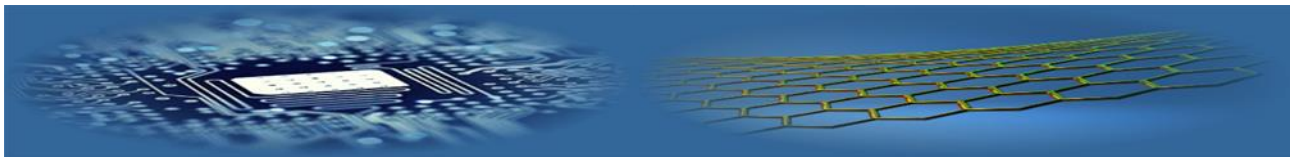

Theory and modelling of real-time physical and bio- nanosensor systems

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Abstract

Our research pursues two important directions of real-time control nanosystems addressed to ecological monitoring and medical applications. We develop physical nanosensors (pressure and temperature) based on functionalized CNTs and GNRs nanostructures. The model of nanocomposite materials based on carbon nanocluster suspension in dielectric polymer environments (epoxy resins) is regarded as a disordered system of fragments of nanocarbon inclusions with different morphologies. Using the effective media cluster approach, disordered systems theory and conductivity mechanisms analysis we have formulated the approach of conductivity calculations for carbon-based polymer nanocomposites and obtained the calibration dependences. We also develop bio-nanosensors based on polymer nanotracks with various enzymes, which provide the corresponding biocatalytic reactions and give reliably controlled ion currents. Particularly, we describe a glucose biosensor based on the enzyme glucose oxidase (GOx) covalently linked to nanopores of etched nuclear track membranes. Using simulation of chemical kinetics glucose oxidation with GOx, we have obtained theoretical calibration dependences. Our objective is to demonstrate the implementation of advanced simulation models providing a proper description of electric responses in nanosensoring systems suitable for real time control nanosystems. Comparisons with experimental calibration dependences are discussed. Prospective ways of developing the proposed physical and bio- nanosensor models and prototypes are considered.

Keywords

real-time nanosensors
functionalized nanocomposites
physical nanosensors
bionanosensors

1 Introduction

Nanosensor systems constitute an essential functional part of any modern devices that provide information processing for information systems, engineering interfaces, healthcare and many others. The talk is about nanosensor systems for various aspects of ecological monitoring and security. The fundamental electron devices are FET-transistors able to provide high sensitivity to various external influences of different nature. Conventional schemes of nanosensoring systems are based on nano-FET-types devices, particularly:

a) unperturbed field-effect transistors based on CNT- or GNR- based FETs are mainly composed of the corresponding semiconducting carbon materials suspended over two electrodes;
b) physical nanosensors: a conducting threshold can be altered when the tube or graphene ribbon is bent;
c) 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 by the presence of donor or acceptor molecules of specific gases or composites;
d) biological nanosensors: ensure monitoring of biomolecular processes such as antibody/antigen interactions, DNA interactions, enzymatic interactions or cellular communication processes, etc. [1, 2].

Another way to design nanosensoring systems is the use of polymer nanoporous structures [3, 4]. In particular, ion tracks are suitable for biosensing applications because they have true nanometric dimensions. Ion tracks can confine chemical reactions in well-defined, pre-determined locations ensuring that their reaction products are highly enriched locally. If the membranes containing such etched tracks are put on the path of ion currents flowing through a vessel, all the ions are subsequently forced to pass through the nanopores, electrically sensing any confined chemical reaction occurring there via the changes of electrical resistance in the pores.

We focus our research on two important directions of real-time control nanosystems addressed to ecological monitoring and medical applications, both of which provide environmental security of human society and every individual. Ecological monitoring has been widely presented at NATO Workshop 2011 Nanodevices and Nanomaterials for Ecological Security June20-24, Riga-Jurmala, Latvia [5].

For individual application, it is necessary to develop nanodevices controlling various functions of the human body, particularly, providing control over the *parameters of human health, the enhancement of human abilities, and the functioning of implants and prosthetics*. Another course in the development of nanosensors, nanoactuators, nanotransducers, etc - is the creation of artificial systems such as artificial intelligence or artificial individual. The main objective of the current study is to demonstrate the implementation of advanced simulation models ensuring a proper description of electric responses in nanosensoring systems [2, 4, 5].

Initially, we consider physical nanosensors (pressure and temperature) based on functionalized CNTs and GNRs nanostructures. The model of nanocomposite materials based on carbon nanocluster suspension (CNTs and GNRs) in dielectric polymer environments (e.g., epoxy resins) is regarded as a disordered system of fragments of nanocarbon inclusions with different morphologies (chirality and geometry) in relation to a high electrical conductivity in a continuous dielectric environment. The electrical conductivity of a nanocomposite material depends on the concentration of nanocarbon inclusions (in fact, carbon macromolecules).

We should evaluate the role of particular conductivity mechanisms using the cluster approach based on the multiple scattering theory formalism, realistic analytical and coherent potentials, as well as effective medium approximation (EMA-CPA) which we have effectively used for modeling of nanosized systems, especially for various conductivity problems [6,7].

We have extensive experience in modelling conductivity calculations in CNT-Metal and GNR-Metal interconnects, where the conductivity mechanism is very sensitive to local morphological disordering [8-10].

Further on, we pay attention to the development of bio-nanosensors based on polymer nanoporous structures (nanotracks) with various enzymes, which provide the corresponding biocatalytic reactions and give reliably controlled ion currents [3, 4, 11].

