C-1. CARBON BASED NANOSENSOR SYSTEMS FOR INTELLIGENT SYSTEMS: MODELLING AND TECHNOLOGY

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Interfaces of carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) alongside with other materials are widely applied for novel nanosensor devices. The fundamental electron devices include field emission transistors (FETs) sensitive to various external influences of different nature such as mechanical, chemical, biological, electrical, magnetic, etc. In CNT- and GNR-based nano-FETs the electrical properties of nanocarbon components change under the influence of local external factors. Unique physical properties of CNTs, GNRs and their various interconnects find application as nanomaterials in different types of sensors (pressure, flow, thermal, gas, optical, mass, position, stress, chemical and biological sensors). There is a set of more complicated nanocarbon systems (e.g. graphene nanofibers (GNF), CNT- and graphene-based aerogels (CNTBA and GBA) etc, which are considered as prospective materials for fast nanoelectronics and nanosensors. The development of carbon-based nanosensors provides the possibilities t o create various interfaces for intelligent complex systems. This is especially important for the human body system when carbon-based nanoinclusions are physically and chemically body friendly.

Electromagnetic properties of carbon-based nanosystems. We pay main attention to CNTs, graphene nanoribbons and nanofibers (i.e., GNR and GNF) as well as CNT and graphene-based aerogels (CNTBA, GBA), consisting of CNTs, graphene nanoflakes, metallic nanowires and nanopores as the basis for high-speed nanoelectronics and potential nanosensors.

Special attention is paid to fundamental properties of CNTs, GNRs as well as various CNT-Me, GNR-Me, CNT-graphene interconnects (e.g., Fig.1, 2). 3D CNTBA and GBA nanosystems are considered as complicated systems of basic nanocarbon interconnected elements.

The developed cluster approach based on the multiple scattering theory formalism as well as effective medium approximation is used for nanosized systems modeling including calculations of dispersion law, electronic density of states, conductivity, etc. [1]. Technological interest to contacts of CNTs or GNRs with other conducting elements in nanocircuits, FET-type nanodevices, CNTBA and GBA is the reason to estimate various interconnect resistances, which depend on chirality effects in nanotubes and nanoribbons. Simulations of electromagnetic properties in interconnects for evaluation of integral resistances, capacitances and impedances of various topologies of nanodevices (1D, 2D and 3D), including frequency properties (GHz&THz) have been performed.

Nanodevices for effective electron transport. 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 (= Fe, Ni, Cu, Ag, Pd, Pt, Au) with the predefined CNT (or GNR) geometry. In the simplest cases, the electronic structure of CNT-Ni interconnects can be evaluated through the DOS for a C-Metal contact considered as a 'disordered alloy' [1]. In the current study, we have developed more complicated structural models of CNT-metal junctions based on a precise description of their atomistic structures.

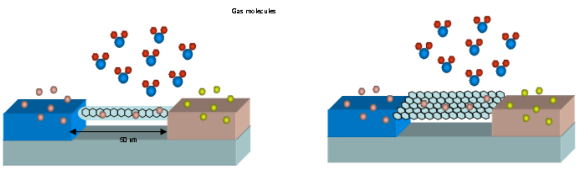

Fig. 1. FET-type nanodevices as prospective nanosensor systems: an example of chemical nanosensors: the same threshold can be altered when the amount of free charges on the tube of graphene ribbon surface is increased or decreased.

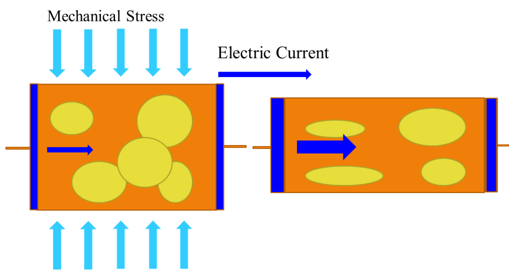

Fig. 2. Mechanical stress and electric current correlation in nanoporous materials: conductivity percolation as a result of fractal dimension changes. *Nanoaerogel conductivity, elastisity and porosity correlation model*.

