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SIMULATION OF TRACK STRUCTURES AS THE BASIS OF BIOSENSORS

Abstract. The main factor determining the functioning of the track biosensor is the influence of the composition of an ionic liquid flowing through the track on the ion current density at a certain external voltage. When any contamination enters the ionic liquid flowing through the track, the current density changes. This change determines the sensitivity of the biosensor. The amplifying electronic circuit of the device makes it possible to vary the sensitivity parameter over a wide range. In this work, it was found that the sensitivity of the biosensor depends on the mode in which it is operated. This means that the mode of operation must be selected depending on what sensitivity is required in each particular case.

Key words: porous, track biosensors, model particles, adsorption centers, sensitivity.

INTRODUCTION

Experts consider bio-nanotechnology to be one of the most intriguing areas of application of nano-science. In recent decades, the applications of nanotechnology in many fields related to biology, such as diagnostics, drug delivery, and molecular imaging, have been intensively investigated and yielded remarkable results.

The importance of monitoring vital processes and parameters in various spheres of life has led to the discovery of small analytical devices known as biosensors. The creation of these devices has provided various applications including drug discovery, disease diagnosis, biomedicine, food safety and processing, environmental monitoring [1; 2].

Biosensors are analytical devices used to detect the presence of an analyte of interest in a sample. They are self-contained integrated devices that provide qualitative and quantitative data about analyte by using a biological recognition element that is coupled to a transduction element. The purpose of these analytical devices is to rapidly provide accurate and reliable information about the analyte of interest in real time [3-6].

Biological sensor elements interact with the investigated substance to generate a signal. The signal generated as a result of the interaction between the sensitive element and the substance under study is then converted into a measurable and quantifiable signal through a transducer. Thus, the signal processing system amplifies the electrical signal and transmits it to the data processor, which produces a measured signal in the form of a digital display, printout, or by other way [7; 8]. The development of efficient biosensors with high functionality has led to significant achievements in various scientific fields. However, the experimental construction of biosensors faces difficulties, which in some cases can be overcome by using computational methods. Computer simulation can be to complement or replace classical experimental methods of biosensor development. Our study is directed to development and improvement of a computer model of track biosensor with an account of results earlier obtained by methods of computer modelling in the field of track biosensor creation.

1. On the possibilities of using track structures

1.1. Electrical peculiarities of tracks

The basis of any track biosensor is a track structure, which, in a particular case, is a polymer film irradiated with fast ions. The resulting structural disorder along the tracks changes electronic behavior of material. The free volume created in this way allows electrolytes to penetrate into the polymer along the hidden surface of the track, thus forming parallel liquid conductive nanowires between the front and back sides of the foil. Thus the irradiated polymer foils can exhibit electronic properties that mimic bioelectronic functional properties, as they somewhat resemble biological membranes that also contain parallel electrolyte-filled nanopores. Carbonaceous accumulations along the hidden tracks act as obstacles to the smooth passage of the ion current along them when a low-frequency direct or alternating current voltage is applied. As a result, charges can accumulate so that their electric field exceeds the intensity of the breakdown field. At this moment, current surges occur, which are associated with negative differential resistance.

1.2. Track structures for detection of spiral bacteria

There are some classes of parasitic bacteria with characteristic spiral morphology (bodies about $\sim 0.15 \dots 0.5 \mu\text{m}$ thick and spiral length $\sim 5 \dots 10 \mu\text{m}$), such as spiroplasma (e.g. E-Coli) and spirochetes (such as Borelli and Treponema). All of them can move at a significant speed (usually $\sim 3-10 \mu\text{m/s}$), but with different mechanisms of migration. While spiroplasma bacteria move through the kinks, spirochetes demonstrate purely longitudinal movement. The peculiar elongated structures of these bacteria allow them to pass along nanopores such as etched tracks. This is used to isolate them by filtration. A combination of ion track filters provides effective sensors for spirochetes. This should be done by measuring their mobility through tracks etched to different diameters over a range of helix diameters. Such measurements provide an interesting insight into the motion limitations of nanometric helical structures. In this way, spirochetes can be distinguished from spiroplasmas.

2. Simulation of optimal operating modes of a track biosensor

The parameters of the biosensor depend on the shape of the tracks, their sizes, and the atomic and electronic structure of the inner surfaces [9-11].

