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Theoretical Simulations on Electric Properties of CNT-Me and GNR-Me Interconnects Using Effective Media Approach

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Abstract

To overcome disadvantages of nowadays microtechnology, a further miniaturization of electronic devices, high integration level as well as increase of both operation frequencies and power density is required, including the use of adequate materials and innovative chip interconnects. Due to their unique physical properties, especially due to a ballistic (without losses) mechanism of conductivity, carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) attract a permanently growing technological interest, for example, as promising candidates for nanointerconnects in a high-speed electronics.

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Keywords: Carbon nanotubes; Graphene nanoribbons; CNT-Me and GNR-Me interconnects; *ab initio* electronic structure calculation; Conductance and resistance; Chirality effects

1. CNT-ME and GNR-ME models in the effective medium approach

The present research has the major concern for the junctions of CNTs and GNRs coming into contact with metallic elements of a nanocircuit. We have simulated interconnects for both single-wall (SW) and multi-wall (MW) carbon nanotubes (CNTs) as well as single-layered (SL) and multi-layered (ML) graphene nanoribbons (GNRs) with different morphology (Fig. 1). The electronic structure of the CNT-Me and GNR-Me interconnects can be evaluated through the electronic density of states (EDOS). C-Me contact is considered a 'disordered alloy', where clusters containing both C and Me atoms behave as scattering centers. The computational procedure that we developed for these calculations is based on the construction of cluster potentials and the evaluation of both scattering (S) and transfer (T) matrices [1].

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) (Figs. 2 and 3).

2. Simulation of CNT-Me and GNR-Me interconnects: *model of 'effective bonds'*

We have developed structural models for CNT-Me and GNR-Me junctions, based on their precise atomic structures, which take into account the chirality effect and its influence on the interconnect resistance for Me (= Ni, Cu, Ag,

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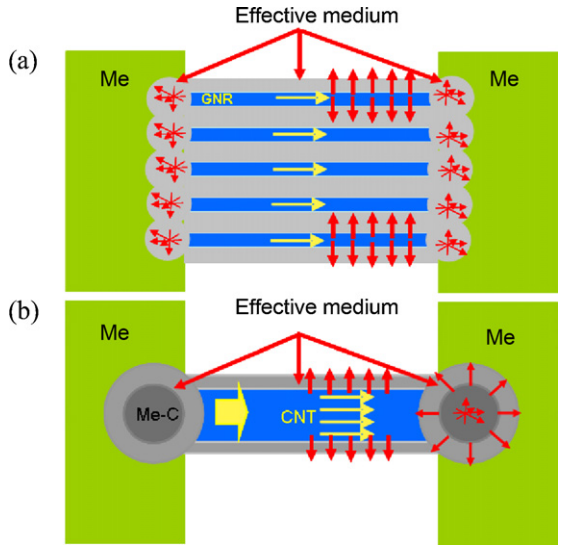

Fig. 1. Prototypes of novel nanodevices based on: a) CNT-Me interconnects; b) GNR (multilayered) - Me interconnects.

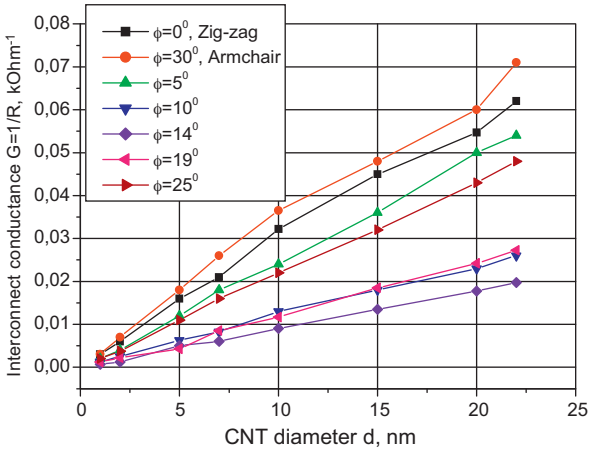

Fig. 2. Parametric calculations of conductance for CNT-Au interconnects with various chirality angles.

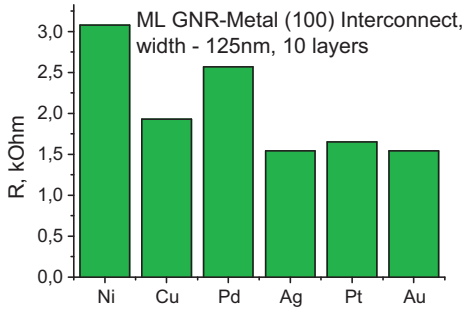

Fig. 3. MLGNR-Me Interconnects resistances.

Pd, Pt, Au) and pre-defined CNT (or GNR) geometry, taking into account the *d*-dimensional properties of atomic structures [1]. The general model of multiple scattering, using the effective media approximation (EMA) combined with a coherent potential approach (CPA) for condensed matter, is based on the atomic cluster formalism. When using

the CPA as EMA approximation, the resistance of interconnect is evaluated through the Kubo-Greenwood formalism [2] or Ziman model [3]. The *'effective bonds'* model of CNT-Me and GNR-Me interconnects is developed in the present research [4]. It consists of two regions supporting the two different electron transport mechanisms: *ballistic* (elastic) and *collisional* (non-elastic). The CNT and GNR chiralities (m, n) are simulated by the corresponding orientation of the chirality vectors within the scattering medium [4]. The resistance for both (SW&MW) CNT-Me and (SL&ML) GNR-Me interconnects is based on evaluation of the interface potential barriers and implementation of Landauer formula [4].

It has been found, that CNT-Au contact is electrically more preferable as compared to contacts of nanotubes with other metal substrates. We have also developed the model of inter-shell interaction for the MW CNTs and multi-layer (ML) GNRs.

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