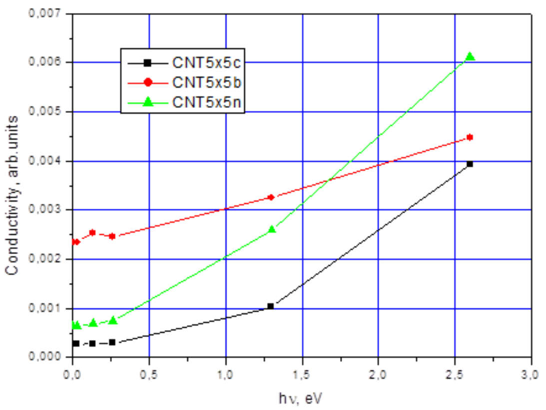

Fig. 3. Conductivities of pure perfect and doped (B or N) CNTs in the limit of non-interacting defects.

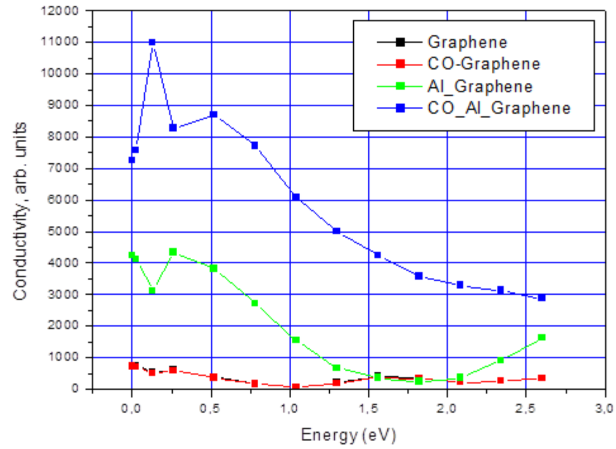

Fig. 4. Conductivities of pure perfect and Al-doped graphene.

When estimating the resistance of a junction between a nanotube and a substrate, the main problem is caused by the influence of the nanotube chirality on the resistance of SW and MW CNT-Me interconnects (Me = Fe, Ni, Cu, Ag, Pd, Pt, Au) which is predefined by CNT geometry [1,2].

Modelling of Nanosensors Systems. Conductivity is an effective tool of nanosensor systems. Usually two basic electron conductivity mechanisms are considered in CNT-based structures. The ballistic mechanism is engaged in electron transport within CNTs (or GNRs), while the collisional mechanism is characteristic of CNT- (GNR-) interconnects [2]. The analysis of Kubo-Greenwood conditions in relation to CNT and GNR morphologies has been presented taking into account $dc(\omega = 0)$, $ac(\omega \neq 0)$ regimes and the temperature factor of the electron transport. Parametrical numerical simulations of conductivity have been carried out for zig-zag *(0,m)*, arm-chair *(m,m)* and chiral *(n,m)* CNTs and GNRs [2], where the sensitivity of conductivity to the local electronic density of states in CNTs and GNRs with local impurities (N and B atoms) are shown (see, e.g., (5,5) CNTs, Fig.3). Similar calculations for graphene-based stuctutures (Graphene, CO-graphene, Al-doped Al-Graphene and Al-CO-Graphene, Fig.4). In particular, this sensitivity implies that CNT- and graphene-based nanodevices can be potentially used as nanosensor systems.

