Ab Initio Simulations on Electric Properties for Junctions Between Carbon Nanotubes and Metal Electrodes

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The cluster approach based on the multiple scattering theory formalism, realistic analytical and coherent potentials, as well as effective medium approximation (EMA-CPA), can be effectively used for modeling of nanosized systems. This allows us to calculate the dispersion law \( E(k) \), electronic density of states, conductivity, etc. The multiple scattering problems are stated for radial (e.g., quantum dots) and axial (e.g., nanowires, nanotubes) symmetry approaches. Basic attention is paid now for applications on carbon nanotubes (CNTs) of varying morphology, including their contacts with other conducting elements of a nanocircuit, which can be applied for interconnects in a high-speed electronics. The main problems solving for the resistance in CNT junctions with metal particles appear due to the influence of chirality effects in interconnects of single-wall (SW) and multi-wall (MW) CNTs with the fitting metals (Me = Ni, Cu, Ag, Pd, Pt, Au) for a predefined CNT geometry. Using the model of ‘effective bonds’ as developed in this study within the formalism of Landauer theory, we can predict the resistivity properties for both SW and MW CNT-Me interconnects. We have also developed the model of the inter-wall interaction inside the MW CNTs, which demonstrates possible ‘radial current’ losses.

Keywords: Carbon Nanotubes, SW and MW Morphology, Junction Between the CNT and Metal Substrate, Scattering Theory, Electronic Structure Calculations, Resistance of CNT-Me Contact, Inter-Wall Transparency in MW CNTs.

1. INTRODUCTION

To overcome disadvantages of nowadays microtechnology, the miniaturization of electronic devices, a high integration level and the increase of the operation frequencies and power density are required, including the use of adequate materials and innovative chip interconnects. Due to their unique physical properties, carbon nanotubes (CNTs) attract permanently growing technological interest, for example, as promising candidates for nanointerconnects in a high-speed electronics.1 The main aim of the current study is the implementation of advanced simulation models for a proper description of the electrical resistance for contacts between carbon nanotubes (both SW and MW) of different morphologies and metallic substrates of different nature. An adequate description of CNT chirality2 is one of the key points for proper simulation on electric properties of CNT-based nanoelectronic devices.

The resistance of contacts between CNTs and metallic substrates can considerably exceed that observed in the separate parts of these junctions.3 The conductance between real metal and CNT still occurs, however, mainly due to the scattering processes, which are estimated to be rather weak.4 Figure 1 represents the contacts of nanotube with both substrates, as a prototype nanodevice. This is a main subject of our current research and modeling. The toroidal region (CNT-Me) is the object of a microscopic approach responsible for the main contribution to the resistance. As to the nanotube itself and the metallic substrate, their resistances may be considered as macroscopic parameters.

The electronic structure of the CNT-Me interconnect can be evaluated through the electronic density of states (DOS) for carbon-metal contact considered as a ‘disordered alloy’, where clusters containing both C and Me atoms behave as scattering centers. The computational procedure developed for these calculations5 is based on the
construction of cluster potentials and the evaluation of both scattering \((S)\) and transfer \((T)\) matrices.

The general model of multiple scattering with effective media approximation (EMA) for condensed matter, based on the approach of atomic cluster, is present in Figure 2. The cluster formalism was successfully applied, e.g., for metallic Cu,\(^5\) as well as for both elemental (Ge, Si, As, Se, Te) and binary (As\(_x\)Se\(_{1-x}\) and Sb\(_x\)Se\(_{1-x}\)) semiconductors.\(^6\) When using the coherent potential approach (CPA) as EMA approximation, the resistance of interconnect can be evaluated through the Kubo-Greenwood formalism\(^7\) and Ziman model.\(^8\) Both Figures 3 and 4 depict the idealized images of contacts between CNTs and the metal substrate.

2. MULTIPLE SCATTERING THEORY AND EFFECTIVE MEDIUM APPROACH FOR CNT SIMULATIONS

2.1. Electronic Structure Calculations

We consider the resistivity 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 (Matissien rule). The scattering paradigm is presented in Figure 5. The computational procedure developed by us for these calculations\(^5,6\) includes the construction of the cluster potentials and the evaluation of the \(S\)– and \(T\)-matrices for scattering and transfer, respectively. This allows us to realize the full-scale electronic structure calculations for condensed matter (‘black box’), where influence, \(\Psi_{in}(r)\), means a set of electronic ‘trial’ energy-dependent wave functions, while response, \(\Psi_{out}(r)\), allows us to calculate sets of scattering amplitudes corresponding to the scattering channels for any ‘trial’ energy. This results in ‘decryption’ of the electronic spectra of ‘black box’.