Features of the passage of ion flows through the tracks determine the quality of the functioning of the track biosensor. As noted earlier [11], this kinetics is significantly affected by adsorption centers on the inner surfaces of the tracks. With their uniform distribution on the surface and the same parameters, the ion flow has ohmic behavior (Fig. 1). It is this option that is optimal for the functioning of the biosensor. However, it is difficult to ensure a uniform distribution of adsorption centers on the inner surface of the track during the creation of tracks during the passage of fast ions through the film. Usually, ohmic current conditions are not created (Fig. 2).

Computer simulation of [11] made it possible to obtain the dependence of the depth of the potential well of the adsorption center on the charge. It turned out that even with a uniform distribution of adsorption centers over the surface, the dependence of the current density on the charge value is nonmonotonic (Fig. 3). However, with their uneven distribution these dependences are more complex and unpredictable (Fig. 4), which is important to consider when creating a biosensor.

An unexpected result was the influence of the flux density of model particles on their deceleration by adsorption centers (Fig. 5).

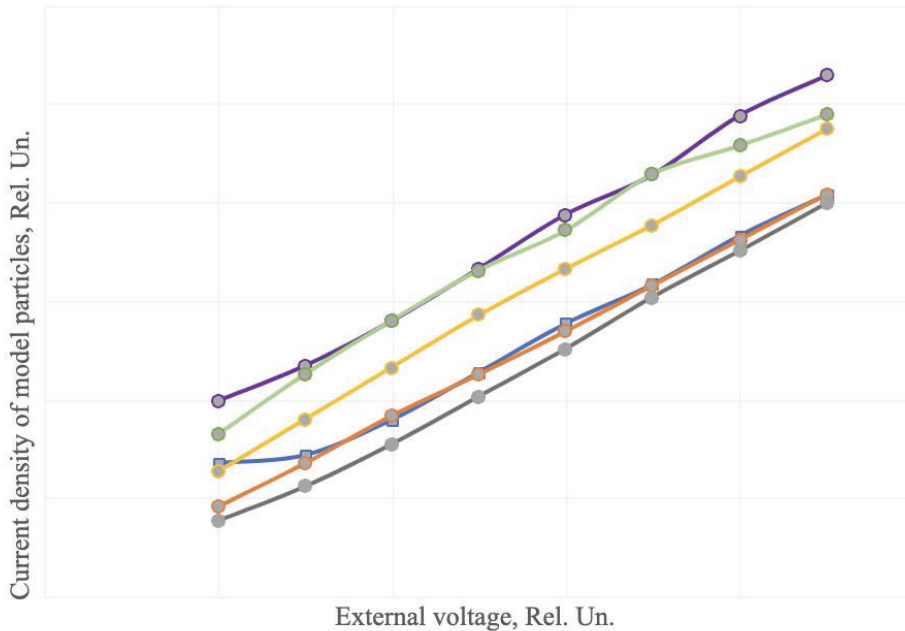


Fig. 1. Dependence of the current density of model particles on the external voltage. Curves of different colors correspond to different values of the initial external voltage. The increase in voltage during subsequent measurements was carried out in the same way in all cases

