THEORETICAL SIMULATIONS OF NANOELECTRONIC DEVICES: QUANTUM DOTS, NANOWIRES AND CARBON NANOTUBES

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Introduction

The miniaturization of electronic devices, the high integration level and increase of the operation frequencies and power density require the use of adequate materials and innovative chip interconnects and vias, to avoid a bottleneck in the existing technologies. Fundamental efforts are directed on the special kinds of nanosystems such as quantum dots, quantum nanowires and nanotubes. Quantum dots, also known as nanocrystals, are a non-traditional type of semiconductor with limitless applications as an enabling material across many industries. They are unique class of semiconductor, because they are so small, ranging from 2-10 nm. (10-50 atoms) in diameter (Figure 1). Basic attention is paid to carbon nanotubes (CNTs), including their contacts with other conducting elements of a nanocircuit. Due to the unique physical properties, CNTs attract permanently growing technological interest, for example as promising candidates for nanointerconnects in a future high-speed electronics (Figures 2,3).

![Figure 1. Quantum dots](image1)

![Figure 2. Carbon nanotubes](image2)

![Figure 3. Model of nanoelectronic device](image3)

Discovered in 1991 by Iijima and co-workers, carbon nanotubes have quickly become one of the most popular materials in nanoscience and nanotechnology, drawing the interest of researchers worldwide. Many potential applications have been investigated, largely based on theoretical and experimental results, including: conductive and high-strength composites; energy storage and energy conversion devices; sensors; field emission displays and radiation sources; nanometre-sized semiconductor devices, probes, and interconnects.

A computational procedure developed for these calculations [1] is based on construction of the cluster potentials and evaluation of the S- and T-matrices for scattering and transfer, respectively. Certain simplifications are necessary to obtain reliable results. For instance, CPA (coherent-potential approximation [1]) is considered as an effective-medium-approach (EMA). The specific conductivity ($\sigma$) can be evaluated through the Kubo-Greenwood formalism [1-3] or in simple cases using the Drude-type formula. The temperature and frequency properties can be also considered in this approach.

The principally important problem for nowadays developed nanodevices is properties of interconnects with a real electronic system to realize the evident advantages of nanotechnologies.

In particular, the electrical resistance of contacts between the carbon nanotubes (CNT) and the nickel catalytic substrate can considerably exceed that observed in separate parts of these interconnects [4,5]. Conductance between real metals and CNT still occurs, however, mainly due to scattering...
processes which are estimated rather weak [6]. Figure 4 depicts the idealized image of contacts between the CNTs and Ni substrate.

The toroidal region (C-Ni) is the object of microscopic approach responsible for the main contribution into resistance. As to the nanotube itself and the metallic substrate, their resistances may be considered as the macroscopic parameters. The electronic structure for the CNT-Ni interconnect can be evaluated through the electronic density of states (EDOS) for C-Ni contact considered as ‘disordered alloy’, where clusters containing both C and Ni atoms are the centres of scattering. The computational procedure developed by us for these calculations [1] is based on the construction of the cluster potentials and the evaluation of the S- and T-matrices of scattering and transfer, respectively (Figure 5). The cluster formalism was successfully implemented for metallic Cu [1] as well as for both elemental (Ge and Si) and binary (As-, Sb-, and Se-containing) semiconductors [7] (see also Figure6). Special attention was paid to the latter since As_xSe_{1-x} and Sb_xSe_{1-x} are not only prospective materials for the optical recording - the concept of statistical weighing was applied here for the binary components [4,5]. Using the coherent potential approach (CPA) as an effective-medium-approximation (EMA) the resistance of interconnect can be evaluated through the Kubo-Greenwood formalism [7] and Ziman model [9].

**The scattering problem and electronic properties calculation algorithm:**

- Multiple scattering

![Figure 4. Fragment of interconnects between the Ni substrate and C nanotubes.](image)

![Figure 5. Scattering principle](image)

![Figure 6. Multiple scattering problem for the system of clusters: strategy of calculations of fundamental properties of condensed medium](image)
1. Effective Media Electronic Structure Calculations of CNT-Ni Interconnects

The scattering theory approach gives us the possibility to calculate an electronic structure and elastic properties of condensed media, which should be considered as static phenomena. At the same time this approach is convenient for the electron transport modelling, which is a dynamical problem for electron scattering. Thus the trial (model) electronic waves in the case of conductivity modelling become realistic ones. A computational procedure developed for these calculations [1] is based on construction of the analytical cluster potentials, based on the potential approximation of Gaspar and a statistical approach of atomic electronic structure (X\text{α} and X\text{αβ} presentations for the electronic exchange and correlation) and evaluation of the S- and T-matrices for scattering and transfer, respectively.