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**Fig. 1.** Model of CNT-Me interconnect as a prototype of nanodevice.

**Fig. 2.** Multiple scattering problem for the system of clusters as a model of condensed matter: strategy of calculations of fundamental properties of condensed medium described within the effective media approximation.

**Fig. 3.** Fragment of interconnects between the Ni substrate and C nanotubes.
We consider a domain where the stationary solutions of the Schrödinger equation are known, and we label them by

\[ \psi_{\text{in}}(r) = \phi_k(r) = \exp(ikr) \] (1)

Scattering of ‘trial’ waves, in a presence of potential, yields new stationary solutions labeled by

\[ \psi_{\text{out}}(r) = \psi_{\pm k}(r) \] (2)

for the modified Schrödinger equation \( \hat{H}\psi_{\pm k}(r) = E\psi_{\pm k}(r) \), where the Hamiltonian operator includes the original potential energy of modeled scattering object.

An electronic structure calculation is considered here as a scattering problem, where the scattering centers are identified with the atoms of clusters.\(^5\) The first step of modeling is the construction of potentials, both atomic and crystalline, which is based on analytical Gaspar’s potential of screened atomic nucleus\(^9\) and \(X/\alpha\) and \(X/\alpha/\beta\) presentations for the electronic exchange and correlation, using the LDA (Local Density Approximation). Figure 6 shows both atomic and crystalline potentials for carbon as compared to the Hartree-Fock atomic potential.

\[ \psi(r) \rightarrow e^{ikz} + f(\theta) \frac{e^{ikr}}{r} \] ("liquid metal" model) (3)

and

\[ \psi(r) \rightarrow e^{ikz} + f(\theta, \varphi) \frac{e^{ikr}}{r} \] (spherical cluster model) (4)

Then, the electronic wave scattering problem is solved, and the energy dependence of the scattering properties for isolated \(MT\) scatterers is obtained, in the form of the phase shifts, \(\delta_{\text{in}}(E)\). The \(T\)-matrix of the cluster is found as a whole. The indices \(l\) and \(m\) arise as a result of expansions of the functions as Bessel’s functions \(j_l\) and \(h_l\) of spherical harmonics \(Y_{lm}\).

In general, the modeling of disordered materials represents them as a set of atoms or clusters immersed in 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.\(^5\) The results of potential modelling and phase shifts in the framework of the \(MT\)-approximation are present elsewhere.\(^5,6\)

The formalism used by us for electronic structure calculations is based on the coherent potential approximation (CPA),\(^7\) the multiple scattering theory\(^10\) and cluster approach.\(^11\) As a first step in the modelling procedure, one postulates the atomic structure on the level of short- and medium-range orders. As a second step we construct a “crystalline” potential and introduce the muffin-tin (\(MT\)) approach. The construction procedure of potentials, both atomic and crystalline, uses the special well-tested realistic analytical potentials based on the Gaspar-like potentials as well as \(X\alpha\) and \(X\alpha\beta\)-presentations for the electronic exchange and correlation, in the form of the electronic density expansions.\(^5\) The scattering paradigm for the simplest cases of spherically symmetrical potential-scatterers (elastic scattering) looks as:

\[ \psi(r) \rightarrow e^{ikz} + f(\theta, \varphi) \frac{e^{ikr}}{r} \] (spherical cluster model) (4)

Then, the electronic wave scattering problem is solved, and the energy dependence of the scattering properties for isolated \(MT\) scatterers is obtained, in the form of the phase shifts, \(\delta_{\text{in}}(E)\). The \(T\)-matrix of the cluster is found as a whole. The indices \(l\) and \(m\) arise as a result of expansions of the functions as Bessel’s functions \(j_l\) and \(h_l\) of spherical harmonics \(Y_{lm}\).

