Electromagnetic Scattering from Multiple Carbon Nanotubes with Experimentally Determined Shapes and Distributions

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Electromagnetic scattering from Carbon Nanotubes (CNT) has received wide interest in the past decade. Many different CNT configurations have been computationally investigated such as single CNTs, infinite planar arrays of CNTs, finite arrays with simple distributions, and bundles of CNTs. In all of the previously reported configurations, the CNTs were perfectly straight and they were arranged in a uniform distribution. However, in commercial CNT composites the CNTs typically exhibit highly complex shapes and distributions. The goal of this work is to simulate and characterize the electromagnetic scattering from multiple CNTs with realistic shapes and distributions that resemble those found in commercial composites.

Actual distributions were obtained experimentally using three-dimensional (3D) Electron Tomography (ET) of CNT composites. The volume reconstructed using 3D TEM was on the order of 0.2 cubic micrometers, which contained tens to hundreds of CNTs. The resolution of 3D ET is on the order of a few nanometers and therefore is capable of elucidating the detailed 3D CNT locations and shapes in addition to any interconnections between the CNTs. In order to reduce the computational time and memory requirements, the CNTs were modelled as thin wires and the Method of Moments (MOM) for Arbitrary Thin Wires (ATW) formulation was employed. For further computational efficiency, the computational bottlenecks in the MOM code were analyzed and the optimum parallelization schemes determined. The simulations show that multiple CNTs exhibit resonances in the total extinction coefficient that are shifted with respect to the resonances of the individual CNTs. The effects of different CNT dispersions and concentrations on this shift in resonances are quantified which acts as a first step in developing electromagnetic scattering as a technique for the non-destructive evaluation of the loading, orientation and distribution of CNTs in a composite .