Certain simplifications are necessary to obtain reliable results, for example, the CPA considered as an effective-medium-approximation (EMA). The specific conductivity (\(\sigma\)) can be evaluated through the Kubo-Greenwood formalism or in simple cases using the Drude-type formula. The temperature and frequency properties can be also considered in this approach. We consider the interconnect system as a disordered system. This allows to apply the scattering principle (see Figures4-6), taking into account any short atomic structure order.

The modelling of disordered materials represent 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:

\[
\Sigma(E) = V_e + \langle \hat{T} \rangle (1 + G_e \langle \hat{T} \rangle)^{-1}, \tag{1}
\]

\[
G(E) = G_e + G_e \langle \hat{T} \rangle G_e = \langle G \rangle, \tag{2}
\]

\[
\langle \hat{T}(E, \mathbf{K}) \rangle = 0, \tag{3}
\]

\[
\Sigma(E) = V_e, \tag{4}
\]

\[
\langle G \rangle = G(E) = G_e, \tag{5}
\]

\[
N(E) = -(2/\pi) \ln|\det[G(E)]| . \tag{6}
\]

Here \(<...,>\) denotes configuration averaging, \(V\) and \(G\) 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 (3) can be re-written in form:

\[
\langle \hat{T}(E, \mathbf{K}) \rangle = \text{Sp} T(E, \mathbf{K}) = \int \langle \mathbf{K} | T(E, \mathbf{K}) | \mathbf{K} \rangle d\Omega_{\mathbf{K}} = 0 , \tag{7}
\]

where \(\mathbf{K} = 4\pi \sum_{\text{lm}} f(kr) Y_{\text{lm}}^*(\mathbf{K}) Y_{\text{lm}}(r)\) is the one-electron wave function and integration is performed over all angles of \(\mathbf{K}\) inside the volume \(\Omega\). Equation (7) enables one to obtain the dispersion relation \(E(\mathbf{K})\) of the effective medium. The calculation of the density of the electronic states in the form of equation (6) can be done using the variation procedure:

\[
\rho(E) = \frac{\delta N(E)}{\delta E} . \tag{8}
\]

The calculations of conductivity are usually performed using Kubo-Greenwood formula [5,8]:

\[
\sigma(\omega) = (\pi \Omega / 4\omega) \int [f(E) - f(E + h\omega)] D_{E,E} \rho(E) \rho(E + h\omega) dE, \tag{9}
\]

where \(\omega\) is a real frequency parameter gives the Fourier transform for the time-dependent functions, \(f(E)\) the Fermi-Dirac distribution function, \(D_{E,E} = \int_{\Omega} \Psi_{E(K)}^* \nabla \Psi_{E} d\mathbf{r}\), where \(\Psi_{E(K)} = A \exp(i\mathbf{K}r)\) 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 \(\Psi_{E(\mathbf{K})}\) on the isoenergy surface in \(K\)-space. The imaginary part of \(\mathbf{K}\) causes damping of the electron wave, due to the absence of long-range structural order.

The second simplest possibility for estimating the conductivity comes from the Thouless model [10], where the loss of phase of the electron wave is linked with the structural disorder and is taken into
account in a purely phenomenological way through the coherence length $\lambda$. The complex wave number $K = K_R + i(1/2\lambda)$ in this model can now be attributed to the calculated dispersion relation $E(K)$, where $K_R$ denotes the real part of wave number $\text{Re}\{K\}$. If we calculate the coherence length $\lambda = (1/2)\text{Im}\{K\}$, then the conductivity can be expressed via Fermi level $\varepsilon_F$:

$$\sigma_e(\omega) = (16/3)\pi^2\lambda_0^2(\varepsilon_F)[1 + \omega^2\lambda_0^2/(4\varepsilon_F)].$$

Using the dispersion law, the effective mass of electrons can be defined as:

$$m^* = (\varepsilon_F E / \partial K_R^2)^{-1}.$$  

Thus, the static conductivity can be re-written using Drude formula [11]:

$$\sigma_{e(K)} = \frac{e^2 n^*}{m^*} \tau,$$

where $n^*$ is the effective electron density, with a relaxation time $\tau \approx \frac{l}{v_h}$, $v_h = \frac{3kT}{m^*}$, and $l(T)$ denoting the free path.