In general, the modeling of disordered materials represents them as a set of atoms or clusters immersed in...
an effective medium, with the dispersion $E(K)$ and a complex energy-dependent coherent potential $\Sigma(E)$ found self-consistently in the framework of the CPA. The basic equations of this approach are:

$$\Sigma(E) = V_{\text{eff}} + \langle T \rangle (1 + G_{\text{eff}} \langle T \rangle)^{-1}$$

(5)

$$G(E) = G_{\text{eff}} + G_{\text{eff}} \langle T \rangle G_{\text{eff}} = \langle G \rangle$$

(6)

$$\langle T(E, K) \rangle = 0$$

(7)

$$\Sigma(E) = V_{\text{eff}}$$

(8)

$$\langle G \rangle = G(E) = G_{\text{eff}}$$

(9)

$$N(E) = -(2/\pi) \ln \left\{ dE \left\| G(E) \right\| \right\}$$

(10)

Here $\langle \ldots \rangle$ denotes averaging, $V_{\text{eff}}$ and $G_{\text{eff}}$ are the potential and the Green’s function of the effective medium, respectively, $T(E, K)$ is the $T$ matrix of the cluster, and $N(E)$ the integral density of the electronic states. Eq. (7) can be re-written in form:

$$\langle T(E, K) \rangle = \text{Sp} T(E, K) = \int_{\Omega_k} \langle K | T(E, K) | K \rangle d\Omega_k = 0$$

(11)

where $|K\rangle = 4\pi \sum_{l,m} (i)^l j_l(kr) Y_{lm}(K) Y_{lm}(r)$ is the one-electron wave function, Sp means the calculation of the matrix trace while the integration is performed over all angles of $K$ inside the volume $\Omega_k$. Eq. (7) enables one to obtain the dispersion relation $E(K)$ of the effective medium. The DOS calculations have been performed using the relation:

$$\rho(E) = \frac{2}{\pi} \int \text{Im} \{\text{Sp} G(r, r', E)\} dr$$

(12)

where $G(r, r', E) = \sum_{l,m} Y_{lm}(r) Y_{lm}(r') G_l(r, r')$ is the angular expansion of Green function.

The paradigm of scattering theory and the developed strategy for simulation of CNTs electronic properties uses the generalized scattering condition for the low-dimensional atomic structures of condensed matter (Quantum Scattering in d-Dimensions):

$$\psi_k^{(\pm)}(r) \sim \varphi_k^{(\pm)}(\Omega) \exp(\pm ikr)$$

(13)

where superscripts ‘+‘ and ‘−‘ label the asymptotic behavior in terms of $d$-dimensional waves:

$$\frac{\partial \sigma_{ab}}{\partial \Omega} = \frac{2\pi}{h\nu} \left| \langle \varphi_b | \hat{V} | \psi_a \rangle \right|^2 \rho_d(E)$$

(14)

where $d$ is the atomic structure dimension. In particular, the scattering model for a cylindrical atomic cluster allows us to calculate the CNTs electronic structure for various diameters and chiralities.

2.2. Calculations of Conductivity and Resistance

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

$$\sigma_{\text{ef}}(\omega) = \frac{\pi n}{4\omega} \int \left| f(E) - f(E + \hbar \omega) \right| D(E)^2 \rho(E) \rho(E + \hbar \omega) dE$$

(15)

where $\omega$ is a real frequency parameter of Fourier transform for the time-dependent functions, $f(E)$ the Fermi-Dirac distribution function, $D_{\text{ef}} = \int_\Omega \psi_{\text{ef}}(r) \nabla \psi_{\text{ef}}^* dr$. $\psi_{\text{ef}}(K) = A \exp(iK\mathbf{R})$ and $K$ is the complex wave vector of the effective medium. The dispersion function $E(K)$ determines the properties of the wave function $\psi_{\text{ef}}(K)$ upon the isoenergy surface in $K$-space. The imaginary part $\mathbf{K}_i$ of $\mathbf{K}$ causes a damping of the electron wave, due to the absence of the long-range structural order.

For static conductivity ($\omega = 0$ and $T = 0^\circ$, K), Eq. (15) gives the Drude-like formula:

$$\sigma_{\text{ef}}(\omega) = \frac{e^2 n^*}{m^* \tau}$$

(16)

where $n^*$ is the effective electron density, with a relaxation time $\tau \approx 1/\nu_{\text{th}}$, $l(T)$ is the free path while a heat velocity is $v_{\text{th}} = (3kT/m^*)^{1/2}$. The effective electron mass can be defined using the dispersion law:

$$m^* = \left( \frac{\partial^2 E}{\partial K^2} \right)^{-1}$$

(17)

where $K_0$ is a modulus of the real part $\mathbf{K}$ vector.

