Simulation of quantum transport in doped carbon nanotube diode controlled by transverse electric field

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Abstract. Using first-principle and semi-empirical methods, optical responses and transport characteristics of hybrid CNT-based diodes are studied. The junction is realized by a combination of doping of one half of a nanotube and applying a transverse electric field to the other. Calculations are carried out in the framework of the density functional theory and the nonequilibrium Green function method. The possibility of using these rectifiers in optical nanoantennas is discussed.

1. Introduction

There are several ways to create pn-junctions based on carbon nanotubes, such as the substitution of boron or nitrogen atoms instead of carbon in the nanotube lattice, doping with charge transfer from electrodes, atoms or molecules, or controlling bands using the transverse electrostatic field (see book [1]). In the latter method, the device can operate in several different modes in a controlled way (by changing the transverse electrostatic field), and there is no need for chemical doping of nanotubes. Examining the effect of a transverse electric field on CNT electronic properties within the Dirac particle formalism in a cylinder, the authors of Ref. [2] showed that the problem obeys supersymmetry that protects low-energy states and ensures the preservation of metallic properties of CNT in arbitrarily large fields. In semiconductor tubes, the band gap decreases with increasing transverse electric field. This behavior is confirmed by the calculations using the density functional theory [3]. The patent [4] states that it is possible to use the influence of transverse electric field on the electrical conductivity and radiation absorption characteristics in such applications as switches, transistors, photodetectors, and polaron generators. When local electric fields are applied to a nanotube, a corresponding number of quantum wells in the nanotube may be formed in several places. Such a configuration is useful for Bragg reflectors, lasers, and quantum computing [4]. At present, there is great interest in the creation of terahertz and infrared nanoantennas based on CNTs. Doping CNTs with nitrogen or boron atoms in some studies is considered as a way to increase the antenna efficiency of CNT arrays. In [5], it is shown that the replacement of 8% carbon atoms in a CNT by nitrogen or boron atoms leads to an increase in conductivity, antenna efficiency, and thermal radiation power.

Here, we calculate the properties of CNT-based junction realized by a combination of doping one half of a nanotube and applying a transverse electric field to the other. This type of CNT-
based diode can be advantageous for optical nano-antennas. As is known, the development of a nanoantenna for infrared and visible frequency ranges of electromagnetic radiation is associated with the problem of a rectifier (diode) operating at terahertz and higher frequencies without large power losses. These losses usually arises due to the effect of pn-junction capacitance. Using the density functional theory (DFT), semi-empirical self-consistent extended Hückel method and the nonequilibrium Green function method (NEGF) implemented in QuantumATK, we calculate optical properties of doped nanotubes and estimate projected local density of states, transmission and current-voltage characteristics of the hybrid CNT-based diodes.

2. Model and method

Using the Kubo-Greenwood approach and the density functional theory, optical characteristics (absorption spectrum, reflections, dispersion law of dielectric susceptibility, and frequency dependence of conductivity) of semiconducting single-walled carbon nanotubes are calculated. The susceptibility tensor is defined by the Kubo-Greenwood formula:

\[
\chi_{ij}(\omega) = -\frac{e^2\hbar^4}{m^2\varepsilon_0 V^2} \sum_{nm} \frac{f(E_m) - f(E_n)}{E_{nm} - \hbar\omega - i\Gamma} \pi_{nm}^{i} \pi_{nm}^{j}
\]

where \(\pi_{nm}^{i}\) is the matrix element of dipole moment \(i\)-th component for states \(n\) and \(m\), \(V\) is volume, \(\Gamma\) is widening, \(f(E)\) is the Fermi-Dirac function. The dielectric tensor and optical conductivity are calculated according to relations

\[
\varepsilon_{ij}(\omega) = 1 + \chi_{ij}(\omega)
\]

\[
\sigma_{ij}(\omega) = -i\omega \varepsilon_0 \chi_{ij}(\omega).
\]

We considered hybrid CNT-based diode, where junction is created by combination of doping with a transverse electric field generated by charged gate electrode. The implementation of the device is based on the so-called screening approximation assuming that properties of the left and right electrodes can be described by solving a problem for a completely periodic cell. The nonequilibrium electron density are calculated by NEGF-method implemented in Quantum ATK. The electronic states in hybrid diodes are calculated by means of the self-consistent Hückel method. Current-voltage characteristics are calculated according to:

\[
I = \frac{e}{h} \int T(E) [f_L(E, T_L) - f_R(E, T_R)]dE,
\]

where \(f_L\) and \(f_R\) are electron energy distribution functions in the left and right electrodes, respectively, \(T(E)\) is a transmission spectrum calculated by the NEGF-method.

