P:30 Electron transport in defective metallic and semiconducting carbon nanotubes: An improved RGF-based O(N) approach

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We present electron transport calculations for metallic and semiconducting carbon nanotubes (CNTs) with randomly positioned realistic defects. For this purpose we use our new and very efficient RGF-based $\mathcal{O}(N)$ algorithm [1]. Based on this approach we are able to handle CNTs of realistic size up to several microns with up to thousands of defects. From our model calculations, simple analytic expressions are derived to express the conductivity of CNTs featuring arbitrary defect mixtures and different chiralities.

Although nearly ideal CNTs can be produced selectively under very clean laboratory conditions, during any step of the device fabrication at the wafer level going towards mass production me- thods, defects are introduced to all CNT devices fabricated so far. While many of the theoretical studies deal with ideal CNTs, it is of big interest to focus more on defective CNTs to know how different defects affect the electronic transport properties of CNTs. We treat this task from a theoretical point of view. This is a challenging task due to the huge number of atoms to be considered for defective systems. The usage of density functional theory (DFT), which scales cubically with the number of atoms, becomes unpractical for this purpose.

We use hybrid models like the density-functional-based tight binding (DFTB) model which com- bine the fastness of the tight binding approach with the good accuracy of DFT. Furthermore, we use the common quantum transport theory in combination with a fast, linearly scaling re- cursive Green's function formalism (RGF), allowing us to treat the electronic transport problem quantum-mechanically. But the further development and improvement of such theoretical me- thods is also an important task to overcome the system size limitations.

In the first part of our contribution we present two new and very efficient RGF-based approaches. The first algorithm accelerates the common RGF for the case of defective quasi-1D systems [1].

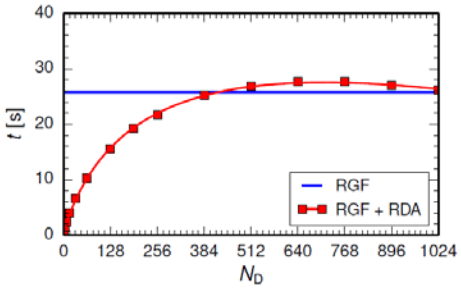

Figure 1: Calculation time as a function of the number of defects within a test system, which contains a fixed number of 1024 cells. The improved RGF+RDA is compared to the common RGF.

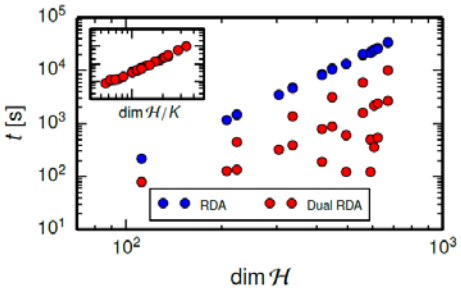

Figure 2: Calculation time as a function of the dimension of the Hamiltonian matrix of the periodic unit cell. The improved Dual-RDA is compared to the common RDA. Inset: Scaled data, where K is the number of sub-cells.

This is achieved by using the iteration steps of the renormalization decimation algorithm (RDA), leading to a smaller effective system. The resulting computational complexity scales linearly with the number of defects, instead of linearly with the total system length for the conventional approach. We show how the scaling of the calculation time depends on the defect density, leading to significant reductions for less defects and small unit cells (RGF+RDA, figure 1). We apply this algorithm to defective metallic armchair CNTs. The second approach treats the problem of periodic quasi-1D systems with large unit cells, which can be treated by the common RDA. However, this gets more inefficient for the larger cells as the calculation time scales

quadratic with the number of atoms. Based on the DFTB model, we present how to reduce the calculation time by simply subdivide and conquer (Dual-RDA, figure 2). We demonstrate the application of the algorithm for semiconducting chiral CNT with different unit cell lengths.

In the second part we show the results we got for the electronic transport through defective CNTs by using our algorithm improvements. For this, we focus on mono- and divacancies, which are the most common defects. In general, our approach can be extended easily to cover arbitrary defect types. In our previous publication [2] transmission spectra of defective metallic armchair CNTs are studied comprehensively and diameter-dependent localization exponents are extracted (figure 3a, 3b). We extend this work to defect mixtures and show that the total localization exponent can be expressed by linear combinations of those of CNTs with one defect type, which can be used to estimate the conductance of arbitrary defective CNTs. Finally, we focus on defective semiconducting (*m*,*n*)-CNTs of different chirality and present the influence of the structural parameters on the conductivity and the localization exponent. The diameter dependence can be described like for the metallic CNTs, but a distinction into three groups must be done. The investigation of the chirality dependence shows no significant influence (figure 3c).

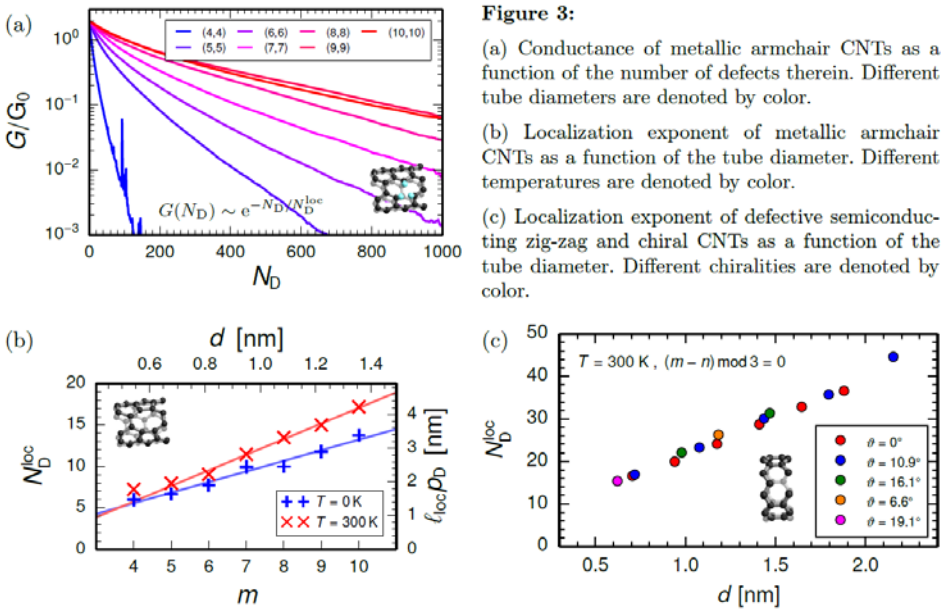

Figure 3:

(a) Conductance of metallic armchair CNTs as a function of the number of defects therein. Different tube diameters are denoted by color.

(b) Localization exponent of metallic armchair CNTs as a function of the tube diameter. Different temperatures are denoted by color.

(c) Localization exponent of defective semiconducting zig-zag and chiral CNTs as a function of the tube diameter. Different chiralities are denoted by color.

[1] F. Teichert et al., J. Comput. Phys., submitted
[2] F. Teichert et al., New J. of Phys. 16 (2014) 123026.