Thus, there exist some ideas to estimate the conductivity in static and frequency regimes and take into account temperature effects. However, in the case of CNT, we must consider not only the diffusive mechanism of conductivity, but also the ‘so-called’ ballistic one. This is an evident complication in the interpretation of electrical properties of CNTs and related systems.

3. ‘LIQUID METAL’ MODEL FOR CNT-METAL JUNCTION: CNT-NI CASE

The term “liquid metal” means the structural disorder of the substance involved, more precisely, only the nearest order (short range order—SRO) is considered as it usually occurs in a liquid. It also means that the inter-atomic distance between the nearest neighbors (first coordination sphere) is fixed, whereas the angular coordinates are random. To implement this model, we focus the matter into a single atom (Fig. 7) which is associated with a ‘crystalline’ potential in MT-approach, to consider the influence of the nearest vicinity. The neighbor atom for the selected atom is spread and, in fact, we are working at one-bond distance.

The area 2 is a sphere of radius $R_c$ (Fig. 7) determined from the condition of average matter density maintenance. However, to consider the influence of medium we need to “load” the sphere 2 with an effective complex potential, which defines the fading of electromagnetic waves, thereby modeling the disordered medium. The region 3 is under the influence of coherent potential $\Sigma(E)$. After that we must sew the wave functions on the border of regions 2 and 3, superposing the Soven condition, which correspond to the statement that disordered media do not allow
the forward scattering. The spherical symmetry of this system allows us to use partial decomposition techniques and the scattered wave outside the MT-sphere 2, where the potential is constant, defined as: \[ \psi^{(2)}_{\text{sc}}(r) = j_{1}(kr) - t g_{\text{sc}} n_{\text{sc}}(kr) . \]

The next step includes determination of the dispersion law for the effective medium and the electronic density of states (EDOS, see Eq.(12)). In “liquid” model, the argument \( K \) of dispersion function \( E(K) \) is a complex: \( K_{x} + iK_{y} \). The CPA approach means: \( \int_{\text{d}k} (|K|/|K|) d\Omega_{K} = 0 \), similar to Eqs. (7) and (11). Another condition is that the average density of matter is maintained also locally. For CNT-Ni junction (Figs. 3, 4), a “liquid metal” model is calculated using the ‘mixed’ dispersion law:\(^5,13\)

\[ E_{C-Ni}(K_{x}) = xE_{e}(K_{x}) + (1 - x)E_{Ni}(K_{x}) . \] (18)

Equation (18) means configurationally-averaged state of the electronic structure within the interconnection space with a variable extent of disorder. The metal alloy model can be used for evaluation of mixed effective mass \( m^{*}_{C-Ni}(E) \). Taking into account the spectral dependence of the effective mass \( m^{*}(E) \) and estimating the spectral resistivity \( \rho_{x}(E) \), we can estimate the average layer resistivity \( \rho_{x,av} \) as:

\[ \rho_{x,av} = \frac{E_{\text{lin}}^{k_{x}} \rho_{x}(E)dE}{E_{\text{lin}}} \] (19)

where \( E_{\text{lin}} \) is the width of conduction band and \( x(z) \) the stoichiometry coefficient depending on the coordinate \( z \) of ring layer (Fig. 4). An evaluation of resistance for the CNT-Ni contact gives \(~105~\text{kOhm} \) for the nanotube with the internal and external radii \( R_{1} = 1.0~\text{nm} \) and \( R_{2} = 2.0~\text{nm} \), respectively. Evidently, the results of resistance evaluation for interconnect depend essentially on both the layer height \( l_{l} \) (C-Ni-CNT space, Fig. 4) and the spectral integration parameter \( E_{\text{lin}} \), which is responsible for the electron transport of really activated electrons.

The “liquid metal” model\(^3\) does not operate with CNT chirality in the interconnect space. Limitations on chirality effect (e.g., chirality angle) in the CNT-Me junction forced us to develop the semi-empirical model which considers the local atomic structure of interconnect. For this aim, we construct a model of ‘effective bonds’ for interconnect with the realistic atomic structure.

4. SIMULATION OF CNT-ME INTERCONNECT: ‘EFFECTIVE BONDS’ MODEL

A model of the CNT-Me nanointerconnect\(^4\) (Fig. 1) is developed in the current study. Within the electronic transport formalism, it consists of two regions supporting the two different electron transport mechanisms: ballistic (elastic) and collisional (non-elastic). These electron transport processes are simulated by the corresponding boundary conditions in the form of the effective medium. The CNT chirality \((m, n)\) is simulated by the corresponding orientation of carbon rings within the scattering medium (Fig. 8).

