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Abstract. As carbon nanotubes (CNT) and graphene nanostructures (GNR) constitute the basis of high-speed nanoelectronics and nanosensors, we examine the fundamental properties of various CNT-metal (Me), GNR-Me, and CNT-graphene interconnects. The cluster approach based on the multiple scattering theory as well as effective medium approximation were used to model the dispersion law, electronic density of states (DOS), and conductivity, etc. Multiple scattering problems were solved for nanostructures with radial (quantum dots) and axial (nanowires, nanotubes) symmetry. Interconnect capacitances and impedances have been evaluated in the GHz and THz regimes. Parametrical numerical simulations of conductivity were carried out for zig-zag \((m; 0)\), armchair \((m, m)\), and chiral \((m, n)\) CNTs, and the sensitivity of conductivity to the local electronic DOS in CNTs with local impurities (N and B atoms) was demonstrated. CNTs, CNT-Me, and GNR-Me based nanostructures are prospective nanosensor structures. © 2012 Society of Photo-Optical Instrumentation Engineers (SPIE). [DOI: 10.1117/1.JNP.6.061706]

Keywords: carbon nanotubes; graphene nanoribbons; scattering theory; electronic structure calculations; resistance of carbon nanotubes and GNR-Me interconnects; nanosensors.

1 Introduction

Carbon nanotubes (CNTs) of various chiralities open new possibilities for modern nanoelectronics. Analogous to CNTs, novel marginal forms of graphene-nanoflakes (GNFs) and nanoribbons (GNRs) demonstrate a wasteless ballistic mechanism of conductivity.

The key point of application of CNTs and GNRs is stipulated by the fundamental properties of innovative chips interconnects as the basis for new nanodevices. Similar 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 resistance for end and side contacts between CNTs and GNRs of different morphologies and metallic substrates of different nature.

The focus of the present research is basically on the junctions between carbon nanotubes (CNTs), graphene nanoribbons (GNRs), and the contacting metallic elements of a nanocircuit. Numerical simulations on the conductance and resistance of these contacts have been performed using the multiple scattering theory and the effective media cluster approach. We have simulated both single-walled (SW) and multi-walled (MW) CNTs as well as single-layered (SL) and multi-layered (ML) GNRs with different morphology. Figure 1 represents the contacts of metal (Me) substrates with CNTs and GNRs, respectively, as prototype nanodevices.

The above-mentioned contacts represent the main subject of our current research and modeling. The contact regions (CNT-Me and GNR-Me) are the objects of the microscopic approach.
responsible for the main contribution to the resistance. Meanwhile, the resistances of nanotubes, nanoribbons, and the metallic substrate per se may be considered as macroscopic parameters.

We made a further step in our simulations directed to nanosensor systems. In this respect, due to the sensitivity of the local electronic density of states (DOS) 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 prospective nanosensor applications.

2 Novel Nanodevices Models

There are two basic important applications of CNT- and GNR-based nanostructures. First, 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 nanosensoring systems for various aspects of ecological monitoring and security.1

2.1 CNT- and GNR-Based Sensors

There are some important applications of CNTs and GNRs based interfaces with other materials for novel nanosensor devices. The fundamental electron devices are FET-transistors, which are very sensitive to various external influences of different nature such as mechanical, chemical, biological, electrical, magnetic etc. (see Fig. 2).

A field-effect transistor (FET) is nano in size, whose on/off threshold depends on the tube dimensions, shape, and temperature, etc. A local deformation of CNT (GNR) creates a change in the on/off threshold voltage of the transistor. The electrical properties of carbon-based interconnects change under the influence of external factors. The advantage of CNTs and GNRs over other materials occurs due to their small size, great strength, high electrical and thermal conductivity, and high specific area. Unique physical properties of CNTs and GNRs and their various interconnects allow considering them as sensing nanomaterials in various kinds of sensors—pressure, flow, thermal, gas, optical, mass, position, stress, strain, chemical, and biological sensors. Taking into account specific physical properties of CNTs/GNRs metal interconnects, which are explained by the presence of “dangling” chemical bonds, we should point out the noticeable sensitivity of electric properties of interconnect space to chemical, electric and magnetic influences. Therefore we consider interconnects as a perspective group of nanosensors.1,2