Thus, there are 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 of the interpretation of electrical properties of CNT and their systems.

### 1.1. Liquid Metal Model of the Ni-CNT interconnect

As the first step we have used the so-called liquid metal model for simulation of electronic properties of Ni-CNT interconnects. The term “liquid” means the structural disorder of the substance involved, more precisely, only the nearest order is taken into account, as usual considered in the liquid. It also means that the interatomic distance with the nearest neighbour (first coordination sphere) is fixed whereas the angular coordinates are random. Another condition is that the average density of matter is maintained also locally. The term “metal” does not mean the applicability of model only for metals, it was successfully implemented for semiconductors too [1-3]. Thin metal layers as well as nanotubes can be also described in the framework of the formalism of a glass-like structure [9,10].

To implement this model, we focus the matter into a single atom (Figure 7) which will be associated with a 'crystalline' potential in $MT$-approach, to consider the influence of the nearest vicinity. The neighbour atom around the studied atom is spread and, in fact, we are working on the one bond distance.

The area $\mathcal{A}$ is a sphere of $R_C$ radius determined from the condition of average matter density maintenance. However, to consider the influence of medium we need to “load” the sphere $\mathcal{A}$ with an effective complex potential, which defines the fading of electromagnetic waves, thereby modelling the disordered medium. The region $\mathcal{B}$ is under the influence of coherent potential $\Sigma(E)$. After that we must sew the wave functions on the border of regions $\mathcal{A}$ and $\mathcal{B}$, superposing the Soven condition [16], which correspond to the statement that disordered media do not allow the forward scattering.

The next step is to find the dispersion law of the effective medium and the electronic density of states. In “liquid” model, the argument $K$ of dispersion function $E(K)$ is a complex: $K_R + iK_I$. CPA approach condition using the effective $\tilde{T}$ - matrix amplitudes ($\int \langle K | \tilde{T} | K \rangle d\Omega_K = 0$ [4]) allows us to get the dispersion law (see Figure 8).

The calculation of the EDOS using the formalism of scattering theory is based on Luttinger theorem [17]. The simplest expression for the EDOS through the Green’s function can be written as:

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

where the Green’s function $G(r, r') = \sum_{l,m} Y_{lm}(r)Y_{lm}(r')G_l(r, r')$ is used [8].
The next step in using of the “liquid metal model” is the possibility to evaluate the specific resistance $\rho$ in the framework of the Ziman’s model [7]. The basic definition is the modified Drude formula for conductivity [11]:

$$\sigma = \frac{1}{\rho} = \frac{ne^2\tau}{m^*}, \quad (14)$$

where the $\tau$ is the effective time of free movement, $m^*$ is the effective mass.

If the atoms of liquid metal (or amorphous metal film) are dispersing centres, their distribution is not completely random (while the amplitude of scattering from two atoms located one from another on a distance, circumscribed by a radius-vector $\mathbf{R}$, is equal: $[1 + \exp(iqR)] f(\theta)$, where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$; and taking into account multiple scattering [14]:

$$\frac{1}{\sigma} = \rho = \frac{3\pi}{\hbar^2 e^2 \nu_f \pi} \int_0^{2\kappa_f} |V(q)|^2 S(q) q^2 dq \frac{4k_F^2}{\pi}, \quad (15)$$

where $\frac{1}{\tau} = N_C \nu_f \int_0^\pi I(\theta)(1 - \cos \theta) 2\pi \sin \theta d\theta$, $I(\theta) = |f(\theta)|^2$, $f(\theta) = \left(\frac{m}{2\hbar^2}\right)^3 \int V(\mathbf{r}) \exp(iqR) d\mathbf{r}$ - is the scattering amplitude function, $S(q) = \frac{1}{N_C} \int (1 + \exp(i\mathbf{q}\mathbf{R})) g(R) d\mathbf{R}$ is the structural factor, whereas

$$V(q) = \frac{1}{\Omega} \int V(\mathbf{r}) \exp(iqR) d\mathbf{r}$$

the Fourier image of potential-scatterer, $L = \nu_f \tau$ the distance of free path, $\nu_f$ the Fermi velocity, $\tau$ the free path time, $N_C$ the number of scattering centres within the volume $\Omega$, $\theta$ - is the scattering angle, $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, $\mathbf{k}$, $\mathbf{k}'$ - are the wave vectors before and after a scattering, $g(R)$ - is the pair correlation function of atomic distribution.