The most problematic regions for simulation are CNT-Me junctions, where atomic structural disorder is observed and the conductivity mechanism is changed. The chirality influence on the resistance in the region of interconnect depends on the number of statistically realized bonds between the CNT and the metallic substrate (e.g., Ni, Cu, Au, Ag, Pd, Pt) formed during the CNT growth above the metallic catalyst surface.

4.1. Mechanism of the Ballistic Conductivity as a Result of the Multiple Scattering

We assume that the conducting nanotubes are limited by the length while their conductivity electrons are not drastically scattered by any defect (imperfection) which is similar to an elastic ‘billiard’. The effect of the charge accumulation is neglected as well. We are dealing with the so-called ‘ballistic’ mechanism of the electronic transport. Such a model is similar to an ideal billiard with moving elastic balls-electrons. This means that the length of CNT as providing the ideal ballistic conductivity in standing-wave conditions of the open resonator. According to the Landauer model,\(^14\) \( g_{mn} = (e^{2}/h)S_{\text{av}}(T_{mn}, T_{mn}) \), \( m \neq n \), where \( g_{mn} \) are the conductance coefficients while \( (e^{2}/h)T_{12} \Delta \mu \) is the current flow between the two reservoirs with a difference between the chemical potentials \( \Delta \mu = \mu_{1} - \mu_{2} \) (\( T_{12} \) is

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**Fig. 7.** The “liquid metal” model.

**Fig. 8.** Modeling of chirality effects: carbon ring rotation within CNT.
the transmission coefficient found to be between 1 to 2 in the one-channel case) based on the conception of the quantum conductance $2e^2/h = 0.077 \text{ kOhm}^{-1}$ (or, the resistance is about 12.92 kOhm).

Using the simulation models presented earlier, we have developed models of resistance for both SW and MW CNT-Me interconnects, based on the interface potential barriers evaluation and Landauer formula, which defines the integrated conductance:

$$I_G = \frac{2e^2}{h} \sum_{i=1}^{N} T_i = \left( \frac{1}{12.92 (k \Omega)} \right) \sum_{i=1}^{N} T_i = 0.0774 \sum_{i=1}^{N} T_i \quad (20)$$

where $N$ is the number of conducting channels and $T_i$ the corresponding transmission coefficient.

### 4.2. Chirality and Thickness Simulations

Figure 9 presents a simulation of catalytic growth of CNT on the metal substrate. This is accompanied by creation of C-Me ‘effective bonds’ upon the (100) surfaces of some fcc-metals. Only more-or-less equilibrium bonds (“effective bonds”) are formed at inter-atomic distances corresponding to the minimum total energies. The evaluation of a number of “effective bonds” is principal for the number of “conducting channels” since conductance is proportional to the number of appearing “effective bonds” within the CNT-Me interconnect.

The calculation of conducting abilities of “effective bond” allows us to estimate the energy-dependent transparency coefficient of a potential barrier C-Me (Fig. 10), which belongs to scattering problems. The scattering within a C-Me potential barrier is also regulated by the effect of “thin film” for conductivity electrons, which leads to quantization in voltaic parameters (in the case of full transparency). The transmission (transparency) coefficient $T$ for the barrier scattering problem (Fig. 10) is defined as:

$$T = \frac{E_2}{E_1} \left( \frac{2 \sqrt{E_1}}{E_1 + \sqrt{E_2}} \right)^2 \quad (21)$$

where $E_1$ and $E_2$ are the corresponding electron energies. Evaluation of resistances for CNT-Ni junctions for various nanotube diameters and chiralities are present in Table I (see also Figs. 9 and 10). These resistances have been estimated taking into account that only thermally activated electrons (i.e., a small part of all electrons) take a part in the conduction process with Fermi velocity $v_F$. This ratio