In particular, we describe a concept for a glucose biosensor based on the enzyme glucose oxidase (GOx) covalently linked to nanopores of etched nuclear track membranes [12, 13]. The main objective of the current study is to demonstrate the implementation of advanced simulation models providing a proper description of electric responses in nanosensoring systems for creation of real-time detection nanodevices.

2 Models CNTs- and GNRs-based nanocomposites

2.1 DC-CONDUCTIVITY MECHANISMS OVERVIEW

Talking about conductivity mechanisms in a medium with practically essential conductivity, it is useful to consider the phenomenon through the contributions of scattering effects that can take place in nanocomposite materails. We focus our attention on the four possible ways (see Figure 1) trying to find the best description, in particular, for functionalized nanocomposites.

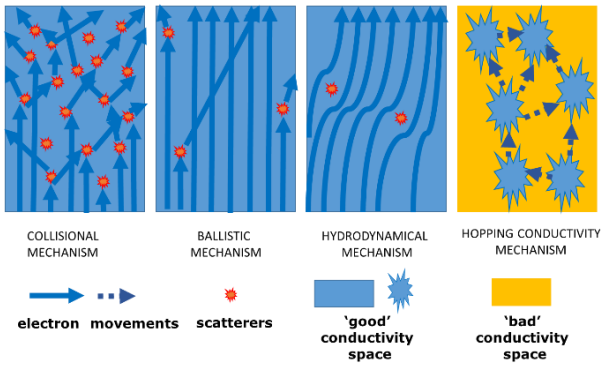


FIGURE 1 Review of general mechanisms of electron DC-conductivity

The key parameter for the analysis is the mean scattering length ℓ_{e-gen} of an electron in the conductive matter. In general, ℓ_{e-gen} includes various contributions in accordance with the well-known Matthiessen's Rule, chapeau stating:

$$\frac{1}{\ell_{e-gen}} = \frac{1}{\ell_{e-e}} + \frac{1}{\ell_{e-a/phon}} + \frac{1}{\ell_{e-o/phon}} + \\ + \frac{1}{\ell_{e-o/phot}} + \frac{1}{\ell_{e-impurity}} + \frac{1}{\ell_{e-defect}} + \frac{1}{l_{e-boundary}} + \ldots , \quad (1)$$

where ℓ_{e-e} is the electron-electron scattering length, $\ell_{e-a/phon}$ is the acoustic phonon (emission and absorption) scattering length, $\ell_{e-o/phon}$ is the optical phonon emission scattering length, $\ell_{e-o/phot}$ is the optical phonon absorption scattering length, $\ell_{e-impurity}$ is the electron-impurity scattering length, $\ell_{e-defect}$ is the electron-defect scattering length, $\ell_{e-boundary}$ is the electron scattering length with the boundary.

Hydrodynamical character of electric conductivity is the fundamental property of certain metals at low temperatures [14, 15]. This quality can be observed for such cases, when the length of electron mean free path is the order of the sample character size, namely, $\ell_{e-boundary} \infty L$ and $l_{e-e} << L$.

The last relation should be precised in cases of collisional and non-collisional electronic plasma with concentrations less than $10^{17} cm^{-3}$. Hydrodynamical behavior of electron liquid is possible to observe in some critical spaces of graphene-based electronic devices [16].

Collisional mechanism is a more expanded conductivity mechanism and takes place in most cases of typical normal conditions, e.g. for metals and semiconductors. In this case $\ell_{e-phon} \infty a << L$, where a is the character distance between 'scatterers'- atoms. This mechanism for DC-conductivity is described by the classical Drude model [17, 18]:

$$\sigma = \frac{ne^2\tau_{e-a/phon}}{m^*},$$

where n is the electron concentration, e is the electron charge, τ_{e-phon} is the time electron-phonon scattering, m^* is the effective mass of electron.

Ballistic character of conductivity is characterized by transport of electrons in a medium having negligible electrical resistivity caused by scattering. Moreover, the scattering character is essentially elastic and the medium should be considered ideally regular. The time of electron-phonon interaction is negligible. This mechanism is observed, for example, in GNRs and CNTs included in FET-type devices. The most popular description of ballistic mechanism was given by Rolf Landauer and is known now as Landauer-Büttiker formalism [19]. Landauer formula:

$$G(\mu) = G_0 \sum_n T_n(\mu),$$

where G is the electrical conductance, $G_0 = e^2/(\pi\hbar) \approx 7.75 \cdot 10^{-5} Ohm$ is the transmission eigenvalues of the channels, and the sum runs over all transport channels in the conductor. The conductance can be calculated as the sum of all the transmission possibilities that an electron has when propagating with an energy E equal to the chemical potential μ. In fact, the phenomenon is similar to optical thin films effect, when the transparency is achieved due to the quantization of the wave length. However, it is impossible to realize the remarkable conductivity property of GNRs and CNTs without any contacts. Appropriate nanocarbon-metal interconnects are characterized as disordered regions with essentially scattering mechanism of conductivity.

Hopping conductivity mechanism was proposed for disordered condensed systems (eg, for composite amorphous semiconductors and dielectrics) for the explanation of the metal-insulator transition [20]. The talk is about the existence of the electron hopping between the conductive clusters in the dielectric, or between the impurity centres of localization. In this model, the medium (insulator-metal) is represented by the following pattern: there is a random distribution of the nodal points related to each other by 'conductivities' exponentially dependent on the interstitial distances. The hopping conductivity model with a variable 'jump' length can be considered the most general one: $\ell_{e-impurity} \propto a$:

$$\sigma = A\exp\left(-\frac{4}{3}\left(\frac{4\alpha r_s}{a}\right)^{3/4}\left(\frac{W}{\kappa T}\right)^{1/4}\right), \quad (2)$$

where a is the characrteristic 'borous radius' of the considered 'doping' centre, r_s is the characteristic radius of the doping centre or conductive region, W is the characteristic potential barrier for electon tunnelling, k is the Boltzmann constant, T is the sample temperature, $\alpha \approx 0.70$ is the empirical constant which can be evaluated only using Monte-Carlo numerical simulations [21].

