Nanocarbon electromagnetics in CNT-, GNR- and aerogel-based nanodevices: models and simulations

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Abstract

Electromagnetic properties of nanocarbon systems are essential for the creation of various nanoelectronic devices. Our major attention is focused on CNTs, graphene nanostructures (*e.g.*, GNR and GNF), graphene-based aerogels (GBA) and CNT-based aerogels (CNTBA) as the basis for high-speed nanoelectronics and prospective nanosensors. Special attention is paid to fundamental properties of CNTs, GNRs and various CNT-Me, GNR-Me, CNT-graphene interconnects. Nanosystems of 3D GBA and CNTBA are regarded as complicated systems made up of basic nanocarbon interconnected elements. Technological interest to contacts of CNTs or GNRs with other conducting elements in nanocircuits, FET-type nanodevices, GBA and CNTBA is the reason to estimate various interconnect resistances, which depend on chirality effects in the interconnects. Simulations of electromagnetic properties in interconnects have been performed to evaluate integral resistances, capacitances and impedances of various topologies (1D, 2D and 3D) in nanodevices, including their frequency properties (GHz&THz).

Keywords: CNTs - carbon nanotubes, GNR – graphene nanoribbons, CBA – Carbon Based Aerogels, Carbon Nanoporous Materials, Carbon-based nanocomposites

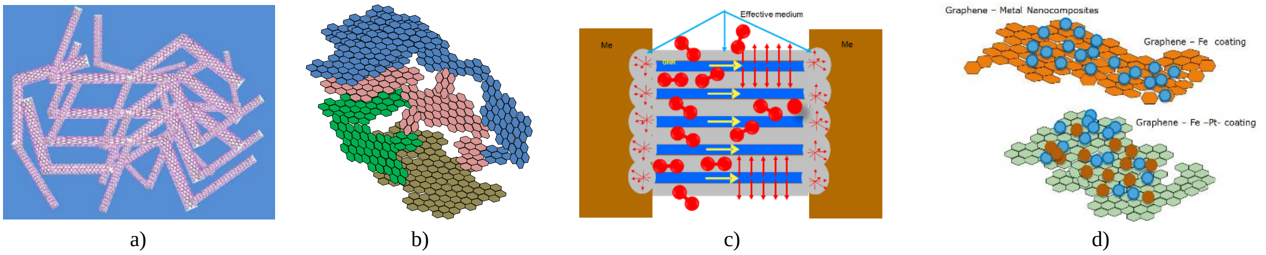
1 Introduction

The objective of the current study is to demonstrate the implementation of advanced simulation models to ensure a proper description of the electronic properties, electrical conductivity, electromagnetic and electromechanical phenomena of functionalized CNT- and GNR-based nanostructures of different morphologies and their interconnects for nanosensor and nanomemory systems. The developed cluster approach based on the multiple scattering theory formalism as well as effective medium approximation is used for nanosized systems modeling supported by calculations of dispersion law, electronic density of states, conductivity, *etc*. [1]. The sensitivity of the local electronic density of states to external influences (mechanical, chemical, magnetic, etc) on the fundamental electromagnetic properties of CNTs, GNRs and their metal interconnects have been analyzed from the point of view of nanosensor applications [1, 2]. We develop a set of prospective models of nanocarbon-based nanomaterials and nanodevices based on various interconnects and interfaces (see Figure 1).

Correlations between multiple external influences (mechanical, chemical, electromagnetic *etc* factors) and fundamental properties of nanocarbon materials are studied.

2 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. 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), with a predefined CNT geometry [2-3].



a) b) c) d)

FIGURE 1 A set of simulation models: a) Structural model of CNTBA; b)Structural model of GBA; c) GNRs-based gas nanosensor device; d) Graphene-metal nanocomposites - Fe and Fe-Pt coatings.

2.1. CONDUCTIVITY AS AN IDENTIFYING 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, while the collisional mechanism is characteristic of CNT-substrate interconnects [4]. Hence the general conductivity σ_{gen} is evaluated as follows:

$$1/\sigma_{gen} = 1/\sigma_{coll} + 1/\sigma_{ball} \,. \qquad (1)$$

For pure CNTs, we clearly observe that $\sigma_{ball} >> \sigma_{coll}$. The collisional contribution is basically connected with the specific morphology of the interconnect space. In the framework of multiple scattering theory formalism and effective medium approximation, we can evaluate both factors of conductivity. A special question for modelling is the dependence of both conductivity mechanisms on the electron free path length, which, in the case of pure CNT, is usually considered as the nanotube length.