<table>
<thead>
<tr>
<th>Diameter, nm</th>
<th>Chirality indices (Fig. 8)</th>
<th>Number of bonds in contact</th>
<th>Modulus of chirality vector, nm</th>
<th>Interconnect resistance, kOhm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.010</td>
<td>(13,0)</td>
<td>12</td>
<td>2.952</td>
<td>665.19</td>
</tr>
<tr>
<td>2.036</td>
<td>(26,0)</td>
<td>24</td>
<td>6.394</td>
<td>333.33</td>
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<td>(65,0)</td>
<td>64</td>
<td>15.990</td>
<td>124.72</td>
</tr>
<tr>
<td>10.100</td>
<td>(130,0)</td>
<td>129</td>
<td>32.002</td>
<td>61.87</td>
</tr>
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<td>20.360</td>
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<td>259</td>
<td>63.940</td>
<td>30.82</td>
</tr>
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<td>(7,7)</td>
<td>12</td>
<td>2.982</td>
<td>665.19</td>
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<td>(37,37)</td>
<td>72</td>
<td>15.765</td>
<td>111.11</td>
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<td>10.041</td>
<td>(74,74)</td>
<td>146</td>
<td>31.531</td>
<td>54.79</td>
</tr>
<tr>
<td>20.084</td>
<td>(128,128)</td>
<td>294</td>
<td>63.062</td>
<td>27.21</td>
</tr>
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<td>3</td>
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<td>2666.66</td>
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<td>500.00</td>
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<td>10.16</td>
<td>(108,36)</td>
<td>36</td>
<td>32.05</td>
<td>222.22</td>
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<td>20.32</td>
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<td>80</td>
<td>64.10</td>
<td>100.00</td>
</tr>
<tr>
<td>0.874</td>
<td>(10.5)</td>
<td>5</td>
<td>3.254</td>
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<td>2.072</td>
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<td>4.973</td>
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<tr>
<td>10.1528</td>
<td>(98,49)</td>
<td>47</td>
<td>31.880</td>
<td>170.21</td>
</tr>
<tr>
<td>20.5128</td>
<td>(198,99)</td>
<td>97</td>
<td>64.410</td>
<td>82.47</td>
</tr>
</tbody>
</table>
can be written as:
\[
\frac{\Delta n}{n} \approx \frac{3}{4} \frac{kT}{E_F} \quad (22)
\]
where \( n \) is the quasi-free electron concentration, for \( T = 300^\circ \text{K}, \ kT = 0.0258 \text{ eV} \).

The role of thermally activated electron is described by the scattering mechanism changing in the space of CNT-Me interconnect. The mean free path \( L \) in the CNT is of order \( 10^2–10^4 \text{ a}_C \), where \( a_C \) is a carbon covalent radius, which can be explained by the ballistic mechanism of electron transport within the energy channel of the CNT. At the vicinity of interconnect, we observe a drastic decrease of the electron mean free path down to \( 1–2 \text{ a}_C \).

From the uncertainty condition \( \kappa L \approx 1 \) (where \( L \sim a_C \sim 2 \text{ a}_\text{u.} \) is a free path), we can evaluate the Fermi electron wave number \( \kappa \sim \kappa_F \approx 1/a_C \approx 0.5 \text{ a}_\text{u.}^{-1} \). It means that \( E_F \sim 0.25 \text{ Ry}, \ i.e., a large increase of resistance occurs in the interconnect space. In particular, the variation of the chirality angle \( \phi \) within the interconnect space leads to a fluctuation of the number of C-Me atomic bonds. In the case of \( 0^\circ < \phi < 30^\circ \), a certain number of non-stable and non-equilibrium bonds can be created. Evidently, this leads to a decrease of interconnect conductance, which is well-observed when performing variation of nanotube diameter (Fig. 11).

Specific results for chirality effect simulations are shown in Figure 12, with an evident maximum of the resistance for \( \phi \approx 15^\circ \), where the large number of non-equilibrium bonds is formed, with higher potential barriers and lower transparency. Figure 13 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 is rather a ‘worse’ substrate for interconnect, although it yields the most effective catalyst 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 a stronger bond to the ends of SW CNTs than noble metals, i.e., some compromise exists between electrical parameters and strengths of the interconnect bonding.

