Electromagnetic Scattering from Crumpled Graphene Flakes

Kalyan C. Durbhakula*[(1)], Ahmed M. Hassan [(1)], Deb Chatterjee[(1)], Fernando Vargas-Lara[(2)], Jack F. Douglas[(2)], and Edward J. Garboczi[(3)]

(1) Computer Science Electrical Engineering Department, University of Missouri Kansas City, Kansas City, MO 64110

(2) Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD 20899

(3) Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO 80305

Graphene, one of the most highly-studied emerging nanomaterials, is used in a wide variety of applications that include integrated circuits, nano-antennas, and composites. In most cases, graphene flakes (GF) are assumed to be perfectly flat whereas realistically all GF exhibit wrinkles, ripples, or crumples that vary in scale from several angstroms to several micrometers. Therefore, the primary goal of this work is to study the electromagnetic properties of crumpled monolayer GF. Realistic crumpled GF were generated using a coarse grained molecular dynamics model detailed in (See F. Vargas-Lara, A. Hassan, E. Garboczi, and J. Douglas, Journal of Chemical Physics, 143, 204902, 2015). The Drude model approximation of the Kubo formula was used to describe the surface conductivity of all the GF used in this work and, therefore, the results are valid in the lower terahertz range ($f \leq 4$ THz) where the intra-band conductivity dominates. The GFs were simulated using two independent electromagnetic solvers and the results showed excellent agreement validating the accuracy of each simulation. All the GF had exactly the same size and at least ten different shapes were studied to provide enough statistical variation to quantify the effect of shape.

The results show that the electromagnetic response of aligned GF with the same size and the same level of "*crumpleness*", but with different shapes, had similar extinction cross sections. However, when the same GF were randomly oriented their extinction cross sections diverged significantly. These results show that the electromagnetic properties are more sensitive to the orientation of the GF than to its exact shape. In addition, some orientations of the crumpled GF showed a broadband response in comparison to that of a flat GF of comparable size and conductivity. To explain this broadband response, we performed the Characteristic Mode Analysis (CMA) of the perfectly flat and the crumpled GF. The CMA analysis showed that, for a perfectly flat square shaped GF, the horizontal and vertical modes resonate at the same frequency due to the geometrical symmetry. However, as the GF became more crumpled, geometrical symmetry breaks down causing the horizontal and vertical modes to resonate at different frequencies. At certain orientations, both the horizontal and vertical modes of the crumpled GF can be excited simultaneously explaining the previously noted broadband response. These results can be used to quantify the electromagnetic response of realistically shaped GF as well as aid in the design of novel graphene-based devices.