ELECTROMAGNETIC PROPERTIES OF CNTs AND GNRs BASED NANOSTRUCTURES FOR NANOSENSOR SYSTEMS

Yu. N. SHUNIN[1,2], V. I. GOPEYENKO[2], N. Yu. BURLUTSKAYA[2], T. D. LOBANOVA-SHUNINA[2], S. BELLUCCI[3]

[1]*Institute of Solid State Physics, University of Latvia*
Kengaraga Str. 8, LV-1083 Riga, Latvia
[2]*Natural Sciences and Computer Technologies Department, Information Systems Management Institute, Lomonosov Str. 1, Bld 6, LV-1019 Riga, Latvia*
[3]*INFN-Laboratori Nazionali di Frascati, Via Enrico Fermi 40, Frascati, Italy*

Fundamental electromagnetic properties of CNTs and GNRs nanostructures with functionalized atomic groups and their various interconnects with the essential concentration of 'dangling bonds' are very sensitive to local external perturbations. The induced changes of local electronic density of states lead to correlated changes of current and spin states. The cluster approach based on the multiple scattering theory as well as an effective medium approximation were used to model the dispersion law, electronic density of states, conductivity, *etc*. Multiple scattering problems were solved for nanostructures with radial and axial symmetry. Parametrical numerical simulations of conductivity using the formalism of Kubo-Greenwood were carried out for zig-zag (*m*,0), armchair (*m*,*m*) and chiral (*m*,*n*) CNTs. The sensitivity of conductivity to the local electronic density of states in CNTs with local impurities (N and B atoms) was demonstrated to be promising for nanosensors.

1. Introduction

Carbon nanotubes (CNTs) of various chiralities open new wide possibilities for modern nanolectronics. Analogously to CNTs, novel 'marginal' forms of graphene, *i.e.* nanoflakes (GNFs) and nanoribbons (GNRs), demonstrate a wasteless ballistic mechanism of conductivity. The key point of application for CNTs and GNRs is stipulated by the fundamental properties of innovative chip-interconnects as the basis for new nanodevices. Similarly to CNTs, a full integration of graphene into conventional device circuitry would require a reproducible large-scale graphene synthesis that is compatible with conventional thin film technology [1].

The main objective of the current study is to demonstrate the implementation of advanced simulation models to ensure a proper description of the electrical conductivity of functionalized CNT- and GNR-based nanostructures of different morphologies and their interconnects to nanosensor systems. In this respect, due to the sensitivity of the local electronic density of states to external influences (mechanical, chemical, magnetic, *etc.*), the fundamental electromagnetic

properties of CNTs, GNRs and their metal interconnects were analyzed from the point of view of nanosensor applications.

2. CNT- and GNR-based nanosensors

There are two basic important applications of CNT- and GNR-based nanostructures. Firstly, we should consider nanodevices as conducting nanoelements for effective electron transport, electronic switching (FET-type) devices, and various novel functionalized nanosystems with the complex morphologies. On the other side, we can talk about nanosensor systems for various aspects of ecological monitoring and security. The fundamental electron devices are FET-transistors which are able to provide high sensitivity to various external influences of different nature (Fig. 1) [1,2].

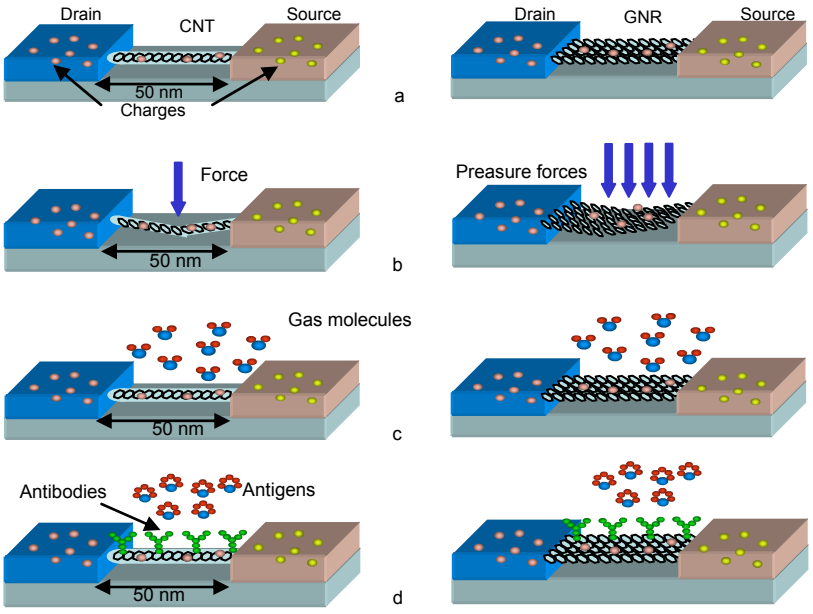

Figure 1. FET-type nanodevices as prospective nanosensor systems: a) the unperturbed field-effect transistors based on CNT- or GNR- based FETs are mainly composed of the corresponding semiconducting carbon materials suspended over two electrodes; b) physical nanosensors: a conducting threshold can be altered when the tube or graphene ribbon is bent; c) chemical nanosensors: the same threshold can be altered when the amount of free charges on the tube of graphene ribbon surface is increased or decreased by the presence of donor or acceptor molecules of specific gases or composites; d) biological nanosensors: monitoring of biomolecular processes such as antibody/antigen interactions, DNA interactions, enzymatic interactions or cellular communication processes.