5. SIMULATIONS ON MW CNT-ME INTERCONNECTS: CONDUCTANCE AND RESISTANCE

Our current study focuses on the development of models describing the growth mechanism of carbon nanotubes upon nanostructured Ni catalyst inside the pores of \( \text{Al}_2\text{O}_3 \) membranes. The scope of these simulations allows us to predict that a specific morphology of CNTs could be formed inside the specific membranes having defined periodicity and hole dimensions. These simulations are necessary, in order to understand the basic mechanism of CNT growth and to achieve the tight control on the fabrication process. We have constructed atomistic models of both SW CNT bundles and MW CNTs which could fit inside a porous alumina with holes diameters \(~20–21 \text{ nm} \). In particular, a multi-shell model of MW CNT is present in Figure 14, with a pre-defined combination of armchair (ac) and zig-zag (zz) shells (Table II). Again, Figure 15
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Four red nanotubes - metallic (ac)
Seven gray nanotubes - semiconducting (zz)

Internal diameter 12.88 nm

Fig. 14. A cross-section of the supercell model for MW CNT with height 6.39 nm and external diameter 19.89 nm.

Table II. Details of the model for MW CNT-Me interconnect.

<table>
<thead>
<tr>
<th>Diameter of CNT shell, nm</th>
<th>Chirality</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.88</td>
<td>(95,95) ac</td>
</tr>
<tr>
<td>13.54</td>
<td>(173,0) zz</td>
</tr>
<tr>
<td>14.24</td>
<td>(105,105) ac</td>
</tr>
<tr>
<td>14.87</td>
<td>(190,0) zz</td>
</tr>
<tr>
<td>15.58</td>
<td>(199,0) zz</td>
</tr>
<tr>
<td>16.27</td>
<td>(120,120) ac</td>
</tr>
<tr>
<td>16.99</td>
<td>(217,0) zz</td>
</tr>
<tr>
<td>17.69</td>
<td>(226,0) zz</td>
</tr>
<tr>
<td>18.44</td>
<td>(136,136) ac</td>
</tr>
<tr>
<td>19.18</td>
<td>(245,0) zz</td>
</tr>
<tr>
<td>19.88</td>
<td>(254,0) zz</td>
</tr>
</tbody>
</table>

shows similar ratios of electric resistances as for SW CNTs (Fig. 13), in favor of Au, Ag and Pd.

Using the simulation models presented earlier, we have developed an “effective bonds” model for MW CNT-Me junction resistance, based on the interface potential barriers evaluation and Landauer formula, Eq. (20). Results of these simulations are present in Figure 15 and Table III. However, in the case of MW CNT-Me junction, the integral mechanical bonding with a corresponding substrate may be not so significant as in the case of SW CNTs, where the weak bonding can be principal.

6. EVALUATION OF CURRENT LOSS BETWEEN THE ADJACENT SHELLS INSIDE THE MW CNT

Using the model of inter-shell potential within the MW CNT we also have evaluated the transparency coefficient, which determines the possible ‘radial current’ losses. Figure 16 shows the inter-shell potential which is calculated using the developed realistic analytical potentials (see comments of Section 2 and the procedure of the potential construction, e.g., in Ref. [3]). In Figure 16, $A$ is the electron emission energy, $E$ the electron energy, $V$ the height of the potential barrier between the nearest atoms in neighboring nanotube shells.

Thus, a radial transparency coefficient $T$ for the two different energy ratios can be defined as:

$$E > V, \quad T = \frac{4E k_2^2}{(E - k_2^2) \sin^2 k_2 a + 4E k_2^2}, \quad k_2^2 = E - V \quad (23)$$

$$E < V, \quad T = \frac{4E k_2^2}{(E - k_2^2) \sinh^2 k_2 a + 4E k_2^2}, \quad k_2^2 = V - E \quad (24)$$

where $k_z$ is the electron wave number in the case of above-barrier motion and $k_2$ the same for under-barrier motion. For example, between the 2nd and 1st shells (zz-ac case, Fig. 14) $a = 13.54 - 12.88 = 0.66$ nm = 12.47 a.u. and $T = 3.469 \times 10^{-6}$ per 1 bond.

Table III. Resistances for the MW CNT-Me interconnects.

<table>
<thead>
<tr>
<th>Metal</th>
<th>Z</th>
<th>Interconnect resistivity, $k\Omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>79</td>
<td>2.313</td>
</tr>
<tr>
<td>Pt</td>
<td>78</td>
<td>2.345</td>
</tr>
<tr>
<td>Pd</td>
<td>47</td>
<td>4.050</td>
</tr>
<tr>
<td>Ag</td>
<td>46</td>
<td>2.062</td>
</tr>
<tr>
<td>Cu</td>
<td>29</td>
<td>2.509</td>
</tr>
<tr>
<td>Ni</td>
<td>28</td>
<td>3.772</td>
</tr>
</tbody>
</table>

