

## THEORETICAL SIMULATION ON ELECTRIC PROPERTIES OF CNT-ME AND GNR-ME INTERCONNECTS

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In order 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, especially due to a ballistic mechanism of conductivity, carbon nanotubes (CNTs) attract permanently growing technological interest, for example, as promising candidates for nanointerconnects in a high-speed electronics. New possibilities for modern nanoelectronics are opened with a novel 'marginal' forms of graphene – nanoflakes (GNFs) and nanoribbons (GNRs), which analogously to CNTs demonstrate a lossless ballistic mechanism of conductivity. Graphene nanointerconnects are also important for nanotechnology. 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. CNT-Me and GNR-Me Nanodevices Models

This research pays the basic attention to the junctions of carbon nanotubes (CNTs) and graphene nanoribbons (GNR) with 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-wall (SW) and multi-wall (MW) CNTs as well as single-layered (SL) and multi-layered (ML) GNRs with different morphology.

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Figs. 1 and 2 represent the contacts of metal substrates with CNTs and GNRs, respectively, as prototype nanodevices. This is a main subject of our current research and modeling. The contact regions (CNT-Me and GNR-Me) are the objects of a 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.

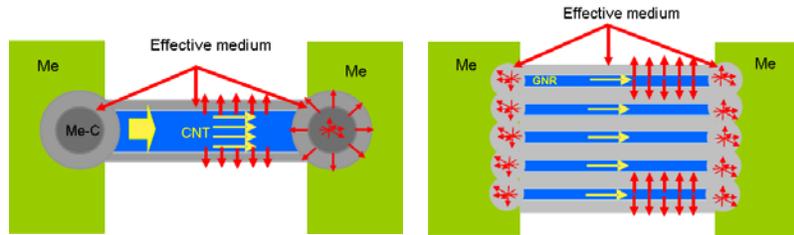


Figure 1. Model of CNT - Me interconnect as a prototype of nanodevice.

Figure 2. Model of GNR (multilayered) - Me interconnect as a prototype of nanodevice.

The electronic structure for the CNT-Me and GNR-Me interconnects 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 by us for these calculations [1] 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 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 resistance of the interconnect is evaluated through the Kubo-Greenwood formalism [2,3] or, in the simplest cases, through Ziman model [3]. 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 (= Ni, Cu, Ag, Pd, Pt, Au) and pre-defined CNT (or GNR) geometry.

## 2. Multiple scattering theory and effective medium approach for CNT and GNR simulations

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 defined as ballistic (Matissien rule). This 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  $\Psi_{in}(\mathbf{r})$  and *response*  $\Psi_{out}(\mathbf{r})$  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’.

We consider a domain where the stationary solutions of the Schrödinger equation are known, and we label them by  $\psi_{in}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\mathbf{r})$ . The scattering of ‘trial’ waves, in the presence of a potential, yields new scattering waves for the modified Schrödinger equation  $\hat{H}\psi_{\mathbf{k}}^{(\pm)}(\mathbf{r}) = E\psi_{\mathbf{k}}^{(\pm)}(\mathbf{r})$ . An electronic structure calculation is considered here as a scattering problem, where the scattering centers are identified with the atoms of clusters [1]. The paradigm of scattering theory and the developed strategy of simulation of CNTs and GNRs electronic properties uses the generalized scattering condition for the low-dimensional atomic structures of condensed matter:

$$\psi_{\mathbf{k}}^{(\pm)}(\mathbf{r}) \underset{r \rightarrow \infty}{\propto} \phi_{\mathbf{k}}(\mathbf{r}) + f_{\mathbf{k}}^{(\pm)}(\Omega) \frac{\exp(\pm ikr)}{r^{\frac{d-1}{2}}}, \quad (1)$$

where superscripts ‘+’ and ‘-’ label the asymptotic behavior in terms of  $d$ -dimensional waves ( $d$  is the atomic structure dimension).

### 3. Simulation of CNT-Me and GNR-Me interconnects:

#### ‘Effective Bonds’ model

A model of the CNT-Me and GNR-Me nanointerconnects (Figs. 1 and 2) 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 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 chirality influence on the resistance in the region of interconnect depends on the number of statistically realized bonds between the carbon nanostructure and the metal contact (*e.g.*, Ni, Cu, Au, Ag, Pd, Pt).

Using the simulation models, presented earlier [1,2], we have determined the resistance for both (SW&MW) CNT-Me and (SL&ML) GNR-Me interconnects, based on evaluation of the interface potential barriers and implementation of Landauer formula [4], which defines the integrated conductance:

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

where  $N$  is the number of conducting channels and  $T_i$  the corresponding transmission coefficient, which is calculated as a scattering coefficient for the interconnect potential barrier. The results of simulations on SW CNT-Me interconnects are presented in Fig. 3.

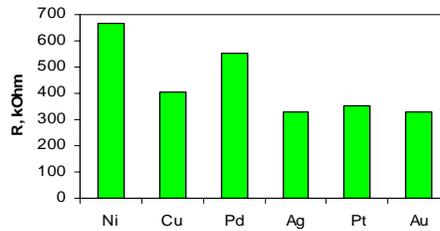


Figure 3. Resistances of the zigzag-type SW CNT-Me interconnects for the CNT diameter  $D \sim 1$  nm.

Using the *effective bonds model* we also have performed similar calculations for MW CNT-Me as well as for SL and ML GRN-Me interconnects.

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