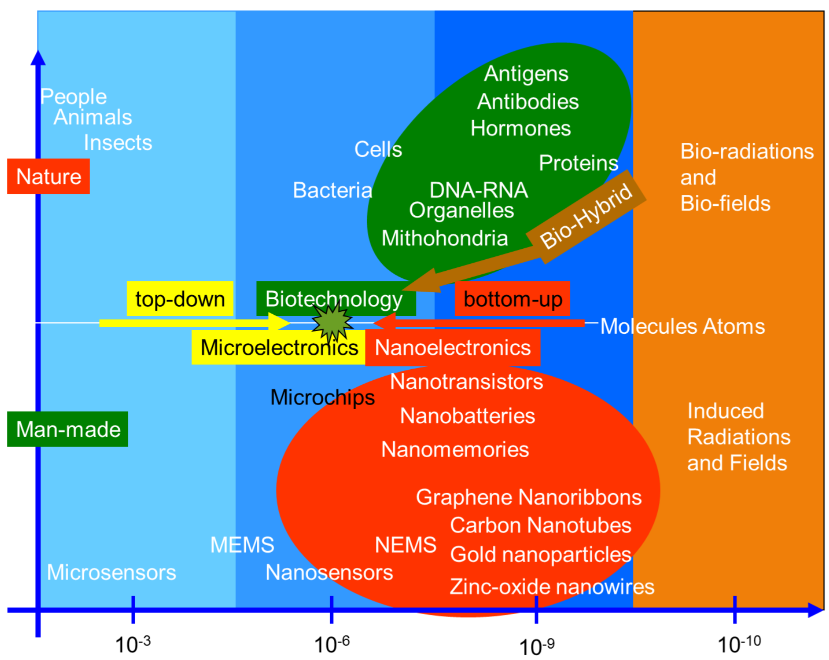

Fig. 5. Top-down, bottom-down and bio-hybrid technologies in creation of basic types of nanosensors.

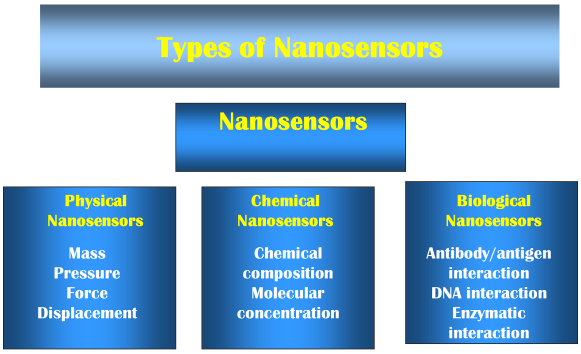

Fig. 6. Basic types of existing nanosensors.

CNTBA and GBA electromechanical properties and nanosensoring. Unique mechanical and electrical properties of CNTBA and GBA make these nanomaterials prospective candidates for new types of nanodevices and nanosensors. The model of electromechanical correlations has been developed based on the fractal dimension induced changes of the aerogel structure. Mechanical stresses or gas inclusions can modify the morphology of CNTBA and GBA changing the resistance.

Thus, the resistance is considered as a function fractal dimension,

$$R \propto \omega^{f(d_S)}, \qquad (3)$$

where ω is the frequency, $f(d_S)$ is the function of fractal dimension d_S. This fractal property of CNTBA and GBA structures provides the possibility to create mechanical and gas nanosensors.

Carbon Based Nanosensors for Intelligent Systems. Why CARBON? Why do we interested in carbon nanosensors especially. The answer is - Humans realize a Carbon-type of Life. Why NANO? The answer is – Nanosized actuators and sensors are adequate to the human body functionalities. A human body is a very harmonious system of 'nanosensors'.

Nanotechnology in reproducing Nature creates various types of certain nanosensors (see, Figs. 5,6). The next step of nanoevolution is the synergy of nanosensoring systems. There are actually four recognizable near future communication needs of nanotechnology in health applications [4]:
i) *information transfer*,
ii) *control data transfer*,
iii) *detection and Identification*,
iv) *localization*.

There are actually three potential areas of communication in nanotechnology:
a) *nanoworld-nanoworld*,
b) *macroworld-nanoworld*, and
c) *nanoworld-macroworld*.

Health applications imply certain requirements on technical parameters of communication unit connected to a micro- or nanodevice. These requirements are:
1) *biocompatibility*,
2) *size comparable to nanosensor*,
3) *communication reach at least in centimeters*.

References

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