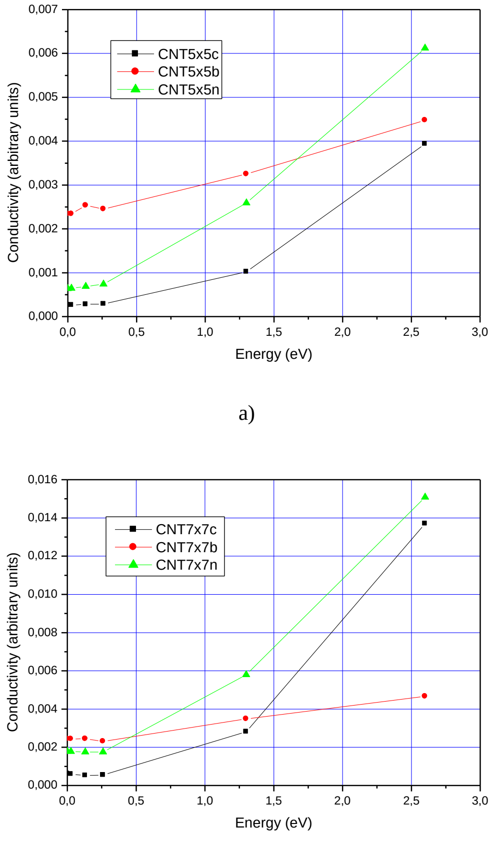
The analysis of Kubo-Greenwood conditions in relation to CNT and GNR morphologies has been presented taking into account *dc* ($\omega = 0$), *ac* ($\omega \neq 0$) regimes and the temperature factor of the electron transport.

The calculations of conductivity are usually performed using Kubo-Greenwood formula [1, 2]:

$$\sigma_E(\omega) = \frac{\pi\,\Omega}{4\omega}\int\left[f(E) - f(E+\hbar\omega)\right]\left|D_E\right|^2 \rho(E)\rho(E+\hbar\omega)dE, \qquad (2)$$

where ω is a real frequency parameter of Fourier transform for the time-dependent functions, *f(E)* is Fermi-Dirac distribution function, $D_{E,E'} = \int\limits_{\Omega} \Psi^*_{E'}\nabla\Psi_E d\mathbf{r}$, where $\Psi_{E(\mathbf{K})} = A\exp(i\mathbf{K}\mathbf{r})$ and **K** is the complex wave vector of the effective medium. The dispersion function $E(\mathbf{K})$ determines the properties of the wave function $\Psi_{E(\mathbf{K})}$ upon the isoenergy surface in **K**-space.

However, *Kubo-Greenwood* formalism is free from this division on ballistic and collisional mechanisms and seems to be more objective. The analysis of Kubo-Greenwood's conditions in respect of CNT morphology has been presented taking into account both *dc* ($\omega = 0$) and *ac* ($\omega \neq 0$) regimes as well as the temperature factor of electron transport [5, 6].



a)

b)

FIGURE 2 Conductivities of pure perfect and doped (B or N) CNTs in the limit of non-interacting defects: a) (5,5); b) (7,7)

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] on the basis of EDOS calculations in [8], 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), (7,7) CNTs, Figures 2a, b). Similar calculations for graphene-based structures (graphene, CO-graphene, Al-doped, Al-Graphene and Al-CO-Graphene, Figure 3) and (N and B doped graphene, Figure 4).

In particular, this sensitivity implies that CNT- and graphene-based nanodevices can be potentially used as nanosensor systems, when local electronic density of states induced by external influences takes place. Similar calculations of conductivities based on the EDOS results have been made for graphene-based materials [9,10] (see Figures 3 and 4).

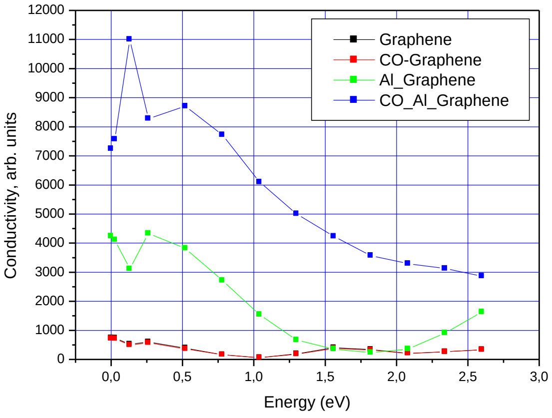


FIGURE 3 Conductivities of pure perfect and Al- doped graphene for EDOS of [9]

