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

Yu.N. Shunin[1,2], Yu.F. Zhukovskii[2], N. Burlutskaya[1], S. Bellucci[3]

[1] Information Systems Management Institute, Ludzas Str. 91, LV-1003 Riga, Latvia,+371 67100593, shunin@isma.lv

[2] Institute of Solid State Physics, University of Latvia, Kengaraga Str. 8, LV-1063 Riga, Latvia,+371 67187480, quantzh@latnet.lv

[3] INFN - Laboratori Nazionali di Frascati,Via Enrico Fermi 40, I-00044, Frascati (Rome), Italy,+39 0694032888,Stefano.Bellucci@lnf.infn.it

INTRODUCTION

This research pays the basic attention to the junctions of CNTs and GNRs with contacting 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).

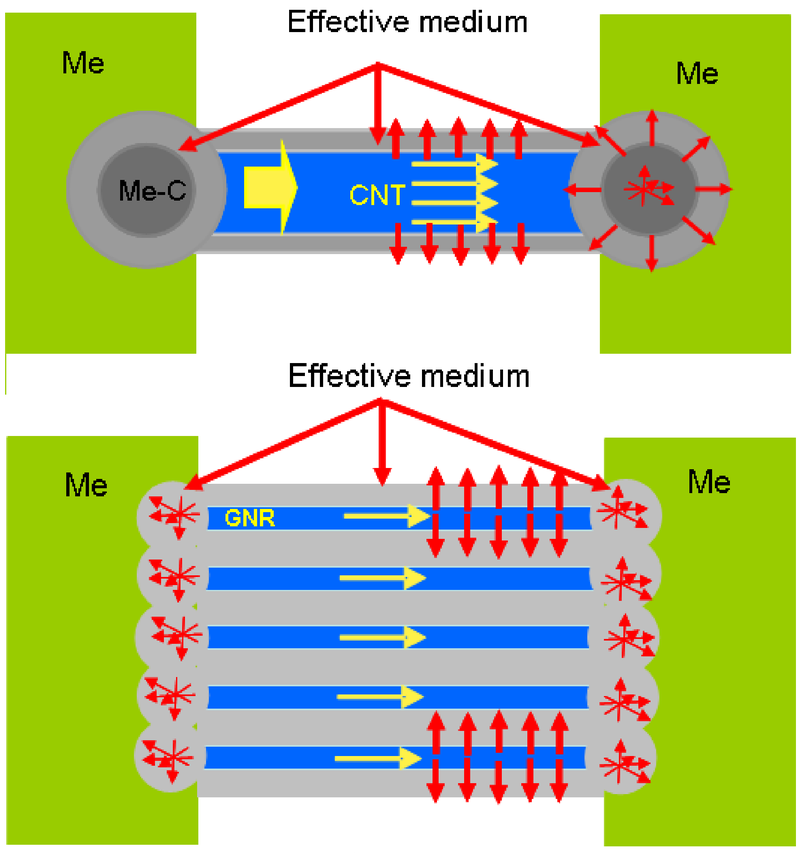

Figure 1. **Prototype of Novel Nanodevices:**
a) CNT-Me interconnect Based Nanodevice
b) GNR (multilayered) - Me interconnect Based Nanodevice

CNT-Me AND GNR-Me MODELS IN THE EFFECTIVE MEDIUM APPROACH

The electronic structure of the CNT-Me and GNR-Me interconnects can be evaluated through the electronic density of states (EDOS) for C-Me 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 is based on the construction of cluster potentials and the evaluation of both scattering (*S*) and transfer (*T*) matrices[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].

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).

We have developed structural models for CNT-Me and GNR-Me junctions, based on their precise atomistic structures, which take into account the chirality effect and its influence on the interconnect resistance for Me (= Ni, Cu, Ag, Pd, Pt, Au) and pre-defined CNT (or GNR) geometry, taking into account the *d*-dimensional properties of atomic structures[1].

