Modeling of percolation in size distributed carbon nanostructures networks

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Many photovoltaic and display devices rely on the use of transparent electrodes, which are generally rigid and brittle. Once a sufficient number of carbon nanotubes (CNTs) and graphene nanoribbon (GNRs) are connected to form a percolative network, their collective electronic and physical properties make these materials promising candidates for flexible transparent electrodes. The description of the underlying physics, along with an optimization of the characteristic of such nanostructures networks, can be efficiently addressed by computational means. Our understanding of the influence of the array structure on the final quality of the electrode can be improved by the modeling of charge transport in various networks, leading to a more selective optimization of their properties.

Models for charge transport have already been developed for percolation systems with high aspect ratio CNTs, but they typically consider a single parameter to describe the CNT-CNT junctions [1]. However, in such complex materials, the propagation of charge carriers is usually limited by contact resistance that is a strongly dependent characteristic of the multiple network properties [2].

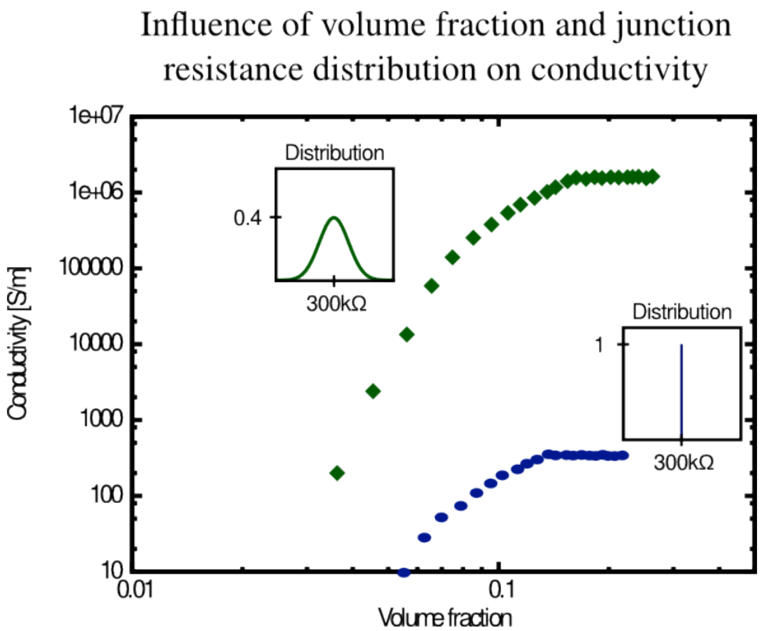
We have developed Monte Carlo (MC) algorithms to study the charge transport in bidimensional networks of CNT and GNR networks by incorporating realistic distributions and descriptions of CNT-CNT (or GNR-GNR) junctions. Our MC algorithms generate random networks with many controlled parameters which can be tuned to represent CNT mats, GNR mats, or other rod-like networks. We then evaluate the total conductance of the generated networks on the basis of individual contacts conductance, which in turn depend on the local network properties. Our results show that the length, diameter, orientation and chirality distributions within the percolative network of the CNT and GNR networks have a great importance on the resulting electrical performances.

References

[1] J. Hicks *et al.*, Phy. Rev. E, **79**, (2009)

[2] P. N. Nirmalraj *et al*., Nano Lett., **9**, (2009)

Figures



The distribution of the resistance values of the tube-tube junctions within a CNTs network has an important impact on the total conductivity of the system. A greater spread in the junction resistances lead in a higher conductivity.