1.2. Simulation results

A liquid metal model for CNT-Ni interconnect is based on calculation of the ‘mixed’ dispersion law:

$$E_{C,Ni}(K_R) = xE_C(K_R) + (1-x) E_{Ni}(K_R). \quad (16)$$

The metal alloy model is used for evaluation of mixed effective mass $m^*_{C,Ni}(E)$. Dependence of effective masses and specific resistance on $x$ are presented in Figure 9 and Table 1, Taking into account the spectral dependence of the effective mass $m^*(E)$ and estimating the spectral resistivity $\rho_s(E)$, we should estimate the average layer resistivity $\rho_{av}$ as follows:

$$\rho_{av} = \frac{\int_{E_{fin}}^{E_{fou}} \rho_s(E) dE}{E_{fin}}, \quad (17)$$

where $E_{fou}$ is the evaluation of conduction band width. The stoichiometry coefficient $x(z)$, where $z$ is the ring layer coordinate.

The integral resistivity of the contact C-Ni ring imaged in Figure 10 can be obtained by integration:
where $S$ is the nanotube cross-section, $r_1$ and $r_2$ are radii of internal and external walls of CNT. If $z = c_0x$ is proposed as linear, where $c_0$ is the scaling coefficient, we can rewrite Eq. (18) as:

$$R = \frac{k_0}{\pi(k_2^2R_2^2 - k_1^2R_1^2)} \int_0^1 \rho_{x,av}(x)dx ,$$

which can be applied for any geometry of the nanotube on the basis of the calculated resistance unit.

### Table 1. Dependence of specific resistivity $\rho_{x,av}$ on alloy composition ($x$)

<table>
<thead>
<tr>
<th>No.</th>
<th>$x$</th>
<th>$\rho_{x,av}$, Ohm-nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00</td>
<td>0.80724504E+02</td>
</tr>
<tr>
<td>2</td>
<td>0.10</td>
<td>0.8133489E+02</td>
</tr>
<tr>
<td>3</td>
<td>0.20</td>
<td>0.8218841E+02</td>
</tr>
<tr>
<td>4</td>
<td>0.30</td>
<td>0.833055E+02</td>
</tr>
<tr>
<td>5</td>
<td>0.40</td>
<td>0.8487165E+02</td>
</tr>
<tr>
<td>6</td>
<td>0.50</td>
<td>0.87061935E+02</td>
</tr>
<tr>
<td>7</td>
<td>0.60</td>
<td>0.90460375E+02</td>
</tr>
<tr>
<td>8</td>
<td>0.70</td>
<td>0.96249458E+02</td>
</tr>
<tr>
<td>9</td>
<td>0.80</td>
<td>0.10819738E+03</td>
</tr>
<tr>
<td>10</td>
<td>0.90</td>
<td>0.14581056E+03</td>
</tr>
<tr>
<td>11</td>
<td>1.00</td>
<td>0.82312308E+04</td>
</tr>
</tbody>
</table>

Resistance of the C-Ni contact = 0.1064E+04 Ohm, where $R_1 = 0.10E$ - 08 m, $R_2 = 0.20E$ - 08 m are the internal and external radii of conventional nanotube, $k_1 = 1, k_2 = 1, k_0 = 20$ nm are the scaling coefficients, $\int_0^1 \rho_{x,av}(x)dx = 0.5015E + 03$ Ohm - nm is the integral resistivity of a contact area, $w = \frac{k_0}{\pi(k_2^2R_2^2 - k_1^2R_1^2)} = 0.2122E+10$ m$^{-1}$, $k_0 = 0.20E-07$ m, $S = 0.9425E-17$ m$^2$.