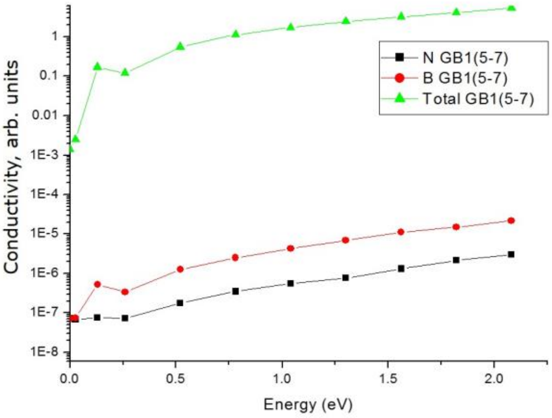


FIGURE 4 Conductivities of pure perfect and N- and B-doped graphene for EDOS of [10]

3 CNT interconnects magnetic phenomena and magnetically stimulated CNT growth in CVD processes

There is a relation between the use of magnetic catalysts and the CVD growth of CNTs determining the most commonly used materials for the CNT growth - Fe, Co and Ni. Nanoparticles of the latter catalysts are magnetically isotropic. It is possible to use magnetically anisotropic nanoparticles such as those in the alloys with a different substitutional disorder (e.g., Fe_xPt_{1-x}) to manage the CVD process with the formation of the predefined CNT chiralities. Limitations in the control after the parameters of CNTs growth are discussed. The role of the number of effective bonds inside interconnects and the descrete character of chiral indeces have been studied in relation to the expected qualities of CNT output in the CVD process. Moreover, it is a way to create effective magnetic nanomemory, where a CNT ‘forest’ provides communication with other parts in novel integrated nanodevices by means of spin waves transport.

Nanocarbon-magnetic metal interfaces open new possibilities for the creation of nanospintronic devices, e.g., nanomemory devices. The model of CNTs growth with the predefined chiralities in a magnetically managed CVD process with the use of magnetically anisotropic Fe_xPt_{1-x} nanoparticles with various substitutional disorders has been developed. The model and magnetically controlled conditions, stimulating the CNT growth in a CVD process, aim at the predictable SWCNT diameter and chirality. The perfect picture of the magnetically stimulated CVD process for CNTs growth can be presented as a CNT forest (see Figure 5). Such a system of nanotubes can also be considered as a prototype of the magnetic memory, where ferromagnetic nanoparticles serve as cells of the magnetic memory – that is, ferromagnetic contacts are controlled by spin pulses, the transport of which is provided by nanotubes.

At the same time, the growth control over chiral and non-chiral nanotubes essentially depends on stoichiometric composition of Pt-Fe nanoparticles. The beginning of the nucleation process providing the growth of nanotubes might be connected with stochastic fluctuations of the magnetic moment in a carbon atom relative to the direction of the local magnetic field in a nanoparticle.

Distribution of the fluctuation angle obeys the Gaussian law:

$$f(\theta)=\frac{1}{\sigma\sqrt{2\pi}}\cdot\exp\left(-\frac{(\theta-\theta_B)^2}{2\sigma^2}\right), \qquad (3)$$

where σ^2 is the angular dispersion of thermal fluctuations of the magnetic moment angle of a carbon atom. To evaluate this dispersion, the potential energy change of the magnetic moment under the influence of the thermal energy should be evaluated: $\mu_C B(1-\cos\theta_T)\approx k_B T_{CVD}$, where μ_C is the induced magnetic moment of a carbon atom $\mu_C=1.25\mu_B$ (see evaluations in [65], $\mu_B=5.788\cdot10^{-5}eV/T$, **B** is the magnetic induction of the catalyst surface, $\theta_T=\theta-\theta_B$ T_{CVD} - is the operating temperature of the CVD process, k_B =8,617 3324(78)$\cdot10^{-5}$ *eV/K*- is the Boltzmann constant. Hence $2\sin^2\frac{\theta_T}{2}\approx\frac{k_B T_{CVD}}{\mu_C B}$. Taking into consideration one of the main problems of the nanotubes growth control – the chirality control – it is necessary to look for the minimal fluctuation angle θ.