2.2 Nanodevices for Effective Electron Transport

The electronic structure for CNT-Me and GNR-Me interconnects can be evaluated through the electronic DOS since a carbon-metal contact can be considered as a “disordered alloy,” where clusters containing both C and Me atoms behave as scattering centers. The computational procedure that we have developed for these calculations3 is based on the construction of cluster

![Fig. 1 Models of C-Me interconnects as a prototype of novel nanodevices: (a) CNT-Me interconnect; (b) multilayered GNR-Me interconnect.](image)
potentials and the evaluation of both scattering ($S$) and transfer ($T$) matrices. The general model of multiple scattering using the effective media approximation (EMA) combined with the coherent potential approach (CPA) for condensed matter is based on the atomic cluster formalism. When using the CPA as EMA approximation, the interconnect resistance is evaluated through Kubo-Greenwood formalism\cite{kubo1957, greenwood1956} or, in the simplest cases, through Ziman model.\cite{ziman1960}

The general model of multiple scattering with EMA for condensed matter based on the approach of atomic cluster is presented in Fig. 3. So far, the cluster formalism has been successfully applied for metals (e.g., Cu, Al) as well as for semiconductors, both elemental (C, Ge, Si, As, Se, Sb) and binary (As$_x$Se$_{1-x}$ and Sb$_x$Se$_{1-x}$).\cite{shunin2012} Special attention has been paid for the latter,

**Fig. 2** FET-type nanodevices as prospective nanosensor systems: (a) The unperturbed FETs based on CNT and GNR are presented. 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: this 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, etc.

**Fig. 3** Zig-zag CNT-Me end-type interconnect formation model.
since the concept of statistical weighing has been applied for the binary components in solid
solutions.

We have developed structural models for CNT-Me and GNR-Me junctions, based on their
precise atomistic structures, which take into account the CNT chirality effect and its influence
on the interconnect resistance for Me (= Fe, Ni, Cu, Ag, Pd, Pt, Au) as well as the pre-defined CNT
(or GNR) geometry.

In the simplest cases, the electronic structure of the CNT-Ni interconnects can be evaluated
through the DOS since the C-Ni contact is considered as a disordered alloy.\(^5\) In the current study,
we have developed more complicated structural models of CNT-metal junctions based on the
precise description of their atomistic structures. When estimating the resistance of a junction
between a nanotube and a substrate, the main problem was caused by the influence of the nano-
tube chirality on the resistance of SW and MW CNT-Me interconnects (Me = Fe, Ni, Cu, Ag,
Pd, Pt, Au) with a pre-defined CNT geometry.

The basic principles of electronic structure calculations and models for carbon-metal inter-
connects, which constitute the basis for our simulations of their fundamental properties and
possible applications, were formulated in Ref. \(^7\).

### 3 Multiple Scattering Theory and Effective Medium Approach for CNT
and GNR Interconnects Simulation

Resistivity can be considered as a scattering problem, where the current carriers participate in the
transport according to various mechanisms based on the presence of scattering centers (phonons,
charge defects, structural defects, etc.), including a pure elastic way, called ballistic. The develop-
ed computational procedure\(^3\) is based on the construction of cluster potentials and the evalua-
tion of the S- and T-matrices for scattering and transfer, respectively. It allows us to realize the
full-scale electronic structure calculations for condensed matter (“black box”), where influence
means a set of electronic “trial” energy-dependent wave functions \(\psi_{\text{in}}(\mathbf{r})\) and response \(\psi_{\text{out}}(\mathbf{r})\)
gives sets of scattering amplitudes corresponding to possible scattering channels for any trial
energy. This allows us to decrypt the electronic spectra of black box (object of scattering
problem).\(^3,5\)