2.2 NANOCARBON-BASED POLYMER COMPOSITE MODEL

We develop a set of prospective models of nanocarbon-based nanomaterials and nanodevices having various interconnects and interfaces. In particular, nanoporous and nanocomposite 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. 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 [8, 22, 23].

In cases when nanocarbon clusters are embedded in high resistance media (instead of vacuum) we come to a nanocomposite material. The utilization of polymeric composite materials (e.g., epoxy resins) supplemented with various morphological nanocarbon groups of carbon nanotube-type (CNTs) and graphene nanoribbons (GNRs) allows us to create effective pressure and temperature sensors. Application of such nanocomposites as coatings can provide continuous monitoring of the mechanical strains in piping systems (for example, in aircraft or automotive applications), when the critical pressure values can indicate malfunctions of the engine. The analysis of possible medical instruments for real-time measuring human body temperature and blood pressure can also be realized.

The interest in CNTs and GNRs-based polymer nanocomposites as prospective pressure and temperature nanosensor materials is based on the observed electric percolation phenomena via the nanocarbon inclusions concentration. In particular, the electrical conductivity of a nanocomposite increases with the increasing CNT loading up to a critical filler concentration, where a dramatic increase in conductivity is observed. This critical filler concentration is called electrical percolation threshold concentration. At percolation threshold concentration, a filler forms a three-dimensional conductive network within the matrix, hence electron can tunnel from one filler to another and, in doing so, it overcomes the high resistance offered by insulating polymer matrix.

Consider the model of composite material with carbon nanocluster inclusions of CNTs- and GNRs- types.

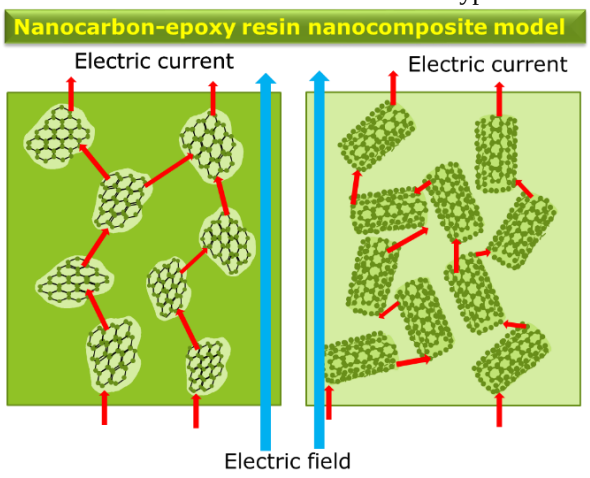


FIGURE 2 Model of composite polymer material with carbon nanocluster inclusions of GNRs- and CNTs- types.

The host material – is a flexible dielectric medium of epoxy resin- type with high resistance [24]. However, a low concentration of nanocarbon inclusions cannot change the mechanical properties of the host material. At the same time, high electrical conductivity of CNTs- and GNRs incurporated in the host material can significantly affect the total conductivity of the nanocomposite material. According to our model, the mechanism of these changes is related to the effects of percolation through the ***hopping conductivity*** (see. Figure 2). This is the only mechanism that takes into account the compliance with our analysis induced morphological changes in the whole nanocomposite matrix. This is a single mechanism, which takes into account accordance with our analysis induced morphological changes in the whole nanocomposite matrix.

Thus, the model of nanocomposite materials based on carbon nanocluster suspension (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 a 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. The hopping mechanism is regulated by the electron hopping between 'nanocarbon macromolecules' (see (1) and [20, 22, 23]:

$$\sigma = A\sigma_0 \exp\left(-\frac{4}{3}\left(\frac{4\alpha r_{tun}}{a}\right)^{3/4}\left(\frac{W_0}{\kappa T}\right)^{1/4}\right), \qquad (3)$$

where r_{tun} 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.

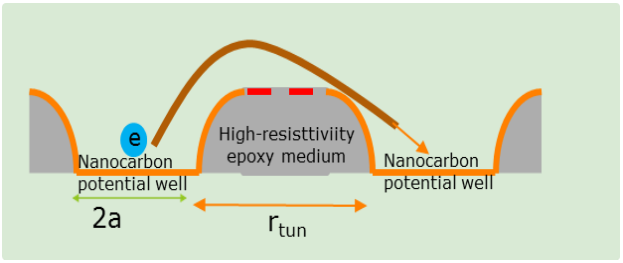


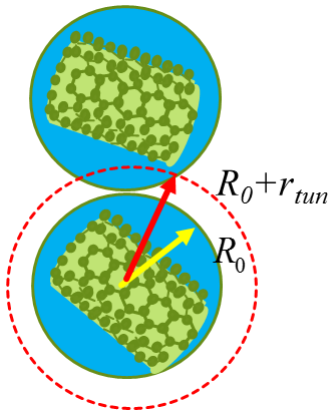
FIGURE 3 Potential wells model for hopping in polymer nanocomposistes, where *2a* is the characteristic size of nanocarbon inclusion, r_{tun} is the length of the tunnel 'jump' of the electron.

