MODELLING OF REAL-TIME PHYSICAL AND BIO-NANOSENSORS FOR MEDICAL APPLICATIONS AND ECOLOGICAL MONITORING

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Two convergent areas of real-time control nanosystems - for ecological monitoring and medical applications are discussed. Functionalized CNTs and GNRs nanostructures serve as a basis for the creation of physical pressure and temperature nanosensors. The development of bio-nanosensors (*e.g.*, glucose biosensors) based on polymer nanotracks with various enzymes is also considered. Both nanosensor models are analyzed in comparison with the experiment.

1. Physical nanosensors based on CNTs- and GNRs-epoxy resin nanocomposites

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 (Fig. 1). The electrical conductivity of a nanocomposite material depends on the concentration of nanocarbon inclusions (in fact, carbon macromolecules). The basic conductivity mechanism for the considered nanocomposites is the hopping conductivity (Eq. 1, Fig. 2). This mechanism can usually be observed, for example, in amorphous semiconductors or some disordered solids. Various nanocomposite morphologies are considered and computer simulation results for pressure and temperature nanosensor models are discussed in comparison with the experimental device prototype [1–3].

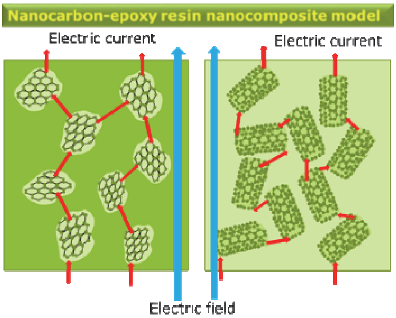


Figure 1. Model of composite polymer material with carbon nanocluster inclusions of GMRs- and CNTs- types.

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

where σ_0 is the normalization constant, which means the conductivity of monolithic dielectric medium.

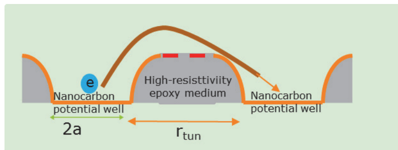
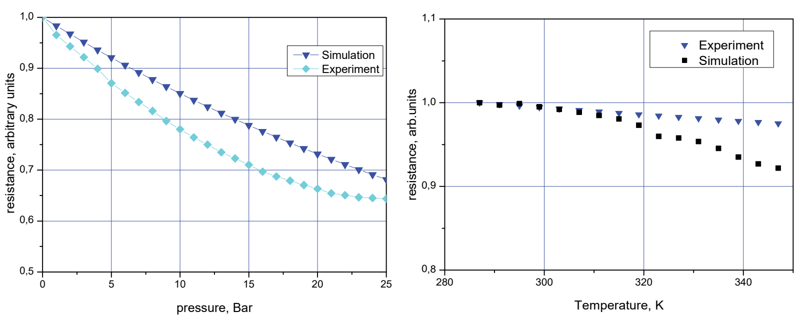


Figure 2. Potential wells model for hopping in polymer nanocomposites, where $2a$ is the characteristic size of nanocarbon inclusion, r_{tun} is the length of the tunnel 'jump' of the electron.

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 Fig. 3a. 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 range of 27 to 90 °C compared with the simulation results is shown in Fig. 3b. The discrepancy in the 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.



a b

Figure 3. Comparison of real pressure and temperature nanosensor indications [4] with more adequate models morphologies simulation: a) pressure nanosensor; b) temperature nanosensor.

Modelling of resistivity dependence via weight fraction of CNTs is presented in Fig. 4, where the sharp changes of resistivity within the weight interval (0.08-0.12) is observed.

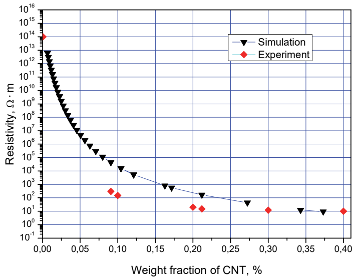
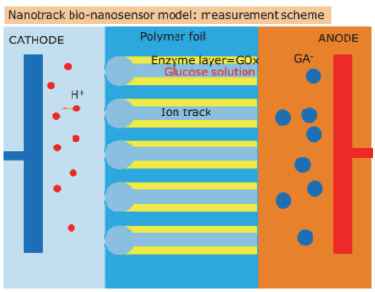


Figure 4. Comparison of resistivity of developed model CNT-based nanocomposite via weight fraction of CNT with the experimental data [5].

2. Polymer nanoporous structures based bionanosensors

We developed bio-nanosensors based on polymer nanoporous structures (nanotracks) with various enzymes, which provide the corresponding biocatalytic reactions and give reliably controlled ion currents [6,7] (Fig. 5).



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

$$O + H_2O \rightarrow H_2O_2$$

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

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

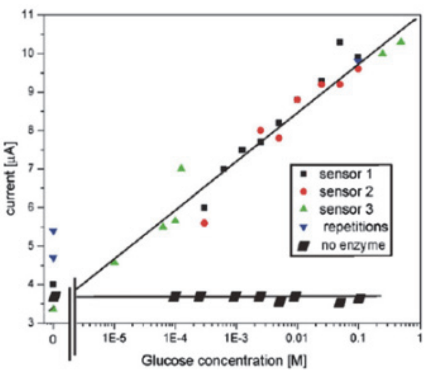
$$\textbf{Anode}:\ H_2O \rightarrow \frac{1}{2}O_2 + 2H^+ + 2e^-$$

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

Ultimate reaction:

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

a



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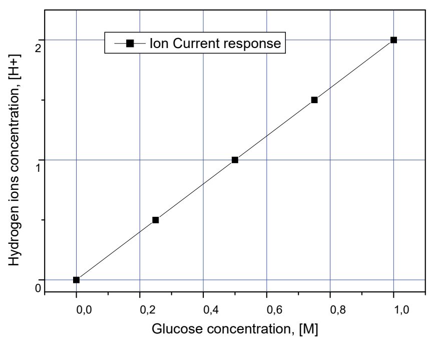

c

Figure 5. 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 dependence; c) Theoretical model of the calibration dependence based on chemical kinetics.

In conclusion, we describe a concept for 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 glucose oxidase we have obtained theoretical calibration dependences, when the concentration of H^+ is proportional to the concentration of the detected glucose. 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 production of diffusible products from the oxidative biomolecular recognition event. Moreover, we can develop a multi-agent packet nanosensor, which can be used for human breathing analyzer in relation to cancer detection, hepatitis, and other applications.

Acknowledgments

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