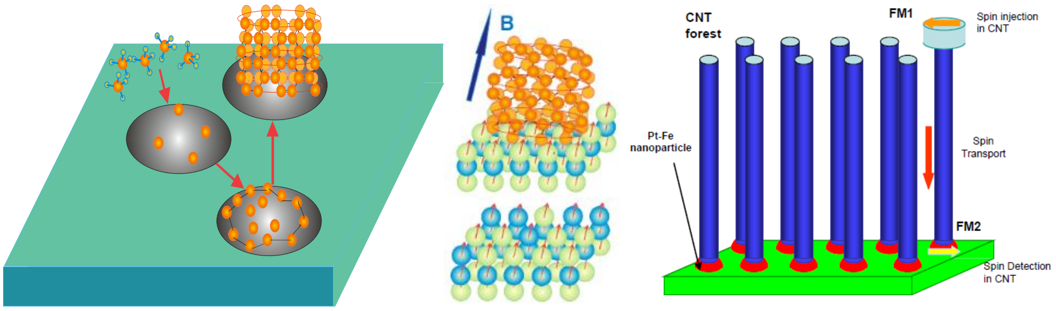


FIGURE 5 Model of CNTs growth in a magnetically controlled CVD process based on Fe-Pt nanodrops catalysts

Then $\sigma^2 = \theta_T^2 = \dfrac{2k_B T_{CVD}}{\mu_C B}$.

The condition of the small fluctuation angle (e.g., $<10^\circ$) at certain temperature of the CVD process imposes limitations on the values of the demanded magnetic induction ***B***. Taking into account the ratio between the chirality angle and the direction of the magnetic field $\phi = \theta_B$, Figure 13 displays the predictable scattering of chiralities for nanotubes of approximately the same diameter.

We are also able to evaluate the necessary value of the magnetic field **B** providing the expected chirality angles scattering, e.g. $\sigma = 0.2$ (approximately 12°) leads to the **B** evaluation for the CVD process temperature $T_{CVD} = 700^\circ C$ as $B = \dfrac{2k_B T_{CVD}}{\sigma^2 \mu_C} \approx \dfrac{16755}{\sigma^2 \mu_C} \approx 57895 \approx 6 \cdot 10^4$ T. For small angle dispersions $\sigma^2 = \theta_T^2 = \dfrac{2k_B T_{CVD}}{\mu_C B}$ the high local magnetic field on the nanoparticle surface is necessary. The result also strongly depends on the carbon atom magnetic moment μ_C [4] (see also Figure 6).

Taking into account the possible errors in diameters of the growing nanotubes, their evaluation from beneath is defined by the minimal variations in parameters of the chirality vector $\vec{c} = (n,m)$ Δn and Δm, which equal 1.

Considering the formula for calculating the diameter of CNT:

$d = \dfrac{\sqrt{3}a}{\pi}\sqrt{m^2 + n^2 + mn}$, where α = 0,142 nm is the distance between the neighboring carbon atoms in the graphite plane.

The relationship between chirality indices (*n* and *m*) and the angle ϕ is presented by the ratio**:**

$$\sin\phi = \frac{m\sqrt{3}}{2\sqrt{m^2 + n^2 + mn}}.$$

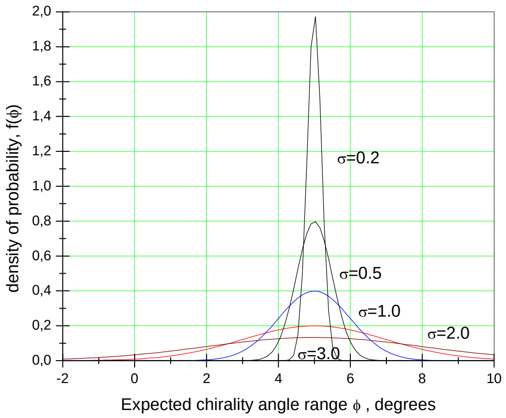


FIGURE 6 The predictable scattering of chiralities for nanotubes of approximately similar diameters

Then the minimum relative error in the diameter of CNT is possible to define as:

$$\varepsilon_d = \frac{\Delta d}{d} \approx \frac{\sqrt{5m^2 + 5n^2 + 8mn}}{2(n^2 + m^2 + mn)}. \quad (4)$$

Particularly, in the case of arm-chair CNT (*m=0*) $\varepsilon_d \approx \dfrac{\sqrt{5}}{2n}$, in the case of zig-zag CNT (*m*=*n*)

$$\varepsilon_d \approx \frac{1}{2\sqrt{2n}}. \quad (5)$$

Thus, the errors in the diameter of the growing CNTs are incorporated in discrete morphological properties. But these minimum estimates are only reinforced, given the obvious errors in the size of catalyst nanoparticles are taken into consideration.