3. Results and discussion

Substitutional doping of different atoms in CNTs is a well known way to functionalize these nanotubes [6, 7]. When SWCNTs are doped with nitrogen or boron, it is assumed that substitutional atoms do not lead to additional atomic rearrangement. It is expected that B and N substitutions lead to the formation of an acceptor and donor states, respectively, in the CNT electronic structure [8]. Here we present results of calculation of optical properties and quantum transport characteristics of hybrid CNT-based diodes, where p- and n-regions are assumed to be formed by combination of doping and applying a transverse electric field. Ref. [9] reported that substitutional doping of multiwalled CNTs with boron lead to a sufficient decrease in the dc resistivity. Ref. [10] described observation of increase in the ratio of metallic nanotubes for the case of nitrogen substitutional doping of mixtures of metallic and semiconducting SWNTs in composite materials.

In Fig. 1, calculated absorption spectra for pristine and doped CNT are shown. Doping with B and N (fractions 10% and 20%) leads to reducing of absorption coefficient and to shift of peaks. It can be seen that substitution of carbon atoms by B and N atoms lead to different
changes of these spectra. In Fig. 2, calculated dispersion of optical conductivity for pristine and doped CNT is presented. Doping with B does not lead to destruction of absorption peaks, while N doping smooths spectra sufficiently.

![Figure 1](image1.png)

**Figure 1.** Absorption coefficient for pristine, B doped and N doped CNT vs photon energy.

![Figure 2](image2.png)

**Figure 2.** Optical conductivity for pristine, B doped and N doped CNT vs photon energy.

The transmission spectra and current-voltage characteristics are calculated for the following hybrid CNT-based diodes. Half of a nanotube is doped with boron or nitrogen and the other is situated in transverse electric field produced by a metallic gate coated by a dielectric layer (Fig. 3,a). The gate potential can be changed.

The current-voltage characteristics for three values of gate voltage for 20% boron-doped hybrid CNT-diode are presented in Fig. 3,b. They show rectifying behavior of this diode for gate potentials 1 and 3 V. The similar behavior is observed for 20% N-doped hybrid diode (Fig. 4). The distribution of electrostatic difference potential and projected local density of states are shown in Fig. 4 for two opposite values of gate potential (±3 V).

The similar behavior of N-doped and B-doped CNT-diodes can be interpreted in the following way. At chosen doping level (20%), CNTs become metallic for both cases of B- and N-doping,
Figure 3. Cut-plane of electron difference density at $U_g = 3$ V (left panel) and current-voltage characteristics for three values of gate voltage.

Figure 4. Distribution of electrostatic difference potential (a,b), projected local density of states (c, d) and the current-voltage characteristics for two values of gate potential $\pm 3$ V.
so we deal some type of Schottky diode. This fact is confirmed by distribution of states Fig. 4,c and d. Positive gate potential leads to curved bands responsible for rectifying behavior.

4. Conclusion

Using first-principle and semi-empirical self-consistent methods, optical responses and transport characteristics of hybrid CNT-based diodes are studied. The junction is realized by a combination of doping of one half of a nanotube and applying a transverse electric field to the other. Calculations of current-voltage characteristics are carried out by means of the semi-empirical self-consistent method and the nonequilibrium Green function method. This type of CNT-based diode can be promising alternative for optical nano-antennas. The dependence of current-voltage characteristics on gate potential are explained by the fact that at chosen doping level (20%), CNTs become metallic and we deal with Schottky nanodiode. This fact is confirmed by calculated projected local density of states.

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