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CARBON NANOCOMPOSITE STRUCTURE AND PROPERTIES: INSIGHTS FROM TEM TOMOGRAPHY AND SIMULATION

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Despite the exceptional properties of individual carbon nanotubes (CNTs), it has proven difficult to produce composites that demonstrate the hoped-for property enhancements. The gap between expectation and reality can be closed by understanding the difference between the ideal morphology and those currently achievable. As a first step in improving our understanding of these materials, and establishing robust process-structure-property models to aid in their optimization, we have made detailed and accurate measurements of aligned multiwall-CNT/epoxy nanocomposite structure by energy-filtered transmission electron microscope (EFTEM) tomography. These tomographic images, together with novel image processing algorithms, are used to quickly generate accurate reconstructions of the three-dimensional morphology of such nanocomposites as a function of CNT volume fraction (Figure 1). These reconstructions can then be analyzed to yield quantitative data on CNT volume fraction, alignment, bundling/network structure, interconnections and waviness/persistence length. This morphological information provides the foundation for effective modeling of the mechanical, electrical, thermal, and electromagnetic properties of CNT nanocomposites and the enterprise of materials design. As an example, we use the method of moments for Arbitrary Thin Wires (ATW) model to characterize the electromagnetic scattering of CNTs having worm-like cylinder configurations similar to those in Figs. 1(a) to 1(d). The key results obtained from the models are that random variations in CNT locations relative to one another and the interfaces of the embedding medium can lead to large variations in the electromagnetic scattering characteristics. We see that the shape and orientation of the CNTs have a strong effect on their individual electromagnetic scattering characteristics. Evidently, certain CNT shapes exhibit plasmonic resonances in the THz range that were absent in other shapes and/or orientations as shown in Figure 1e. Bundles of multiple CNTs have resonances that are shifted from the resonances exhibited when each CNT in the bundle is simulated by itself, as shown in Figure 1f. In principle, these resonance features, in conjunction with modeling, can be used to interrogate the nanoscale distribution of CNTs and their shapes at the *high throughputs* necessary for manufacturing process and quality control. In this talk, I will describe both the high resolution tomographic data and the models of electromagnetic response derived from it.

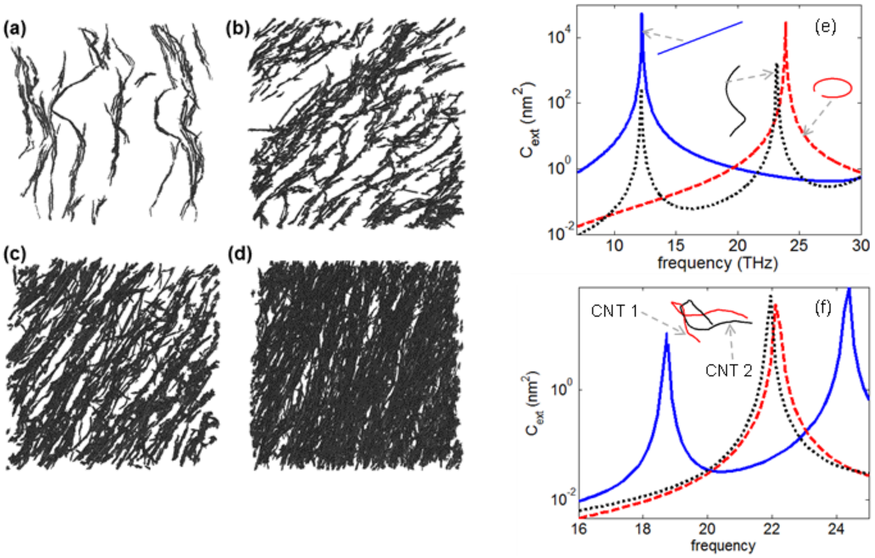

Figure 1. *Volume-rendered reconstructions of a) 0.44 % b) 2.6 % c)4 % and d) 6.9 % volume fraction aligned CNT nanocomposites. The reconstructed volumes are (a) 1327 nm × 1349 nm × 320 nm (b) 859 nm × 840 nm × 152 nm (c) 854 nm × 848 nm × 220 nm and (d) 840 nm × 840 nm × 199 n, (e) calculated total extinction coefficient (C_{ext}) of three CNTs with the same length but different shapes, (f) C_{ext} of a bundle of two CNTs (shown as a blue solid line) and C_{ext} of each individual CNT by itself (shown as a dashed red line for CNT 1 and as a dotted black line for CNT 2).*