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. If we introduce the volume part as an indicator of the nanocarbon inclusions concentration:

$$\eta = \left(\frac{R_0}{R_0 + r_{tun}}\right)^3,$$

where R_0 is the average nanocarbon macromolecule radius, r_{tun} is, as earlier, the statistically averaged width of the potential barrier between the nearest nanoclusters, which is responsible for percolation ability of the model nanocomposite. We should also diminish the hopping phenolmena and percolation probability taking into account the nanocarbon macromolecule orientation within a hypothetical sphere embedded into high resistance dielectric medium. Based on this definition, we can obtain a contribution of potential nanocarbon clusters to nanocomposite conductivity as follows (see also Figures 2, 3):

$$\ln\left(\frac{\sigma}{\sigma_0}\right) = -\frac{4}{3}\left(\frac{4\alpha}{3} R_0 (\eta^{-1/3} - 1)\right)^{3/4}\left(\frac{W_0}{\kappa T}\right)^{1/4}. \qquad (4)$$



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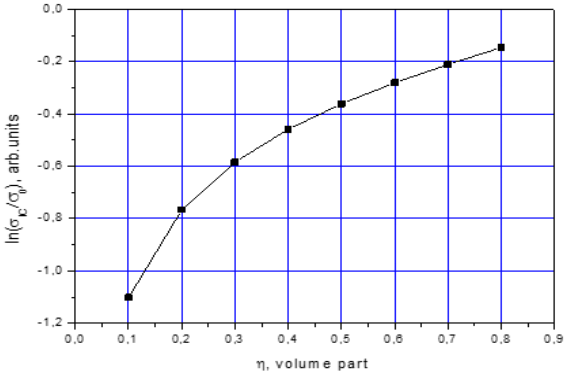


b)

FIGURE 4 Typical statistically averaged morphology of CNT-polymer nanocomposite: a) structural model; b) The hopping conductivity correlation via the average nanocarbon macromolecules volume part within continuous dielectric medium

3 Simulation of stress- and temperature-induced resistance of carbon-based nanocomposite sensors: models and experiment

The overall conductance of nanocomposite material is evaluated using equivalent electric scheme [23]:

$$\Sigma \approx \Sigma_D + \Sigma_{NC},$$
$$\Sigma_{NC} = \sum_{i=1}^{N} (R_i)^{-1}, \quad , \qquad (5)$$
$$R_i = A\sum_{k=1}^{N_i} (\sigma_{nano,ik}^{-1} + \sum_{k=0}^{N_i} (N_{eff,ik}\sigma_{jump,ik})^{-1})$$

where N - is the number of conductivity channels, N_i – is the number of nanocarbon clusters in the conductivity channel, N_{eff} is the number of effective tunneling bonds including the contact region, $\Sigma_D = (R_D)^{-1}$ is the conductance of dielectric medium, σ_{nano} is the conductivity nanocluster, σ_{jump} - is the hopping conductivity of the effective bond, which creates interconnect for large nanocarbon inclusion concentrations.

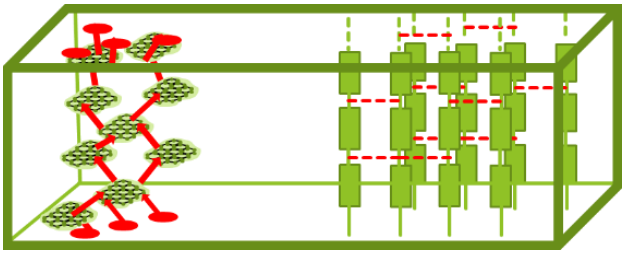


FIGURE 5 Principle equivalent scheme of nanocomposite model for resistance calculation

Basic nanocomposite models for simulation are presented in Figure 6.

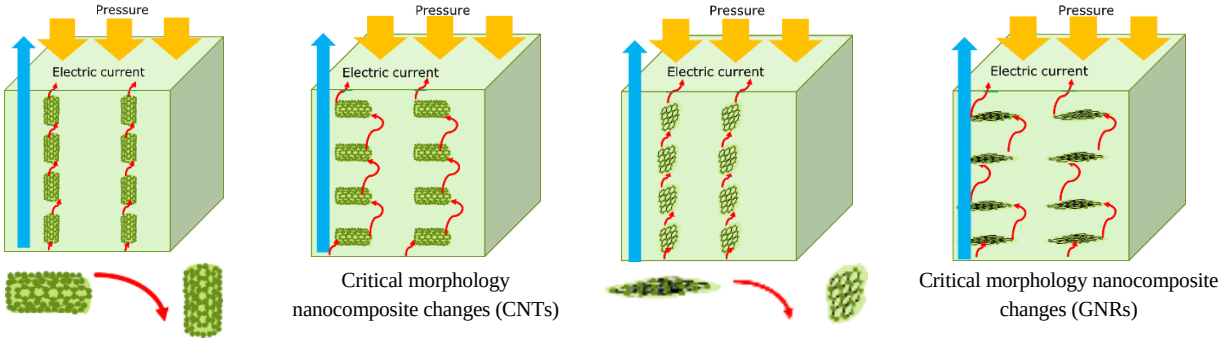


FIGURE 6 Models of nanocarbon-based functionalized polymer nanocomposites: CNT configuration 1, CNT configuration 2 , GNR configuration 1, GNR configuration 2, ⬆ - electric field direction

3.1 SIMULATION RESULTS

The basic dimensions of nanocarbon clusters (CNTs and GNRs) are as follows: the diameter of the CNT - 5 nm, the height - 10 nm, the width of the expanded CNT, i.e., the width of the GNR = $\pi \cdot 5 \approx 15,6$ nm.