#### 2. Mechanism of the Ballistic Conductivity as a Result of the Multiple Scattering

We assume that the conducting nanotubes are not so long and the electrons are not scattered too much by any defect (imperfection) of this nanomaterial [12,13]. The effect of charge accumulations can be neglected. We are dealing with the so called ‘ballistic’ mechanism of the electronic transport. This situation is similar to an ideal billiard with moving elastic balls-electrons. This mechanism works well far from the interconnect space. But the electric current is regulated by the transmission properties of interconnect. This simple approach gives us the well-known result $j_{LR} = n(2e^2/h)V_{bi}$, where $j_{LR}$ is the corresponding current density, $V_{bi}$ the bias voltage, $n$ the number of the ‘conducting channels’ per cross-section of CNT and $2e^2/h = 0.0777$ kOhm$^{-1}$ the quantum conductance (i.e., the resistance is about 12.92 kOhm). This model can be considered in terms of a scattering problem. According to the Landauer model [14], $G_m = (e^2/h)TR(T_{m}T_{m}^\ast )$, $m \neq n$, where $G_m$ are the conductance coefficients while $(e^2/h)T_{m}^\ast = T_{m}^\ast \Delta \mu$ the current flow between the two reservoirs with a difference between the chemical potentials $\Delta \mu = \mu_1 - \mu_2$ ($T_{12}$ is transmission coefficient found to be between 1 to 2 in the one-channel case).

#### 3. CNT Simulation in the CPA

For CNT simulation, the cylindrical symmetry scattering formalism is used. Thus, this means that the trial electronic waves after a scattering give the radial and axial ($z$-axis) components as shown in Figure 11. According to this symmetry demands the potential models are developed (see Figure 12). The potential
modelling is based on the well-tested analytical procedures of Gaspar’s type with the use of exchange-correlation corrections ($X_{\alpha}$ and $X_{\alpha\beta}$-approximations) and muffin-tin (MT) models [1-3, 12, 13].

To solve the central problem of simulation, i.e., the problem of chirality we use the ring cluster conception (Figures 13-15). The main idea is the rotation of carbon ring in respect to the axis of CNT.

![Figure 11. Scattering model for a nanotube fragment: expansions on the radial and axial scattering.](image1)

![Figure 12. Potential models for nanotubes and nanowires](image2)

![Figure 13. C-rings in CNT as clusters](image3)

![Figure 14. The EDOS for graphene ring in the effective medium (CPA calculations)](image4)

![Figure 15. Modelling of chirality effects and expected results: EDOS and energy gap via chirality angle $\phi$.](image5)
### 4. Simulation Chirality Effect of CNT-Ni Nanointerconnect

Model of the CNT-Ni nanointerconnect [3] (Figure 16) is developed in the current study. Within the formalism of electronic transport it consists of two regions supporting 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.
- CNT chirality \((m,n)\) is simulated by the corresponding orientation of C rings within the scattering medium (see, Figures 13, 15).
- The most problematic regions of simulation are CNT-Ni interconnects, where the atomic structural disorder is observed and conductivity mechanism is changed.
- The chirality influence on the resistivity in the region of interconnect depends on the numbers of statistically realized numbers of bonds between the CNT and catalytic substrate (e.g., Ni or Cu, Au, Ag, etc.) formed during the CNT growth above the surface of catalyst.

**Thus, we formulate the Postulate:** The local contact conductivity is proportional to the number of active connecting C-Ni bonds.

The results of resistivity simulation of interconnect for various chiralities are presented in the Table 2 and on the Figures 18 and 19.