SIMULATION OF CNT-Me AND GNR-Me INTERCONNECTS: *MODEL OF 'EFFECTIVE BONDS'*

The *'effective bonds'* model of the CNT-Me[4] and GNR-Me interconnects (Fig. 2) is developed in the current study. It consists of two regions supporting the two different electron transport mechanisms: *ballistic* (elastic) and *collisional* (non-elastic).

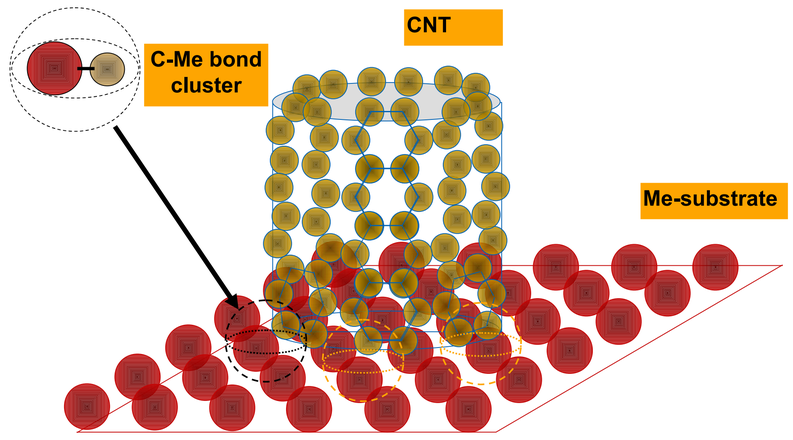

Figure 2. **The SW CNT-Me interconnect: model of *"effective bonds".***

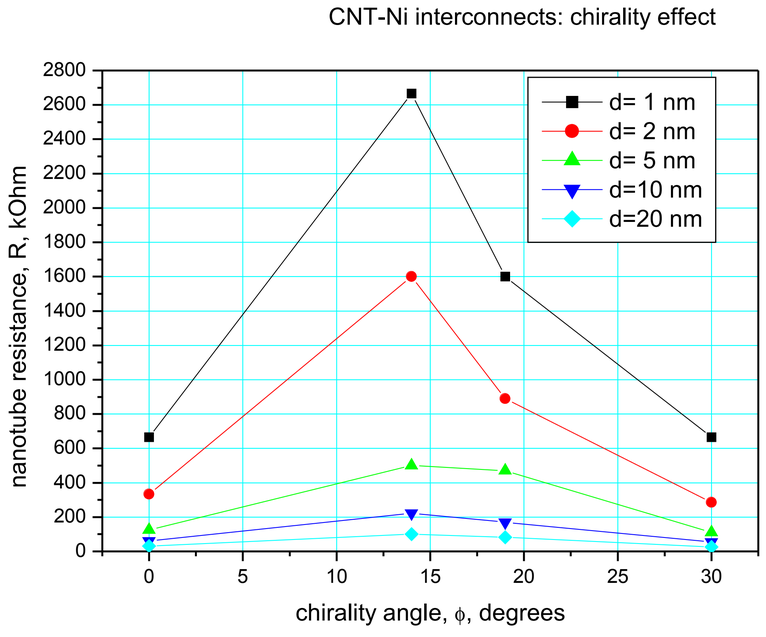

Figure 3. **Resistance of CNT-Ni junction *vs.* NT diameter**