The average statistical distance between nanocarbon clusters is - 5 nm. This is the key distance for the mechanism of hopping conductivity. Nanocarbon cluster is considered as a potential well with a typical size *2a*. Neighboring potential wells are separated by a distance r_{tun}. These two parameters are ultimately determine the morphology of the nanocomposite material. For modeling it also necessary to recalculate a microscopical parameter of relativive jumpimg length to macroscopic strain parameter $\varepsilon = \Delta L / L$ in Hook's law $\sigma = E\varepsilon$, where L is the total sample length. In cases of longitudinal orientation of CNTs (configuration CNT 1) the recalculation looks as:

$$\varepsilon = \frac{\Delta L}{L} \approx \frac{\Delta r}{r} \cdot \frac{1}{1 + \frac{1}{1+(1/n)} \cdot \frac{l}{r}},$$

where *l* is the CNT length (close to *2a*) and n is the number of CNT inclusion along the line (current direction). For transversal CNTs orientations (configuration CNT 2) the similar recalculation looks as:

$$\varepsilon = \frac{\Delta L}{L} \approx \frac{\Delta r}{r} \cdot \frac{1}{1 + \frac{1}{1+(1/n)} \cdot \frac{d}{r}},$$

where *d* is the diameter of the CNT. The proposed model of hopping conductivity for current percolation in carbon-based epoxy-resin nanocomposite takes into account basically the percolations along the nanocluster sets which are located along the stress direction. Interactions between the neighbouring sets are not considered for a low general concentration of nanocarbon inclusions.

Figure 7 demonstrates resistance correlations via static stresses for ideal morphologies of a nanocomposite when CNTs and GNRs are oriented pure longitudinally, pure transversely. Configurations CNT 2(min) and CNT 4(max) correspond to the minimal and maximal tunnelling (jumping) distances due to the angle deviation of CNTs relatively longitudinal orientation.

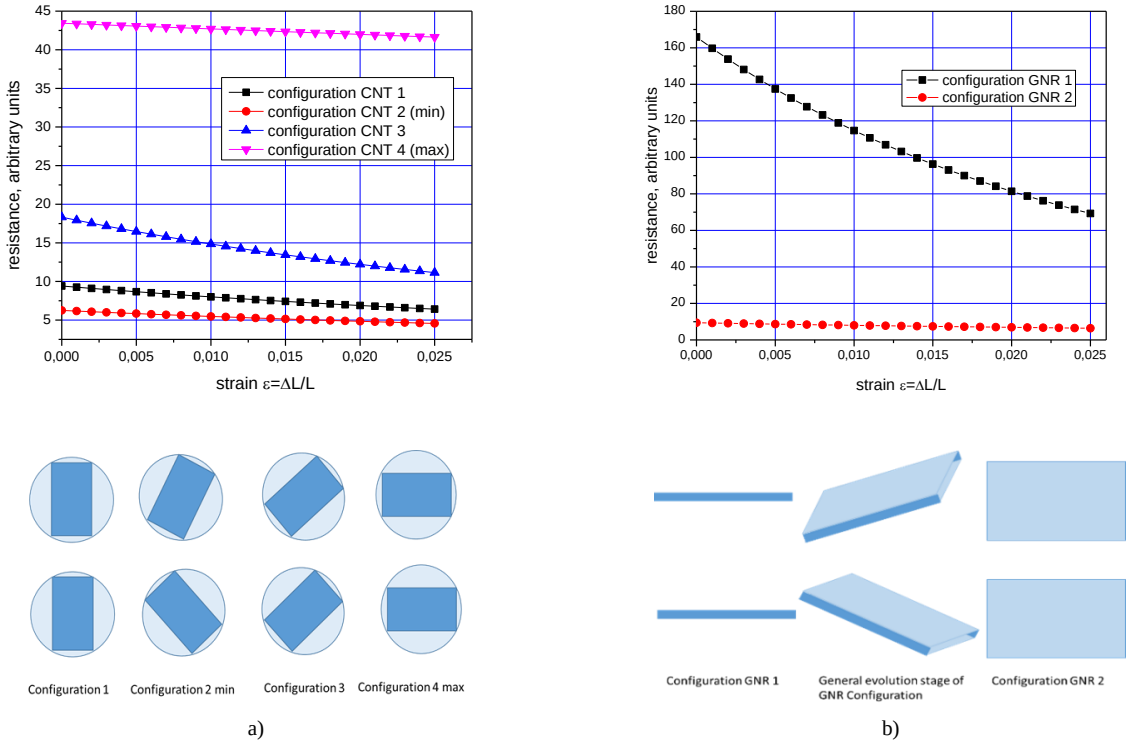


FIGURE 7 Simulation of nanocarbon composites resistances via strain: a) CNTs configurations, b) GNRs configurations

From the technological point of view, it is not so simple to provide such ideal orientations for host polymer materials similar to epoxy resins. The first problem of the nanocomposite morphology is the selection of CNTs and GNRs with identical parameters. The second problem is the polymer-nanocarbon mixture creation when we evidently should expect a homogenous random distribution of nanocarbon orientations.

Figure 8 demonstrates the marginal rotational disordering of CNTs inclusions from 'ideal' longtitudinal orientation. Deviations of orientations give the characterictic intercluster distances of 3.82 and 7.02 nm taking into account basic 5 nm in the ideal case.