#### Table 2. Resistivity simulation results for CNT-Ni interconnect

<table>
<thead>
<tr>
<th>Diameter of nanotube (d), nm</th>
<th>Chirality vector</th>
<th>Bond number in contact</th>
<th>Chirality vector modulus</th>
<th>Interconnect conductivity, kOhm(^{-1})</th>
<th>Interconnect resistivity, kOhm</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Zig-zag, (\varphi = 0^\circ)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.010</td>
<td>C(13,0)</td>
<td>12</td>
<td>2.952</td>
<td>0.0396</td>
<td>25.22</td>
</tr>
<tr>
<td>2.036</td>
<td>C(26,0)</td>
<td>24</td>
<td>6.394</td>
<td>0.0796</td>
<td>12.56</td>
</tr>
<tr>
<td>5.092</td>
<td>C(65,0)</td>
<td>64</td>
<td>15.990</td>
<td>0.207</td>
<td>4.83</td>
</tr>
<tr>
<td>10.100</td>
<td>C(130,0)</td>
<td>129</td>
<td>32.002</td>
<td>0.411</td>
<td>2.43</td>
</tr>
<tr>
<td>20.360</td>
<td>C(260,0)</td>
<td>259</td>
<td>63.940</td>
<td>0.826</td>
<td>1.21</td>
</tr>
<tr>
<td><strong>Armchair, (\varphi = 30^\circ)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.949</td>
<td>C(7,7)</td>
<td>12</td>
<td>2.982</td>
<td>0.0396</td>
<td>25.22</td>
</tr>
<tr>
<td>2.035</td>
<td>C(15,15)</td>
<td>28</td>
<td>6.391</td>
<td>0.090</td>
<td>11.00</td>
</tr>
<tr>
<td>5.021</td>
<td>C(37,37)</td>
<td>72</td>
<td>15.765</td>
<td>0.235</td>
<td>4.25</td>
</tr>
<tr>
<td>10.041</td>
<td>C(74,74)</td>
<td>146</td>
<td>31.531</td>
<td>0.476</td>
<td>2.10</td>
</tr>
<tr>
<td>20.084</td>
<td>C(128,128)</td>
<td>294</td>
<td>63.062</td>
<td>0.952</td>
<td>1.05</td>
</tr>
<tr>
<td><strong>C(3m,m), (\varphi = 14^\circ)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.847</td>
<td>C(9,3)</td>
<td>3</td>
<td>2.66</td>
<td>0.009</td>
<td>100.60</td>
</tr>
<tr>
<td>1.694</td>
<td>C(18,6)</td>
<td>5</td>
<td>5.32</td>
<td>0.016</td>
<td>61.77</td>
</tr>
<tr>
<td>5.082</td>
<td>C(34,18)</td>
<td>16</td>
<td>15.96</td>
<td>0.050</td>
<td>19.78</td>
</tr>
<tr>
<td>10.16</td>
<td>C(108,36)</td>
<td>36</td>
<td>32.05</td>
<td>0.116</td>
<td>8.55</td>
</tr>
<tr>
<td>20.32</td>
<td>C(216,72)</td>
<td>80</td>
<td>64.10</td>
<td>0.259</td>
<td>3.85</td>
</tr>
<tr>
<td><strong>C(2m,m), (\varphi = 19^\circ)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.036</td>
<td>C(10,5)</td>
<td>5</td>
<td>3.254</td>
<td>0.016</td>
<td>61.50</td>
</tr>
<tr>
<td>2.972</td>
<td>C(20,10)</td>
<td>9</td>
<td>6.508</td>
<td>0.025</td>
<td>39.05</td>
</tr>
<tr>
<td>4.973</td>
<td>C(40,20)</td>
<td>17</td>
<td>15.614</td>
<td>0.055</td>
<td>18.10</td>
</tr>
<tr>
<td>10.1528</td>
<td>C(98,49)</td>
<td>47</td>
<td>31.880</td>
<td>0.153</td>
<td>6.50</td>
</tr>
<tr>
<td>20.5128</td>
<td>C(198,99)</td>
<td>97</td>
<td>64.410</td>
<td>0.317</td>
<td>3.15</td>
</tr>
</tbody>
</table>
5. Model of Metal - Multi-Wall (MW) CNT Interconnects

In the case of MW CNT and bundle of SW CNTs the main attention is paid for CNT’s interaction and its effect on the total resistivity and current losses taking into account the dispersion properties of effective medium as a model of interstitial space. Using the simulation models, presented earlier [1,3,12,13], we develop a MW CNT-Me interconnects resistance model, based on the interface potential barriers evaluation and Landauer formula (see division 2).

Evaluation of Fermi energy for metals $E_F(0) = \frac{50.1}{\left(\frac{r_s}{a_0}\right)^2} eV$, where $n = 0.602 \cdot 10^{31} \frac{Z \rho_m}{A}$ is the electron concentration, $Z$ is the number of valent electrons, $\rho_m$ is the mass density, $r_s = \left(\frac{3}{4 m \pi \alpha}\right)^{1/3}$ is the Seitz radius (see Table 3).

