Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electric and Magnetic Polarizability Tensors of Carbon Nanotubes and Graphene Sheets with Different Morphologies: A Numerical Study FERNANDO VARGAS-LARA, NIST-RICE University, JACK F. DOUGLAS, AHMED HASSAN, EDWARD GARBOCZI, NIST, RICE UNIVERSITY TEAM, NIST TEAM — The addition of Carbon Nanotubes (CNTs) and Graphene Sheets (GSs) in polymeric melts affects the electromagnetic response of the resulting composites. This effect strongly depends on the shape of the CNTs and GSs. In this study, we explore how the morphology of individual CNTs and GSs immerse on a dielectric material is related to their electromagnetic signature. In the microwave region, the wavelength is much larger than the size of the CNTs or GSs. Hence, their electromagnetic response in the far field is determined by the electric polarizability tensor, the magnetic polarizability tensor, and the dielectric properties of the CNTs. To determine these properties, we first generate CNTs and GSs with different morphology via molecular dynamic simulations of coarse-grained models for CNTs and GSs, whose mechanical properties mimic the ones predicted by atomistic simulations and experiments. We, next compute the electric polarizability tensors of the aforementioned objects using the path integrator ZENO. Considering this information as a reference, we calculated the magnetic polarizability tensor using finite element calculations (low frequency 3D COMSOL simulations). We finally report these properties as well as their connection with other shape descriptors.

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Date submitted: 15 Nov 2013 Electronic form version 1.4