Another possibility for the creation of magnettic memory devices is the magnetoresistance phenomenon. The giant magnetoresistance (GMR) was discovered in 1988 as a large change in resistance of magnetic Fe/Cr multilayer in the presence of an applied magnetic field [11] and tunnelling magnetoresistance (TMR) was discovered in 1975 by M. Jullière [12] in a device that consisted of two Fe films separated by Ge, namely, trilayer structures, i.e. sandwiches of two ferromagnetic metals separated by a thin spacer layer of **normal metal** (see e.g. Figure 2) **or semiconductor.** They are called spin-valves and are used as magnetic field sensors. The resistance of the device is dependent on the relative magnetization orientation of the ferromagnets. It is R_P when the magnetizations are parallel and R_A when they are antiparallel. The GMR ratio is defined as $\mathrm{GNR} = \frac{R_A - R_P}{R_P}$ as well as for TMR is $\mathrm{TNR} = \frac{R_A - R_P}{R_P}$ (Moodera,1995). It was first in 1995 when room temperature TMR was discovered by Julliére [2] and caused a great interest in spintronics after GMR was discovered in 1988 (Baibich et al [3]). Our idea is that the same effect can be reached by introducing metal or semiconductor-like CNTs into the N space. The TMR signal operates in the same way as the GMR, where R_P and R_A are the resistances of the device for parallel and antiparallel orientations respectively of the ferromagnets magnetization.

The sign and size of the interlayer exchange coupling is dependent on the thickness of the nonmagnetic spacer. The coupling can thus be ferromagnetic and antiferromagnetic dependent on the spacer thickness.

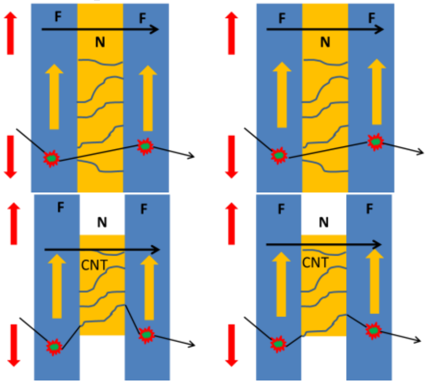


FIGURE 7a Giant magnetoresistance (GMR) device. A thin normal metal spacer (N) separates two ferromagnets (F). The current flows perpendicular to the plane of the sample. N space can be filled by introduced (or grown) CNT, e.g. – metal-like

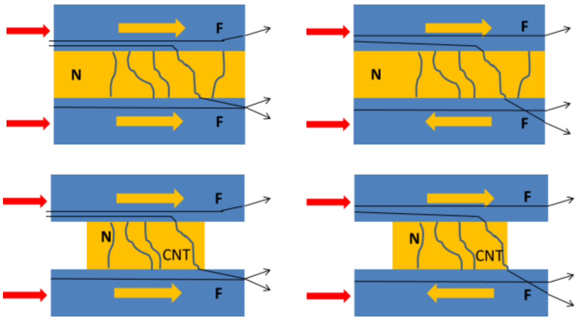


FIGURE 7b Current in Plane (CIP) spin-valve and equivalent resistor mode. Separate channels are for minority and majority spins. The electrons scatter from one F layer to the other on the way through the sandwich

The device shown in Figure 7 is the so-called current perpendicular to the plane (CPP, Figure 7a) geometry. The resistance of such geometry is very low and difficult to detect. For practical applications, structures with the current in the plane (CIP, Figure 7b) are used because they have higher resistance and thus higher difference with the magnetic field.

4 Nanoporous and nanocomposite material models

Nanoporous systems are considered as complicated ensembles of basic nanocarbon interconnected elements (e.g., CNTs or GNRs with possible defects and dangling boundary bonds) within the effective media type environment (Figures 1a, 1b, 1c). Interconnects are essentially local quantum objects and are evaluated in the framework of the developed cluster approach based on the multiple scattering theory formalism as well as effective medium approximation [1,2]. Particular properties of carbon-based nanoporous systems in dependence on the porosity extent, morphology and fractal dimension are practically studied to find useful correlations between their mechanical and electrical properties.