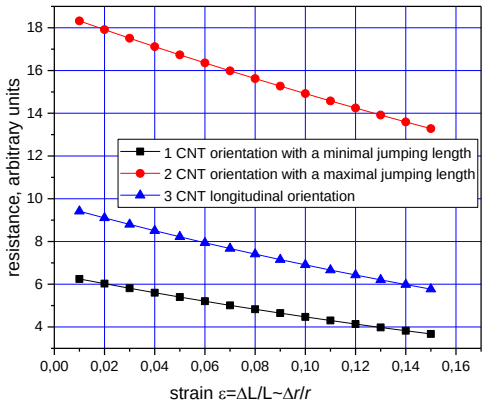


FIGURE 8 Simulation of nanocarbon composites resistances via strain for rotational deviations of CNTs inclusions

Figures 7 and 8 present the full-scale simulation of CNTs orientation deviations within a host material. The results show various sensitivity of the model nanocomposite as a potential pressure nanosensor in dependence of its morphology. Configurations of the 4th type (see Figure 6) are more sensitive and, evidently, more practically preferable.

The model uses morphologically compatible carbon nano-configurations with the same number of carbon atoms, the same surface area of model CNTs and GNRs, and the same chirality. In this way, the model CNTs and GNRs are interconnected by a simple topological transformation from a cylinder to a rectangular fragment.

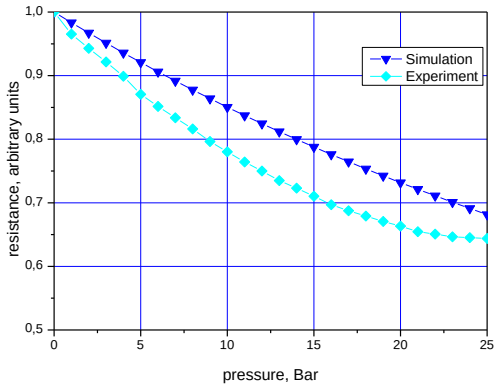
3.2 COMPARISON OF MODELLING AND EXPERIMENTAL RESULTS SIMULATION OF STRESS-INDUCED RESISTANCE OF CARBON-BASED NANOCOMPOSITE SENSORS

In this section, we will discuss the correlation of simulation results for pressure and temperature nanosensors with the experimental data of the particular prototype of similar devices [25], where the developed technology of functionalised nanocomposite based on epoxy resin (ED-20, GOST 10587-84. Epoxy- Diane Resins Uncured, elasticity modulus E=3,05 GPa) with multi-wall CNTs inclusions was applied. The testing of the mentioned nanosensors with various CNTs morphologies and mass concentrations (1, 2, 3 %) was carried out for temperatures ranging from 27 till 90 °C and the pressure ranging from 1 till 30 Bars.

When testing the pressure sensor, the load ranged from 0 to 500 N, which corresponds to the change in pressure from 0 to 30 Bars. The typical dependence of the sensor resistance on the pressure changes, as compared with the

simulation results, is shown in Figure 9a. Small deviations are connected with technological problems in the reproduction of perfect morphology, which reduces the percolation limit of the nanocomposite.

The typical dependence of the temperature sensor in the temperature range of 27 to 90 °C compared with the simulation results is shown in Figure 9b. The discrepancy in behavior between the experimental and theoretical dependencies is associated with morphological imperfections of the real sensor induced the orientation dispersion of CNTs. This effect can diminish the hopping mechanism efficiency, especially, for the higher temperatures.



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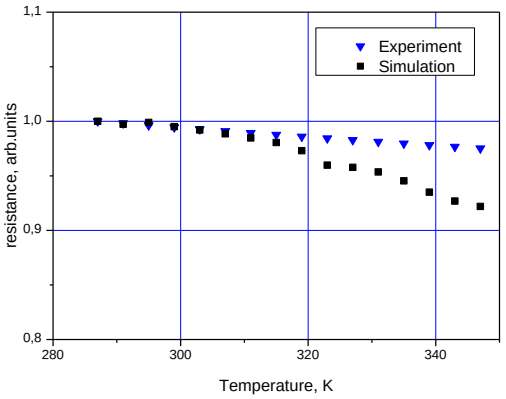


b)

FIGURE 9 Comparison of real pressure and temperature nanosensor indications [25] with more adequate models morphologies simulation: a) pressure nanosensor ; b) temperature nanosensor

4 Polymer nanoporous structures based bionanosensors: biosensor model testing and experimental results

Since the sixties of the past century, it has been known that energetic (with tens of MeV or more) heavy (with atomic masses being usually larger than that of Ar) ion irradiation ("swift heavy ions", SHI) introduces very narrow (~ some nm) but long (typically 10-100 μm) parallel trails of damage in irradiated polymer foils, the so-called latent ion tracks. The damage shows up primarily by the formation of radiochemical reaction products. Whereas the smaller ones readily escape from the irradiated zone, thus leaving behind themselves nanoscopic voids, the larger ones tend to aggregate towards carbonaceous clusters. Thus, emerging structural disorder along the tracks modifies their electronic behaviour (see Figure 10).

