Simulation of electron transport in realistic carbon nanostructures: the role of defects and the conductivity of macro materials

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Carbon nano materials are promising candidates for numerous applications such as transistors, sensors, or as electrical conductors. However, only the ideal defect-free materials show the excellent electronic properties carbon nanotubes (CNTs) and graphene are known for. The presence of defects or contaminations will reduce the electrical conductivity as well as the mechanical stability drastically.

In our contribution, we focus on how we can quantify the loss of conductivity due to defects. Based on an efficient implementation of a recursive Green's functions algorithm we are able to perform statistical studies on micron-sized carbon nanostructures with hundreds of defects and thousands of unit cells [1-3]. We illustrate our approach by showing results obtained for structural defects in CNTs and for edge roughness in graphene nanoribbons. For both systems, the electronic transport occurs in the strong localization regime. Consequently, the conductivity depends exponentially on the number of defects. In addition, we show that besides the defects also defect induced long-range deformations influence the conductivity of CNTs [4]. For proper conductivity modeling, the system size has to be large enough that such defect-induced deformations can build up.

In order to show, how the properties of the nanoscopic building blocks and its arrangement enter into the properties of a macroscopic material, we present a network model for graphene based electrical conductors [5]. Again, a computationally efficient approach is of vital importance, such that we are able to perform statistical studies. Based on a large number of model calculations we can derive guidelines for the production of optimized graphene-based conductor materials. The packing density and the in-plane conductivity of graphene flakes determine the overall conductivity. In contrast, flake sizes and out-of-plane connections decide how close a given material gets to this maximum.

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