In cases when nanocarbon clusters are embedded in high resistance media (instead of vacuum) we come to the model of nanocomposite material. Now we pay attention to the model of nanocomposite materials based on carbon nanocluster suspensions (CNTs and GNRs) in dielectric polymer environments (e.g., epoxy resins) is considered as a disordered system of fragments of nanocarbon inclusions with different morphology (chirality and geometry) in relation to a high electrical conductivity in a continuous dielectric environment. Presumably, the electrical conductivity of nanocomposite material will depend on the concentration of nanocarbon inclusions (in fact, carbon macromolecules). Isolated nanocarbon inclusions will provide conductivity due to the hopping conductivity mechanism through dangling bonds up to the percolation threshold, when at high concentrations (some mass %) a sustainable ballistic regime appears, which is characteristic of pure carbon systems.

Considering the *Kubo-Greenwood* relationship for small $\hbar\omega$ we can take $\rho(E) \approx const$.

A wave function ψ_a of Hamiltonian with the central symmetric potential energy for large distances is proportional to $\exp(-\alpha R)$, where $\alpha \sim a^{-1}$, a is the characteristic ‘Bohr-like’ radius. The interaction between the electronic states localized at points $\mathbf{R}_\mathrm{i}$ and $\mathbf{R}_\mathrm{j}$ describes the *overlapping integral*: $I = \int \psi_a^*(\mathbf{r}-\mathbf{R}_\mathrm{i})\psi_a(\mathbf{r}-\mathbf{R}_\mathrm{j})\,\mathrm{d}^3\mathbf{r} \sim \exp\left\{-\left|\mathbf{R}_\mathrm{i}-\mathbf{R}_\mathrm{j}\right|/a\right\}$

If two states are divided by a distance R, then D can be approximated: $D = \frac{m\omega R}{\hbar}\exp(-\alpha R)(\alpha a)^{3/2}$.

If two centres are close and wave functions are in resonance: $D = \frac{m\omega R}{2\hbar}(\alpha a)^{3/2}$

Following to Mott [13] we can see:

$$\sigma(\omega)=\frac{\pi e^2}{2\hbar}\left\{\rho(E_F)\right\}^2(\hbar\omega)^2 aR_\omega^4,$$

where

$$R_\omega=\frac{1}{\alpha}\ln\left(\frac{2I_0}{\hbar\omega}\right),$$

when, e.g., $I_0=e^2\alpha\left[\frac{3}{2}(1+\alpha R)+\frac{1}{6}(\alpha R)^2\right]$ is the amplitude of overlapping integral for hydrogen-type wave functions.

When the centers are strongly separated from each other, the overlap integral is very small, but strictly speaking, it never turns into zero.

However, in the material, which is considered an insulator, it is easy to detect very small currents due to tunneling of electrons from site to site, possible because of this overlap of the wave functions. Actually implemented mechanisms of electron hopping throughout "islands" of conductivity (nanocarbon clusters) is very complex.

However, we should accept that the probability of electron transition from the center point $\mathbf{R}_i$ to the center point $\mathbf{R}_j$ is proportional to the quadrat of overlapping integral: $I\sim\exp(-2\left|\mathbf{R}_i-\mathbf{R}_j\right|/a)$.

A macroscopic conductivity can be estimated as : $\sigma\sim\exp(-4\alpha R/a)$.

The constant α is evaluated as 0,70. This is approved by Monte-Carlo numerical simulations [14]. Only the most favourable ways for the electron hopping i.e. some of their share ξ should be taken into account. Evaluation of conductivity in this case is modified by: $\sigma(\xi)\sim\exp(-4\alpha\xi^{-1/3}R/a-\frac{1}{3}\xi W/kT)$.

The most precise averaged evaluation of the overall conductivity of the system [15], which is regulated by the hopping of electron between 'nanocarbon macromolecules',then will be: $\sigma_{IC}=\sigma_0\exp(-\frac{4}{3}\left(\frac{4\alpha r_{IC}}{a}\right)^{3/4}\left(\frac{W_0}{kT}\right)^{1/4})$,

where r_{IC} - is the length of the tunnel 'jump' of the electron equal to the distance between 'nanocarbon' clusters, σ_0 is the normalization constant which means the conductivity of monolithic dielectric medium.

If we introduce the volume part as an indicator of the nanocarbon inclusions concentaration: $\eta=\left(\frac{R_0}{R_0+R}\right)^3$,

where R_0 is the average nanocarbon macromolecule radius, R is, as earlier, the width of potential barrier between the nearest nanoclusters which is responsible for percolation ability of the model nanocomposite. We should also diminish the hopping phenomena and percolation probability taking into account the nanocarbon macromolecule orientation within a hypothetical sphere embedded into high resistance dielectric medium.