Table 3. Physical parameter metal for simulation

<table>
<thead>
<tr>
<th>Metal</th>
<th>$V$, Height of barrier C-Me</th>
<th>$V$, Height of barrier C-Me, Ry</th>
<th>$E_F(0)$, Ry</th>
<th>k$_s$, a.u.</th>
<th>k$_l$, a.u.</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>10.2297</td>
<td>0.7544</td>
<td>0.4085</td>
<td>0.6391</td>
<td>1.0783</td>
<td>0.934</td>
</tr>
<tr>
<td>Pt</td>
<td>9.819508</td>
<td>0.7241</td>
<td>0.4395</td>
<td>0.6629</td>
<td>1.0787</td>
<td>0.943</td>
</tr>
<tr>
<td>Ag</td>
<td>10.2528</td>
<td>0.7561</td>
<td>0.4048</td>
<td>0.6362</td>
<td>1.0774</td>
<td>0.933</td>
</tr>
<tr>
<td>Pd</td>
<td>9.741504</td>
<td>0.7184</td>
<td>0.4318</td>
<td>0.8430</td>
<td>1.1954</td>
<td>0.970</td>
</tr>
<tr>
<td>Cu</td>
<td>8.927904</td>
<td>0.6584</td>
<td>0.5176</td>
<td>0.7194</td>
<td>1.0844</td>
<td>0.959</td>
</tr>
<tr>
<td>Ni</td>
<td>8.639076</td>
<td>0.6371</td>
<td>0.8650</td>
<td>0.9300</td>
<td>1.2256</td>
<td>0.981</td>
</tr>
</tbody>
</table>

The transparency coefficient for the barrier scattering problem is as follows:
where $E_1$ and $E_2$ are the corresponding electron energy, see Figure 13). Landauer formula gives:

\[
G = \frac{2e^2}{h} \sum_{i=1}^{N} T_i = \left( \frac{1}{12.92(kT)} \right) \sum_{i=1}^{N} T_i = 0.0774 \sum_{i=1}^{N} T_i ,
\]

(21)

Resistance evaluations have been carried out taking into account only thermally activated electrons, namely, the small part only $\Delta n = \frac{3}{4} \frac{kT}{E_F}$ at the vicinity of Fermi level where $kT = 0.0258$ eV – for $T=300^\circ$ K. Resulting evaluations for interconnects resistance of considered MWCNT are presented in the Table 4.

Table 4. Resistivity simulation results for MWCNT-Me interconnects

<table>
<thead>
<tr>
<th>Metal</th>
<th>Z</th>
<th>$n, 10^{17}$ cm$^{-3}$</th>
<th>$r$, pm</th>
<th>$r/a_0$</th>
<th>$E_F(0)$, eV</th>
<th>Factor $\frac{\Delta n}{n} = \frac{3}{4} \frac{kT}{E_F}$</th>
<th>CNT Interconnect resistivity, kOhm (thermally activated)</th>
<th>CNT Interconnect conductance, kOhm$^{-1}$ (thermally activated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>79</td>
<td>5.90</td>
<td>159.0</td>
<td>3.005</td>
<td>5.54</td>
<td>0.00349</td>
<td>2.313</td>
<td>0.432</td>
</tr>
<tr>
<td>Pt</td>
<td>78</td>
<td>6.60</td>
<td>153.4</td>
<td>2.899</td>
<td>5.96</td>
<td>0.00324</td>
<td>2.345</td>
<td>0.426</td>
</tr>
<tr>
<td>Pd</td>
<td>47</td>
<td>13.5</td>
<td>120.6</td>
<td>2.279</td>
<td>9.639</td>
<td>0.00200</td>
<td>4.050</td>
<td>0.247</td>
</tr>
<tr>
<td>Ag</td>
<td>46</td>
<td>5.86</td>
<td>160.0</td>
<td>3.02</td>
<td>5.49</td>
<td>0.00354</td>
<td>2.062</td>
<td>0.485</td>
</tr>
<tr>
<td>Cu</td>
<td>29</td>
<td>8.49</td>
<td>141.1</td>
<td>2.67</td>
<td>7.02</td>
<td>0.00275</td>
<td>2.509</td>
<td>0.398</td>
</tr>
<tr>
<td>Ni</td>
<td>28</td>
<td>18.26</td>
<td>109.3</td>
<td>2.066</td>
<td>11.73</td>
<td>0.00167</td>
<td>3.772</td>
<td>0.265</td>
</tr>
</tbody>
</table>

Figure 21. The potential barrier forming for CNT-Me interconnect

Figure 22. Resistances MWCNT-Me interconnects
Conclusions

The proposed models of conductivity for CNT-Me device based on the scattering theory principles and effective medium approach take into account the atomic short range order peculiarities in a flexible way. This allows us to simulate all possible technological variants for production of CNT-based electronic systems with a definite symmetry, various chiralities and structural disorder elements.

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References