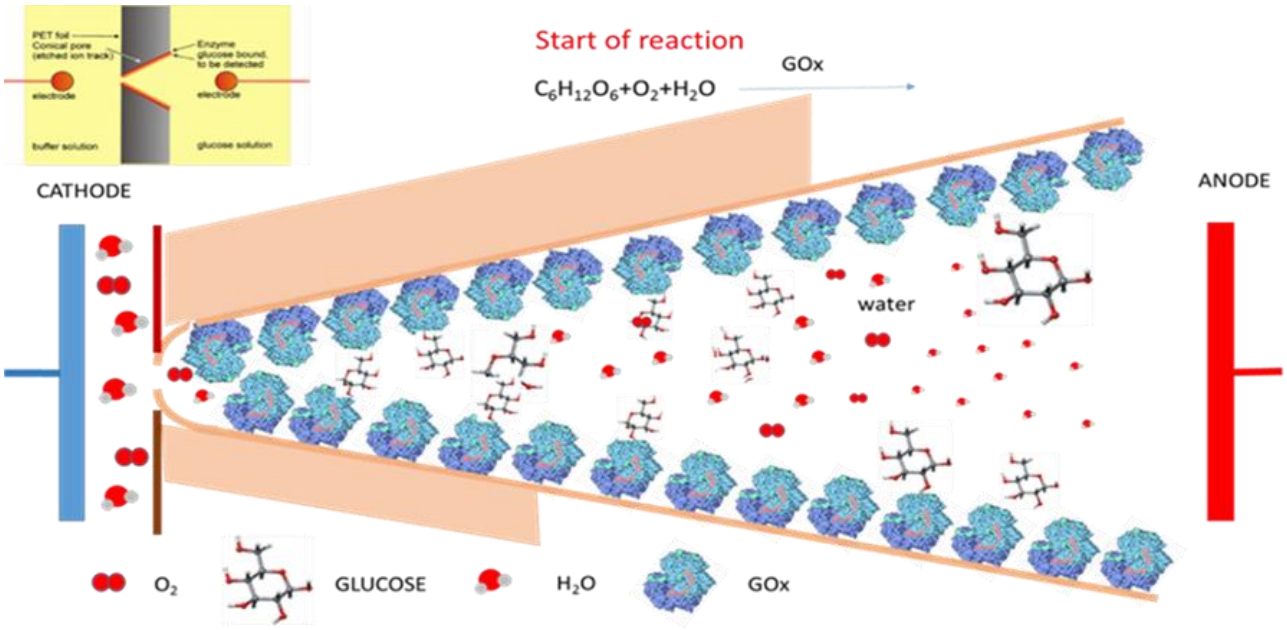


FIGURE 10 General scheme describing the detection scheme and modified polymer. Principle arrangement of experimental setup to study voltage-current dependences in ion track-containing foils embedded in electrolytes.

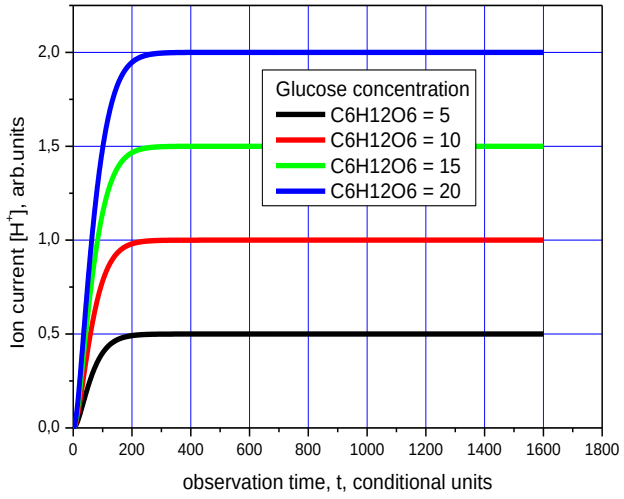
Description of the sensing reaction of glucose with the enzyme GOx looks as follows:

a) the overall net reaction is: Glucose ($C_6H_{12}O_6$) + O_2 (due to enzyme-induced oxidation) $\rightarrow$ gluconic acid ($C_6H_{12}O_7$) + O;
b) This remaining O attaches to some H_2O to form peroxide H_2O_2 ;
c) the product: gluconic acid dissociates around pH=7: $C_6H_{12}O_7 \rightarrow C_6H_{12}O_7^- + H^+$; thus the conductivity of the liquid changes (essentially if the product is enriched in the track's confinement); this is what is measured by the sensor.

In particular, a complicated biochemical kinetics of basic reaction of glucose detection depends on track qualities (e.g., track creation mechanism, foil material properties), enzyme (GOx) distribution on the track surface, geometry of the etched track etc. All these factors are the subject for the nearest special research. Moreover, the detailed kinetics of reaction is the object of 3D-modelling to design the optimal geometry of nanosensor active space. This allows creating optimal nanosensors with the increased efficiency.

The newly created intrinsic free volume enables electrolytes to penetrate into the polymer, thus forming parallel liquid nanowires. In case of tracks penetration through all the foil, the conducting connections emerge between the front and back sides of the foil. The ion track technology is particularly intended to biosensing applications. In this case, the ion tracks are functionalized directly by attaching organic or bioactive compounds (such as enzymes) to their walls.

Using simulation of chemical kinetics glucose oxidation with glucose oxidase (see Figure 11), we have obtained theoretical calibration dependences, when the concentration of H^+ is proportional to the concentration of the detected glucose.



$$H_2O_2 \xrightarrow{catalaza} O_2 + 2H^+ + 2e^-,$$

$w_1 = k_1[C_6H_{12}O_6][O_2][GOx], w_2 = k_2[H_2O_2]-$ reaction rates.