On the basis of this definition we can obtain a contribution of potential nanocarbon interconnects to nanocomposite conductivity as follows (see also Figure 8):

$$\ln\left(\frac{\sigma_{IC}}{\sigma_0}\right)=-\frac{4}{3}(\frac{4\alpha}{a}R_0(\eta^{-1/3}-1))^{3/4}\left(\frac{W}{kT}\right)^{1/4}. \tag{6}$$

Added to this is the effect of intrinsic nanocarbon cluster conductivity, which is dependent on its morphology. The electric conductivity will also depend on the spatial orientation of nanocarbon inclusions. It will be greater for the longitudinal electric field orientations and lower for the transverse ones.

Of course, any spatial orientations are technologically possible. The overall conductivity of nanocomposite material is:, $\Sigma\approx\Sigma_D+\sum_{k=1}^{L}R_k^{-1}$, where

$$R_k=\sum_{j=1}^{M}\sum_{i=1}^{N}(\sigma_{nano,i.j,k}^{-1}+(N_{eff-in,i\,j,k}\sigma_{IC-in,i,j,k})^{-1}+(N_{eff-out,i,j,k}\sigma_{IC-out,i,j,k})^{-1}), \tag{9}$$

where M - is the number of conductivity channels, N – is the number of nanocarbon clusters in the conductivity channel, N_{eff} is the number of effective bonds of tunneling bonds, $\Sigma_D=(R_D)^{-1}$ is the conductance of dielectric medium, σ_{nano} is the conductivity nanocluster, σ_{IC} - the hopping conductivity of the *in-* and *out-type* effective bond, which for large nanocarbon inclusion concentrations create their interconnect.

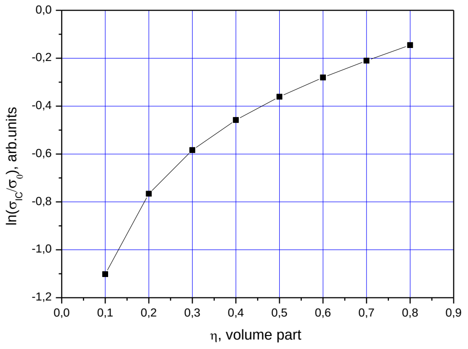


FIGURE 8 The hopping conductivity correlation via the average nanocarbon macromolecules volume part within continuous dielectric medium

A natural application of this kind of nanocomposite materials is nanosensors of pressure and temperature.

5 Instead of conclusion. CNTBA and GBA electromechanical properties

Talking about porous materials in general and, in particular, about nanocarbon-based systems such as CNTBA and GBA, we meet new complications for Solid state theory. We lose a strong dimension, regularity and continuity. In some sense, porous materials are ‘pure’ surfaces. We should also control the fractal dimention of porous materials as a key parameter of their morphology. A porous material in certain cases present a mixture where one component is a substance (for example – a metal) and the other - emptiness. To describe the properties of porous bodies, the percolation theory can be used.

One important difference: the system can not exist as finite metal clusters, since they cannot hang in a vacuum. Consequently, the metal component is always connected - all metals belong to the infinite cluster.

In a conventional two-component mixture two percolation transitions occur at different values of x, corresponding to the formation of an infinite cluster for each of the two components.

These properties are largely similar to the properties of gels.

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 by the 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, $R \propto \omega^{f(d_s)}$, 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 of creating mechanical nanosensors.

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Scientific interests: His current research activities concern nanophysics, nanoelectronics, nanodevices, nanomaterials, nanotechnologies, nanorisks, nanoeducation, and nanothinking

Publications: over 470, 1 book with Springer

Experience: director of NATO ARW “Nanodevices and Nanomaterials for Ecological Security,” Riga, Latvia, 2011, a visiting researcher at Gesellschaft für Schwerionenforschung mbH, Darmstadt, Germany (1995), INFN—Laboratori Nazionali di Frascati, Frascati-Roma, Italy (2010 to 2015), participation in EU FP7 Projects CATHERINE (2008 to 2011) and CACOMEL (2010 to 2014), education practitioner in Higher Education from 1975 till nowadays

Stefano Bellucci

Current position, grades: PhD, Professor, currently coordinates all theoretical physics activities at INFN Laboratori Nazionali di Frascati (Italy).

Universisty studies: April 1982: Laurea in Physics (Magna cum Laude), University of Rome "La Sapienza" July 1984: Master in Physics of Elementary Particles, SISSA and University of Trieste, PhD in physics of elementary particles in 1986 at SISSA, Trieste, Italy.