#### 3.1 Electronic Structure Calculations: Coherent Potential Approximation

We consider a domain where the stationary solutions of the Schrödinger equation are known,
and we label them as

\[
\psi_{\text{in}}(\mathbf{r}) = \phi_k(\mathbf{r}) = \exp(\text{i}kr).
\]

The scattering of trial waves, in the presence of a potential, yields new stationary solutions
labeled as

\[
\psi_{\text{out}}(\mathbf{r}) = \psi_{\text{in}}^{(\pm)}(\mathbf{r})
\]

for the modified Schrödinger equation \(\hat{H}\psi_{\text{in}}^{(\pm)}(\mathbf{r}) = E\psi_{\text{in}}^{(\pm)}(\mathbf{r})\). An electronic structure calculation
is considered here as a scattering problem, where the centers of scattering are identified with the
atoms of clusters.\(^3\)

The first step to modeling is the construction of potentials, both atomic and crystalline, which
is based on analytical Gaspar’s potential of screened atomic nucleus,\(^8,9\) \(X_\alpha\) and \(X_{\alpha\beta}\) presentations
for the electronic exchange and correlation, using the local density approximation.

To obtain the electronic structure, the calculations on scattering properties are necessary,
generally, in the form of S- and T-matrices. These calculations start with the definition of
the initial atomic structure to produce a medium for the solution of the scattering problem
for a trial electronic wave. The results of potential modeling and phase shifts in the framework
of MT-approximation are presented elsewhere.\(^3\)

The formalism used here for calculations on the electronic structure is based on the CPA,
the multiple scattering theory and cluster approach.\(^10,11,12\) As a first step, we postulate the atomic
structure at the level of short- and medium-range orders. As a second step, we construct a crystalline potential and introduce the muffin-tin (MT) approach. This is accomplished by the use of realistic analytical potential functions. Further on, the electronic wave scattering problem is solved. The energy dependence of the scattering properties for isolated MT-caterers is obtained by the use of a realistic analytical potential functions. Further on, the electronic wave scattering problem is resolved by the multiple scattering model of condensed matter is formulated. The paradigm of the scattering theory and the developed strategy of CNTs electronic properties simulation use the generalized scattering condition for low-dimensional atomic structures of the condensed matter:2,7

The basic equations of this approach are as follows:

\[ \Sigma(E) = V_{\text{eff}} + \langle T \rangle \left(1 + G_{\text{eff}}(T)\right)^{-1}, \]  
\[ G(E) = G_{\text{eff}} + G_{\text{eff}}(T)G_{\text{eff}}, \]  
\[ \langle T(E, \mathbf{K}) \rangle = 0, \]  
\[ \Sigma(E) = V_{\text{eff}}, \]  
\[ \langle G \rangle = G(E) = G_{\text{eff}}. \]

Here (\ldots) denotes averaging, \( V_{\text{eff}} \) and \( G_{\text{eff}} \) are the potential and the Green’s function of the effective medium, respectively, \( T(E, \mathbf{K}) \) the \( T \) matrix of the cluster, and \( N(E) \) the integral density of the electronic states. Equation (5) can be also presented in the form:

\[ \langle T(E, \mathbf{K}) \rangle = \mathbf{S}_{\mathbf{p}}T(E, \mathbf{K}) = \int_{\Omega_{\mathbf{K}}} \langle \mathbf{K}|T(E, \mathbf{K})|\mathbf{K}\rangle d\Omega_{\mathbf{K}} = 0. \]

where \( |\mathbf{K}\rangle = 4\pi \sum_{l,m}(i)^{l} \psi_{l,m}(kr)Y_{lm}(\mathbf{K})Y_{lm}^{*}(\mathbf{r}) \) is the one-electron wave function, \( \mathbf{S}_{\mathbf{p}} \) means the calculation of the matrix trace while the integration is performed over all angles of \( \mathbf{K} \) inside the volume \( \Omega_{\mathbf{K}} \). Equation (5) enables one to obtain the dispersion relation \( E(\mathbf{K}) \) of the effective medium. The DOS calculations have been performed using the relation:

\[ \rho(E) = \frac{2}{\pi} \int \text{Im}[\mathbf{S}_{\mathbf{p}}G(\mathbf{r}, \mathbf{r}, E)]d\mathbf{r}, \]

where \( G(\mathbf{r}, \mathbf{r}, E) = \sum_{l,m}Y_{lm}(\mathbf{r})Y_{lm}^{*}(\mathbf{r})G_{l,m}(\mathbf{r}, \mathbf{r}) \) is the angular expansion of Green’s function.

The paradigm of the scattering theory and the developed strategy of CNTs electronic properties simulation use the generalized scattering condition for low-dimensional atomic structures of the condensed matter:

\[ \psi_{k}^{(\pm)}(\mathbf{r}) \propto \phi_{k}(\mathbf{r}) + \int_{r_{\text{co}}<r}^{(\pm)}(\mathbf{\Omega}) \frac{\exp(\pm ikr)}{r^{d/2}}, \]

where \( \Omega \) describes the integrated space in angular units while superscripts “+” and “-” label the asymptotic behavior in terms of \( d \)-dimensional waves, where \( d \) is the atomic structure dimension.
3.2 Calculations of Conductivity and Resistance

The calculations of conductivity are usually performed using Kubo-Greenwood formula:13

\[
\sigma(E) = \frac{\pi \Omega}{4 \omega} \int [f(E) - f(E + \hbar \omega)] |D_E|^2 \rho(E) \rho(E + \hbar \omega) dE, \tag{12}
\]

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

3.2.1 Conductivity as a tool of nanosensing systems

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 characteristic of CNT-substrate interconnects.5 Hence the general conductivity \( \sigma_{\text{gen}} \) is evaluated as follows:

\[
\frac{1}{\sigma_{\text{gen}}} = \frac{1}{\sigma_{\text{coll}}} + \frac{1}{\sigma_{\text{ball}}}. \tag{13}
\]

For pure CNTs, we clearly observe that \( \sigma_{\text{ball}} \gg \sigma_{\text{coll}} \). The collisional contribution is basically connected with the specific morphology of interconnects space.14 In the framework of multiple scattering theory formalism and effective medium approximation, we can evaluate both factors of conductivity. A special question for modeling is the dependence of both conductivity mechanisms on the electron free path length that, in the case of pure CNT, is usually considered as the nanotube length.

The analysis of Kubo-Greenwood’s conditions in respect of CNT morphology has been presented taking into account dc (\( \omega = 0 \)), ac (\( \omega \neq 0 \)) regimes and the temperature factor of electron transport. Parametrical numerical simulations of conductivity have been carried out for zig-zag (\( m, 0 \)), armchair (\( m, m \)), and chiral (\( m, n \)) CNTs,13,14 where the sensitivity of conductivity to the local electronic DOS in CNTs with local impurities (N and B atoms) have been demonstrated. In particular, this sensitivity means that the potential possibility of CNT-based nanodevices is to be used as nanosensing systems (see Part 2).

4 CNT- and GNR-Metal Interconnects Simulation Results

4.1 Model of “Effective Bonds” for Simulations of CNT-Me and GNR-Me Junctions

The model of “effective bonds” for CNT-Me and GNR-Me nanointerconnects (Fig. 1) has been developed in the current study. Within the electronic transport formalism, it consists of two regions supporting two different electron transport mechanisms: ballistic (elastic) and collisional (non-elastic). These electron transport processes are simulated using the corresponding boundary conditions in the form of the effective medium. The CNT and GNR chiralities (\( m, n \)) are simulated by the corresponding orientation of the chirality vectors within the scattering medium. The most problematic regions for simulation are Carbon-Me junctions, where atomic structural disorder is observed and the conductivity mechanism is changed. The atomistic models of interconnect space are based on the developed earlier analytical atomic potentials.3,8,9 The superposition procedure of these potentials allows reproducing the details of interconnect potential barrier taking into account its real morphology (see also Fig. 8). The chirality influence on the resistance in the region of interconnect depends on a number of statistically realized bonds between a carbon nanostructure and a metal contact (e.g., Fe, Ni, Cu, Ag, Pd, Pt).

