characteristic Modes (TCM), which allows the predictions of the resonances achieved by CNTs given their shape and orientation with respect to the incident waves. Also, the TCM analysis shows fundamental differences between the CNTs and perfectly conducting wires of the same shape and size.

Understanding the relationship between the shape of a CNT and the electromagnetic waves it scatters will allow better understanding of the interaction of electromagnetic waves with CNT composites. This understanding will help advance several fields, such as the Nondestructive Evaluation (NDE) of CNT composites using electromagnetic waves as well as the development of novel materials with unique electromagnetic properties.