Publications: over 400 papers in peer-reviewed journals (with h = 40), and more than 10 invited book chapters, the editor of ten books with Springer

Scientific interests: research interests include theoretical physics, condensed matter, nanoscience and nanotechnology, nanocarbon-based composites, and biomedical applications.

Experience: He worked as a visiting researcher at theBrandeis University, Waltham, MA, USA (1983 to 1985); at the M.I.T., Cambridge, MA, USA (1985 to 1986); the University of Maryland, USA (1986 to 1987); at the University of California at Davis, USA (1987 to 1988). He is an editorial board member of the Springer Lecture Notes in Nanoscale Science and Technology, as well as the editorial board member of the Global Journal of Physics Express and the Journal of Physics & Astronomy

Yuri Zhukovskii

Current position, grades: Dr.Chem., Head of Laboratory of Computer Modeling of Electronic Structure of Solids, Institute of Solid State Physics (University of Latvia).

Publications: He is the author of over 120 regular and review papers in international scientific journals. His Hirsch index is 16.

Experience: From 1977 until 1995 he was a researcher at the Institute of Inorganic Chemistry, Latvian Academy of Sciences. Since 1995 he has been a leading researcher at the Institute of Solid State Physics, University of Latvia. Within the last 20 years he has been granted several fellowships for collaboration, visiting activities and positions at seven universities and scientific centers of Canada, Finland, Germany, United Kingdom, and the United States. He has also been actively engaged in developing active collaboration with some scientific groups in Belarus, Italy, Russia, and Sweden. Simultaneously, he has been a contact person and participant in a number of collaboration projects under support of European Commission. His current research activities concern theoretical simulations on the atomic and electronic structure of crystalline solids (with 3D, 2D and 1D dimensionalities).

Victor Gopeyenko

Current position, grades: professor, Dr.Sc.Eng Vice-Rector on scientific issues at Information System Management University and the director of ISMU Computer Technologies Institute.

University studies: Riga Civil Aviation Engineering Institute (Latvia), obtained his doctor's degree (Dr. Sc. Eng., 1987) at Riga Civil Aviation Engineering Institute (Latvia).

Scientific interests: current research activities concern nanophysics, nanoelectronics, nanodevices, and nanotechnologies in the EU FP7 Project CACOMEL (2010 to 2014). His special interests concern carbon nanotubes and graphene systems applications and modeling.

Publications: 80 regular papers in international scientific journals

Experience: he was the member of local organizing committee of NATO ARW "Nanodevices and Nanomaterials for Ecological Security," Riga, Latvia, 2011, he is the editor-in-chief of the journal 'Information Technologies, Management and Society' and editorial board member of the journal 'Innovative Information Technologies'.

Nataly Burlutskaya

Current position, grades: a researcher at the Information Systems Management University and the Institute of Solid State Physics, University of Latvia

University studies: Master degree in computer systems (2011) at Information Systems Management University, Riga, Latvia.

Scientific interests: current research activities concern theoretical simulations of the electronic and electrical properties of carbon nanotubes and graphene nanoribbons in the EU FP7 Project CACOMEL (2010 to 2014).

Publications: 30 regular papers

Experience: Nataly Burlutskaya was the secretary of organizing committee of NATO ARW "Nanodevices and Nanomaterials for Ecological Security," Riga, Latvia, 2011.

Tamara Lobanova-Shunina

Current position, grades: Associate Professor at Riga Technical University, Aeronautics Institute, PhD, Dr.edu

University studies: University of Latvia, She obtained her PhD (2009) on innovative education at South-Ukrainian National University

Scientific interests: current research activities concern nanotechnologies, nanomanagement, nanoeducation, nanorisks, and nanothinking in the EU FP7 Project CACOMEL (2010 to 2014), special interests are connected with the systemic approach to nanosystems applications.

Publications: 53 regular papers

Experience: She was a member of the NATO ARW Local Organizing Committee 'Nanodevices and Nanomaterials for Ecological Security', Riga, Latvia, 2011. She has been working as a visiting researcher at INFN-Laboratori Nazionali di Frascati, Frascati-Roma, Italy (2010 to 2015). She was the Head of International Business Communications Department, Director of the study programme 'International Business Communications' at Information Systems Management University (till 2013). She is the Editorial Board member of the journal 'Innovative Information Technologies'. She is the author of over 53 scientific papers in international scientific journals.