Using the simulation models, presented earlier,3,5 we have determined the resistance for both (SW and MW) CNT-Me and (SL and ML) GNR-Me interconnects, based on the evaluation of the interface potential barriers and implementation of Landauer formula,15 which defines the integrated conductance:
\[ I_{G} = \frac{2e^2}{h} \sum_{i=1}^{N} T_i = \left( \frac{1}{12.92 \text{ (kOhm)}} \right) \sum_{i=1}^{N} T_i = 0.0774 \sum_{i=1}^{N} T_i. \] (14)

The chirality \((m, n)\) is simulated by the corresponding orientation of carbon rings within the scattering medium. The most problematic areas for the proper simulation are CNT-Me and GNR-Me end to junctions (Figs. 3 and 4), where the atomic structural disorder is observed and the conductivity mechanism is changed.

In the case of side-type contact for GNR-Me interconnects, the number of effective bonds per contact square is essential (see Fig. 5).

**4.2 SW- and MW-CNTs Interconnects Resistance Simulations**

Figures 4 and 5 present a creation of C-Me “effective bonds.” We consider here (100) substrates of fcc-metals. We should also underscore that this is a probabilistic process when only more-or-less equilibrium bonds (effective bonds) are formed at interatomic distances corresponding to the minimum total energies. The evaluation of a number of effective bonds using Eq. (13) is principal for the number of conducting channels, since the conductance is proportional to the number of appeared effective bonds within the CNT-Me interconnect.

The calculations of conducting abilities of effective bond lead us to estimate the energy-dependent transparency coefficient of a potential barrier C-Me (Figs. 6 and 7). The scattering process for this potential barrier is regulated by the effect of “thin film” for conductivity electrons, which leads to quantization in voltaic parameters (in the case of full transparency).7

Figure 8 shows the generalized results of simulations on resistance of junctions obtained for various metallic substrates. It is clear that Ag and Au substrates are more effective electrically, while Ni appears a worse substrate for interconnect, although it yields the most effective catalyst.

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**Fig. 4** Armchair GNR-Me end-type interconnect formation model.

**Fig. 5** GNR-Me side-type interconnect formation model.
for CNT growth. On the other hand, the catalysts, which are usually used for the SW CNT growth (e.g., Fe, Co, and Ni), have stronger bonds to the ends of SW CNTs than noble metals,\textsuperscript{16} therefore, some compromise exists between electrical parameters and strengths of the interconnect bonding.

We have constructed atomistic models of MW CNTs, which could fit into a porous alumina with diameters of holes $\sim 20$ nm. In particular, a model of MW CNT with a pre-defined combination of armchair (ac) and zig-zag (zz) shells, namely, 12.88 to 19.88 nm, with chiralities

Fig. 6 Interconnect potential model for the scattering problem: CNT-Me, GNR-Me.

Fig. 7 Formation of a potential barrier for SW CNT-Me (SL GNR-Me) junction.

Fig. 8 Resistances of the zig-zag-type SW CNT-Me interconnects for the CNT diameter $\sim 1$ nm.
Using the simulation models presented earlier, we have developed an effective bonds model for MWCNT-Me junction resistance. The results of these simulations are presented in Fig. 9. For MWCNT-Me junction, the integral bonding with a corresponding substrate may be not as significant as in the case of SW CNTs, where a weak bonding can be principal. Figure 9 shows similar ratios of electric resistances for SW CNTs (Fig. 8), in favor of Au, Ag, and Pt. It should be noted, that technological qualities of CNT-Me interfaces pre-define the resulting resistance. In particular, experimental evaluations of CNT-Pt interconnect resistances for side-type and end-type contacts are 50 kΩ and 50–300 kΩ, correspondingly (see Ref. 18).