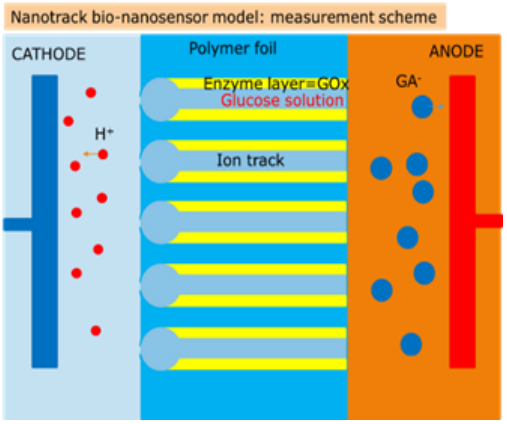
$$\begin{cases} \frac{d}{dt}[C_6H_{12}O_6] = -w_1 \\ \frac{d}{dt}[H_2O_2] = w_1 - w_2 \\ \frac{d}{dt}[C_6H_{12}O_6] = -w_1 + w_2 \\ \frac{d}{dt}[C_6H_{12}O_6] = 2w_1 \end{cases}$$

FIGURE 11 Simulation of H+ ion current via observation time in case of saturation and corresponding chemical kinetics equations

Experimental and theoretical calibration dependences demonstrate similar trends. The proposed device can serve to detect physiologically relevant glucose concentrations. The catalytic sensor can be made re-usable due to the formation of diffusible products from the oxidative biomolecular recognition event. Moreover, we can develop a multi-agent packet nanosensor, suitable for application as a human breathing analyser in relation to cancer detection, hepatitis, and so on.

The recent advancements in the field of nanosensor design allow monitoring and tracking biomolecules in such areas as the environment, food quality and healthcare. The presently developed ion track-based nanosensors provide high sensitivity, reliable calibration (see Figure 12), small power and low cost.

The creation of novel biosensors and their further improvement requires a careful study of the mechanisms of electrolytes passing through the tracks. Experimental and theoretical calibration dependences demonstrate similar trends. The proposed device can serve to detect physiologically relevant glucose concentrations. The catalytic sensor can be made re-usable due to the formation of diffusible products from the oxidative biomolecular recognition event. Moreover, we can develop a multi-agent packet nanosensor, which can be used as a human breathing analyzer in relation to cancer detection, hepatitis, and so on.



a)

$$C_6H_{12}O_6 + O_2 \xrightarrow{GOx} C_6H_{12}O_7 + O$$

$$O + H_2O \rightarrow H_2O_2$$

$$H_2O_2 \xrightarrow{catalaza} \frac{1}{2}O_2 + H_2O$$

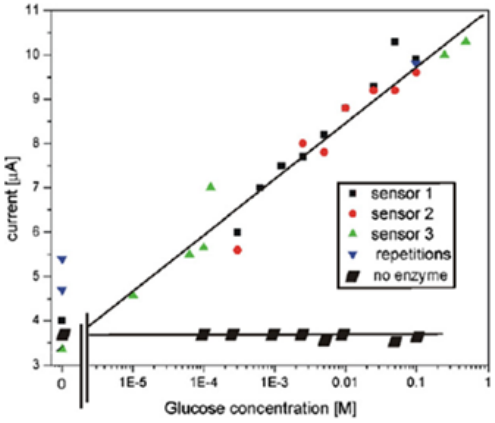
$$C_6H_{12}O_7 \rightarrow C_6H_{12}O_7^- + H^+$$

$$Anode:\ H_2O \rightarrow \frac{1}{2}O_2 + 2H^+ + 2e^-$$

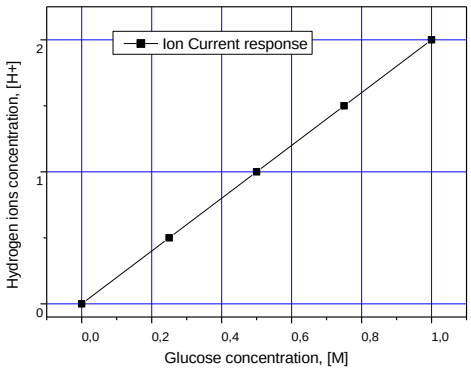
$$Cathode:\ 2H^+ + 2e^- \rightarrow H_2$$

$$Ultimate\ \ reaction:$$

$$C_6H_{12}O_6 + H_2O \rightarrow C_6H_{12}O_7 + H_2$$



b)



c)

FIGURE 12 a) General model of glucose detection process on the ion track-containing foils embedded in electrolyte and basic set of biochemical reaction; b) Experimental calibration dependenceerformance comparison of three identically produced track-based glucose detectors against a calibration curve I (+5 V) vs. glucose concentration; c) Theoretical model of typical calibration dependence based on chemical kinetics results: simulation of induced H^+ ion current via Glucose concentration.

5 Conclusions

A nanocomposite pressure and temperature nanosensor prototypes have been simulated. The hopping conductivity mechanism gives the adequate description of possible nanosensor qualities. An important problem of manufacturing sensors based on CNTs and GRNs is nanocarbon inclusions orientation, which determines the electrical properties of the future sensor.

Our work has demonstrated that ion track-based glucose sensors can be effectively created. Furthermore, they show good sensitivity, they cover a wide range of medical applications, and they can be re-used at least 10 times. This study also proves that track-based biosensors with other enzymes can be similarly developed.

Both nanosensoring schemes use simple electrical response outputs for device calibrations of parameters to be measured and can be considered as real-time tools.

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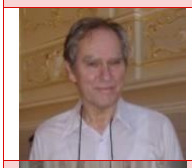

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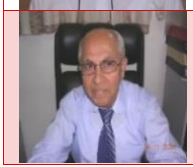

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