# Polarizability Tensors of Carbon Nanotubes and Graphene Sheets with Realistic Shapes

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Carbon Nanotube (CNT) and Graphene Sheets (GS) dispersed in composites exhibit a variety of shapes that are controlled by many factors such as how the CNT/GS are fabricated, how they are dispersed, and the material in which the CNT/GS are embedded. The goal of this work is to study how the shape of the CNT and GS affects their electromagnetic properties. A large number of worm-like CNT and crumpled GS with realistic shapes were generated using a coarse-grained molecular dynamics model. The static electric and magnetic polarizability tensors of these worm-like CNT and crumpled GS were calculated. The electric polarizability tensor is defined as the polarizability tensor calculated when the ratio between the dielectric permittivity of the CNT/GS and the dielectric permittivity of the embedding environment is equal to infinity. The magnetic polarizability tensor is the polarizability tensor calculated when the ratio between the dielectric permittivity of the CNT/GS and the dielectric permittivity of the embedding environment is equal to zero. The electric polarizability tensors were calculated using ZENO, which is a Monte Carlo numerical path integration package, and the magnetic polarizability tensors were calculated using the commercial finite element package COMSOL.

The perfectly conducting and the perfectly insulating intrinsic conductivity of the CNT/GS were defined as one third the trace of the electric and magnetic polarizability tensors, respectively. The intrinsic conductivity corresponds to the polarizability of the CNT/GS particles averaged over different orientations. The scaling of the perfectly conducting and the perfectly insulating intrinsic conductivity with size was evaluated for the worm-like CNTs and the crumpled GS. This scaling was contrasted with how the intrinsic conductivity of straight CNTs and flat GS scale with their sizes. The results show that the shape of the CNT/GS has a strong effect on the scaling of the intrinsic conductivity with size especially in the perfectly conducting case.

Finally, it was shown by (E.J. Garboczi and J.F. Douglas, Physical Review E 53, 6169-6180) that the knowledge of the intrinsic conductivities at the perfectly conducting and the perfectly insulating limit is sufficient to construct Páde approximants that can calculate, with high accuracy, the intrinsic conductivity at any contrast in the dielectric permittivity between the CNT/GS and the embedding environment. In this work, Páde formulations were developed for the CNT and GS with realistic shapes and they were found to provide excellent agreement with COMSOL calculations. The evaluation of the polarizability tensors and intrinsic conductivities accomplished in this work has several applications such as the calculation of Rayleigh scattering from CNT/GS and the calculation of the effective properties of CNT/GS composites.