Figures 10 and 11 show parametric simulations of SWCNT (zig-zag)-Au interconnect impedances Z via chiralities and curvature. These results correlate with calculations in the framework of semiclassical approach of Maksimenko et al., where the GHz–THz range has demonstrated essential changes of interconnect resistance.

### 4.3 SL GNR-Me and ML GNR-Me Interconnects Resistances and Capacitances

Similar calculations on resistances and capacitances have been carried out for special configurations of SL GNR (zig-zag)-Me interconnect (Fig. 12) and for ML GNR (zig-zag)-Me interconnect (end-type contacts) (Figs. 12 to 15), which is essential, e.g., in case of planar technology in nanodevices design.
Fig. 11 SWCNT (zig-zag)-Au (100) interconnect impedance via the curvature parameter (chirality index) $m$.

Fig. 12 Resistances of the SLGNR (zig-zag)-Me end-type interconnects.

Fig. 13 Resistances of the MLGNR (zig-zag)-Me end-type interconnects.
Fig. 14 Capacitances of the SLGNR (zig-zag)-Me end-type interconnects.

Fig. 15 Capacitances of the MLGNR (zig-zag)-Me end-type interconnects.

Fig. 16 Conductance of GNR-Au interconnect (side-type contact) via the depth "y" parameter of contact overlapping.
For cases of side-type contact the number of effective bonds per contact square is essential. Figure 16 shows the conductance of GNR-Au interconnect via the depth “y” of contact overlapping.

### 4.4 Parametric Calculations of CNT-Me Interconnects Resistances

We have also performed parametric calculations of resistances for Ni, Pd, and Au CNT interconnects, where CNT diameters have been varied from 1 to 22 nm, and chirality angles from 0 to 30 deg (with the step 5 deg) for the two basic metal substrate orientations [(100) and (111)]. The aim of these detailed simulations is to create approximation dependences and the database of interconnect compositions for various technological applications. Technologically reasonable results of these simulations [CNT-Me interconnect, (100), (111)] are shown in Fig. 17. The dependence of interconnect resistance on the number of effective bonds ($R_{\text{interconnect}} \times N_{\text{eff.bonds}}$) is the constant value. In the cases of CNT-Au, CNT-Pd, and CNT-Ni interconnects (100) it equals approximately 4000, 6666, and 8000 kΩ, correspondingly.

**Fig. 17** Results of parametric calculations of resistances for Me-CNT interconnects: (a) to (f).
5 Conclusions

Using the effective bonds model, we have predicted the resistivity of interconnects between the metal substrate and SW or MW CNTs (SL GNR or ML GNR). We have underscored that conductance and other current-voltaic parameters depend on the morphology of the nearest shells in MWCNTs and MLGNRs, which leads to complications for technology and production of nanodevices with stable electric characteristics.

We have the potential now to create the database of CNT-Metal and GNR-Metal junction combinations taking into account a set of parameters; namely, the angle of chirality, the CNT diameter, the number of walls or layers, the type of a metal substrate (Me), and the orientation of a metal substrate [e.g. (100), (111), or (110)]. Thus we are able to forecast interconnect properties for various SW-, MW CNT, SL- and MLGNR configurations.

Potential nanosensor devices based on CNTs, GNRs, and their interconnects are possible to design and use for effective detection of external influences of various nature. They can change the electron transport regime and promote the current losses. At the same time, the interconnect interfaces can also be sensitive to chemical adsorbents, electrical and magnetic fields, while changing the properties of interconnect potential barrier and the efficiency of conducting channels. Both these nanosensoring mechanisms are possible to simulate in the framework of the proposed models.

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