COMSOL Calculations of the Electric and Magnetic Polarizability Tensors of Carbon Nanotubes, Graphene Sheets, and Superballs with Different Morphologies

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Carbon Nanotubes (CNT) and graphene sheets (GS) dispersed in composites exhibit a variety of random shapes. At low frequencies, the wavelengths are much larger than the size of the CNT. Hence, the electromagnetic signature of a CNT or GS in the far field is determined by the magnetic polarizability tensor, the electric polarizability tensor, and the dielectric properties of the CNT. Therefore, it is important to develop computational techniques to calculate the electric and magnetic polarizability tensors of individual CNTs and GS with realistic morphologies. The electric and magnetic polarizability tensors of CNT and GS of different morphologies were calculated using electrostatic 3D COMSOL simulations. The correlation between the individual elements of the electric and magnetic polarizability tensors and different shape parameters of the CNT and GS was also investigated. To further understand the relationship between the polarizability tensors and the different shape parameters, canonical 3D objects were simulated using COMSOL. In particular, “superballs” defined by the formula $x^m + y^m + z^m = 1$ cover a wide variety of regular shapes by simply varying the exponent “$m$”. The electric and magnetic polarizability tensors of superballs with various exponents “$m$” were calculated using electrostatic 3D COMSOL simulations, since an analytical solution only exists for $m = 2$ (sphere) and again correlated to different shape parameters. The talk will focus on how to use COMSOL to set up electrostatic simulations of the complex geometries previously mentioned and how to use these simulations to extract the polarizability tensors.