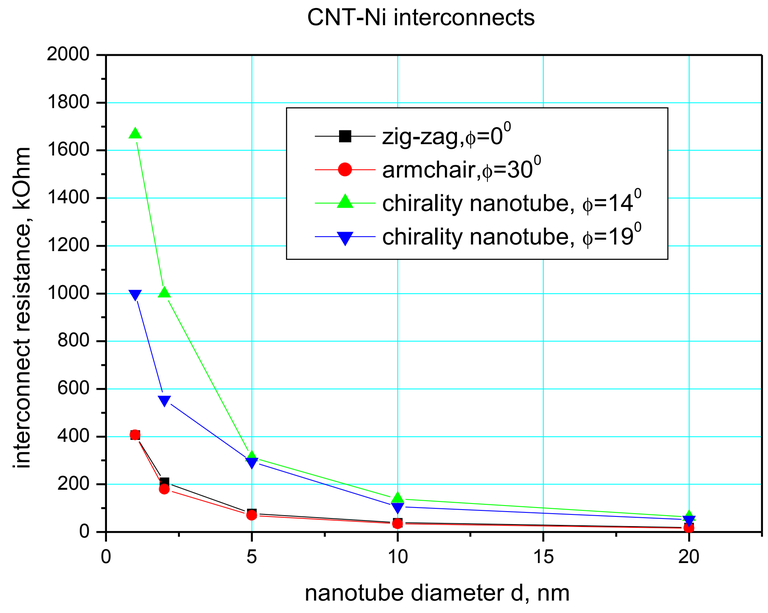

Figure 4. **CNT-Ni interconnect: *chirality effects***

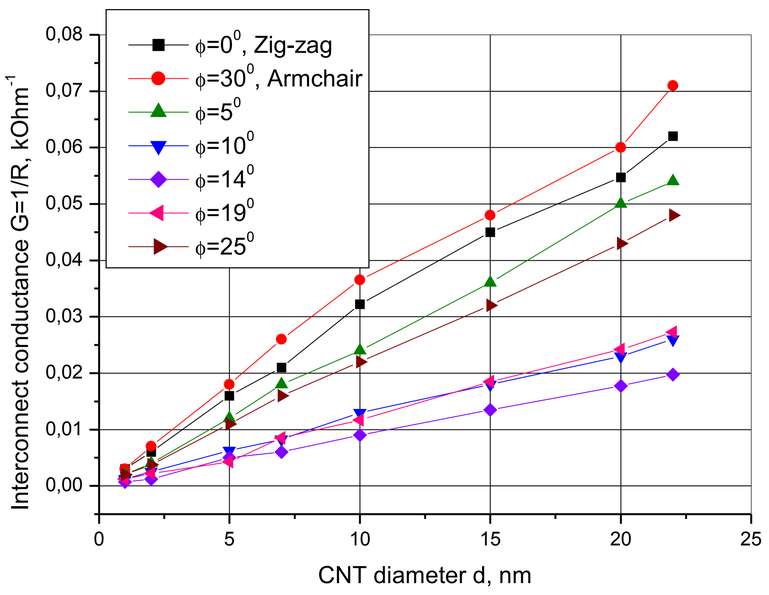

Figure 5. **Parametric calculations of conductance for CNT-Au interconnects with various chirality angles**

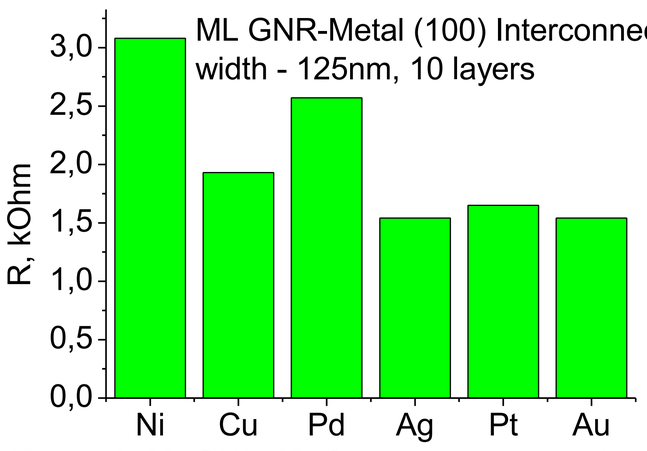

Figure 6. **MLGNR-Me Interconnects resistances**

Resume: 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, which allows us to estimate the transparency coefficient as an indicator of possible 'current' losses.

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