3. Conductivity as a tool of nanosensor systems

The calculations of conductivity are usually performed using Kubo-Greenwood formula [1,2]:

$$\sigma_E(\omega) = \frac{\pi\Omega}{4\omega}\int\left[f(E) - f(E+\hbar\omega)\right]\left|D_E\right|^2 \rho(E)\rho(E+\hbar\omega)dE, \quad (1)$$

where ω is the real frequency parameter of the Fourier transform for the time-dependent functions, $f(E)$ is the Fermi-Dirac distribution function, $D_{E,E'} = \int_{\Omega} \Psi^*_{E'} \nabla \Psi_E d\mathbf{r}$, where $\Psi_{E(\mathbf{K})} = A\exp(i\mathbf{Kr})$ and $\mathbf{K}$ is the complex wave vector of the effective medium. The dispersion function $E(\mathbf{K})$ determines the properties of the wave function $\Psi_{E(\mathbf{K})}$ upon the isoenergy surface in $\mathbf{K}$-space.

Usually two basic electron conductivity mechanisms in CNT-based structures are considered. The ballistic mechanism is engaged in electron transport within CNTs while the collisional mechanism is a characteristic of CNT-substrate interconnects. The general conductivity σ_{gen} is evaluated as:

$$1/\sigma_{gen} = 1/\sigma_{coll} + \sigma_{ball}. \quad (2)$$

For pure CNTs, we clearly observe that $\sigma_{ball} >> \sigma_{coll}$. But, Kubo-Greenwood formalism is free from this division on ballistic and collisional mechanisms and seems to be more objective. The analysis of Kubo-Greenwood's conditions in respect of a CNT morphology has been presented taking into account both *dc* ($\omega = 0$) and *ac* ($\omega \neq 0$) regimes as well as the temperature factor of electron transport.

We use in this research the results of *ab initio* electronic structure calculations of P. D'yachkov's group [3] based on the linear augmented cylindrical wave (LACW) theory of the perfect SW CNT band structure. The developed generalization of this method allows one to treat the electronic structure of various defects in the SW CNTs. The method combines the advantages of the density-functional *ab initio* theory with the Green's function approach to the point defects electronic structure.

The main aim of our research is a simulation on sensitivity of SW CNTs to various defects which evidently change the local EDOS and then, as a result, give the changes of conductivity. The detailed properties of EDOS at the vicinity of Fermi level are essential for expected conductivity values.

Fig. 2 shows the parametric simulations of *ac*-conductivity for armchair (*m*,*m*) CNTs, where the essential sensitivity to the radius of SW CNT for energies more than 0.5 eV is shown. There is no essential dependence on chirality number *m* for THz-range, excluding $m = 4$. Fig. 3 demonstrates the

comparison of conductivity calculations for pure perfect and doped (B or N) CNTs in the case of non-interacting defects. Numerical simulations of conductivity have been carried out for zig-zag (*m*,0), armchair (*m*,*m*) and chiral (*m*,*n*) CNTs, where the sensitivity of conductivity has been demonstrated to the local electronic density of states in CNTs with local impurities (N and B atoms). In particular, this sensitivity means that the potential possibility of CNT-based nanodevices is to be used as nanosensor systems. This means that the calibration of such nanosensors on current is possible.

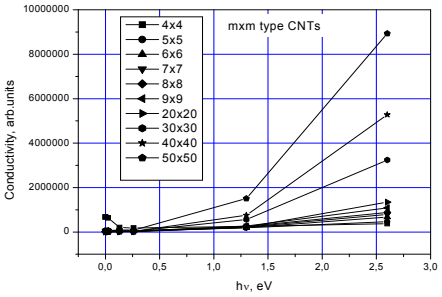

Figure 2. Conductivities of perfect *armchair* SW CNTs of various morphologies. *Note:* The critical frequency of about 0.25 eV corresponds to 60 THz.

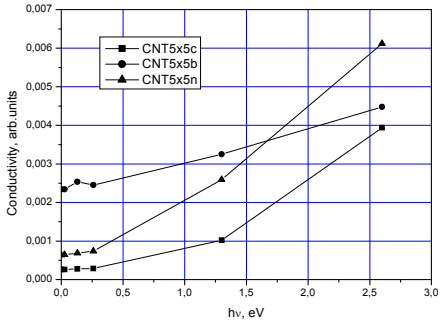

Figure 3. Conductivities of pure perfect and doped (B or N) CNTs in the limit of non-interacting defects.

Acknowledgments

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