The total radial conductance is proportional to $T$ and the number of effective potential barriers. It is also clear that the ‘radial current’ losses (or, simply radial current) are similar to the Hall current due to the induced magnetic field of the basic axial current. A pure scattering mechanism is also possible. However, the radial conductance per CNT length depends on chirality of the nearest nanotubes, when the number of shortest effective barriers is varied in a probabilistic way. This also means that current–voltage parameters of MW CNTs can be less stable, than in the case of SW CNTs. It was found that the inter-shell interactions, such as inter-shell tunneling of electrons and Coulomb interactions, cause a reduction of the total MW CNT conductance. This is also in agreement with evaluations in Ref. [22].

7. PARAMETRIC SIMULATIONS OF SW-CNT-METAL INTERCONNECTS

Using the approach presented in Section 5, we have also performed the large-scale parametric calculations of resistances for CNT interconnects with Ni, Pd and Au, where CNT diameter varies from 1 to 22 nm, and chirality angle from $0^\circ$ to $30^\circ$ (with the step $5^\circ$), for two basic metal substrate orientations ([100] and [111]). These simulations clarify dependences of the used approximations on CNT properties and determine the data base for CNT-Me interconnect important for technological applications.

Technologically reasonable results of these simulations are shown in Figure 17. The resistance of interconnect produced by a number of effective bonds ($R_{\text{interconnect}} \times N_{\text{eff.bonds}}$) yields constant values. In the case of a CNT interconnect with Au(100) substrate this value equals $\sim$4000 kOhm.

The presented results of interconnect resistance simulations are useful, in order to consider a parametric analysis of SWCNT effective conducting channels with arbitrary chirality. The synergy and consistency of electric properties of CNT as well as CNT-Me spaces will, evidently, allow for the correct description of CNT-based nanodevices as a whole.

8. CONCLUSIONS

We consider conductivity and resistivity as a scattering problem, where the current carriers participate in the transport, according to mechanisms based on presence of the scattering centers (charge and structural defects, phonons, etc.). Computational procedure developed for these calculations is based on both construction of cluster potentials and evaluation of matrices for scattering and transfer, respectively. Models of CNT-Me junctions developed in the current study consist of two regions supporting the two different electron transport mechanisms: ballistic (elastic) and collision-type (non-elastic). These transport processes are simulated within a general scattering problem where precise solutions of modeled CNTs and CNT-Me junctions are accorded self-consistently with the effective medium of the rest space possessing the conventional and pre-defined boundaries.

The CNT $(m,n)$ are simulated by the corresponding orientation of the chirality vectors within the scattering medium. Inside the regions of C-Me junctions, where atomic structural disorder is observed, the conductivity mechanism is changed. The chirality influence on the resistance of junction depends on the number of statistically realized bonds between the carbon nanostructure and the metal substrate.

Using the ‘effective bonds’ model, we have predicted the resistivity of interconnects between the metal substrate (e.g., Ni) and the SW or MW CNTs. There also exists a qualitative compatibility of results obtained for the CNT-Me junctions using both approaches considered in this paper:

(i) first principles ‘liquid metal’ model and
(ii) semi-empirical ‘effective bonds’ model based on the Landauer’s relationship.

At the same time, the latter results are quantitatively comparable with those measured experimentally, i.e., within the range from several up to 50 kOhm.

We have also developed the model of inter-shell interaction for the MW CNTs, which allows us to estimate the transparency coefficient as an indicator of possible ‘radial current’ losses. We have underscored that a conductance and other current–voltage parameters depend on the morphology of the nearest shells in MW CNTs, which leads to complications for the production of nanodevices with the stable electric characteristics.

Detailed parametric simulations of CNT-Me interconnect resistances in the case of Ni, Pd and Au substrates give us the data base of corresponding resistance values via CNT diameters, chiralities and substrate orientations.
([100] and [111]) for design of possible nanodevices and technological applications. In particular, we point out that the CNT-Au interconnect is electrically preferable.

Acknowledgments: This study has been supported by grant EC FP7 ICT-2007-1, Proposal for 21625 CATHHERINE Project (2008–2010): Carbon nAnotube Technology for High-speed nExt-geneRation nano-InterconNEcts. We thank Professor E. A. Kotomin, Professor M.-S. Sarto and Dr. A. Tamburrano for stimulating discussions.

References and Notes


Received: 26 January 2011. Accepted: 17 February 2011.