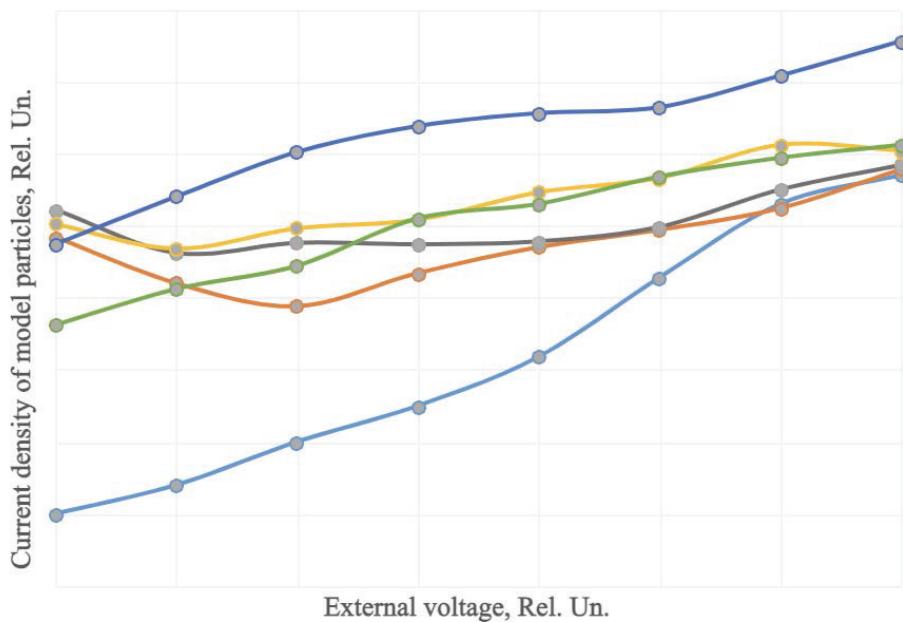


Fig. 2. Dependence of the current density of model particles on the external voltage. Curves of different colors correspond to different values of the initial external voltage. The increase in voltage during subsequent measurements was carried out in the same way in all cases

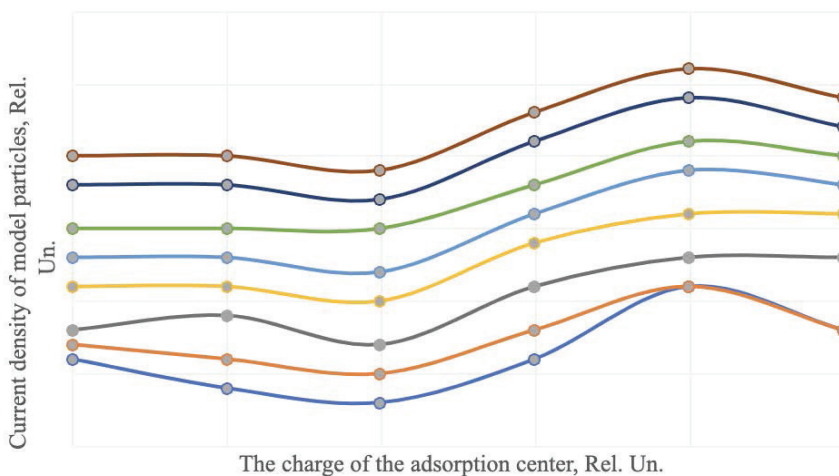


Fig. 3. Dependence of the current density of model particles on the charge of the adsorption center in the case of uniform distribution of adsorption centers on the inner surface of the track. Curves of different colors correspond to different values of the initial external voltage. The increase in voltage during subsequent measurements was carried out in the same way in all cases

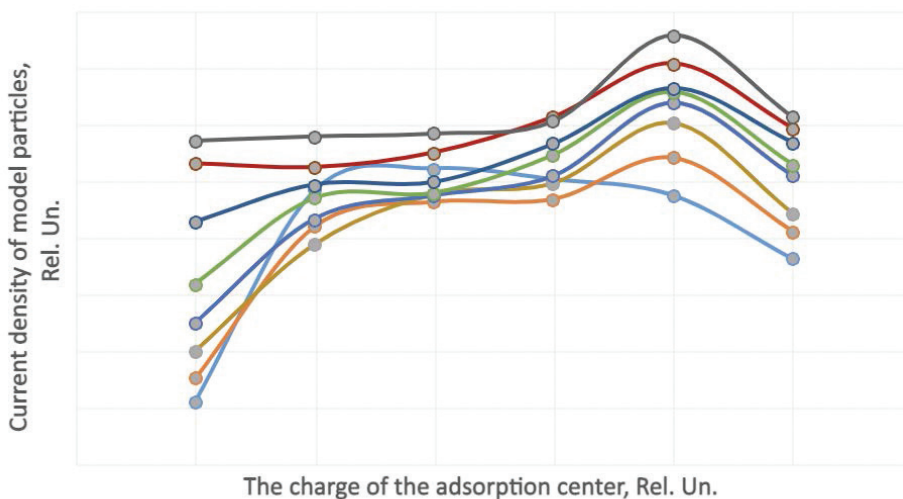


Fig. 4. Dependence of the current density of model particles on the charge of the adsorption center in the case of random distribution of adsorption centers on the inner surface of the track. Curves of different colors correspond to different values of the initial external voltage. The increase in voltage during subsequent measurements was carried out in the same way in all cases

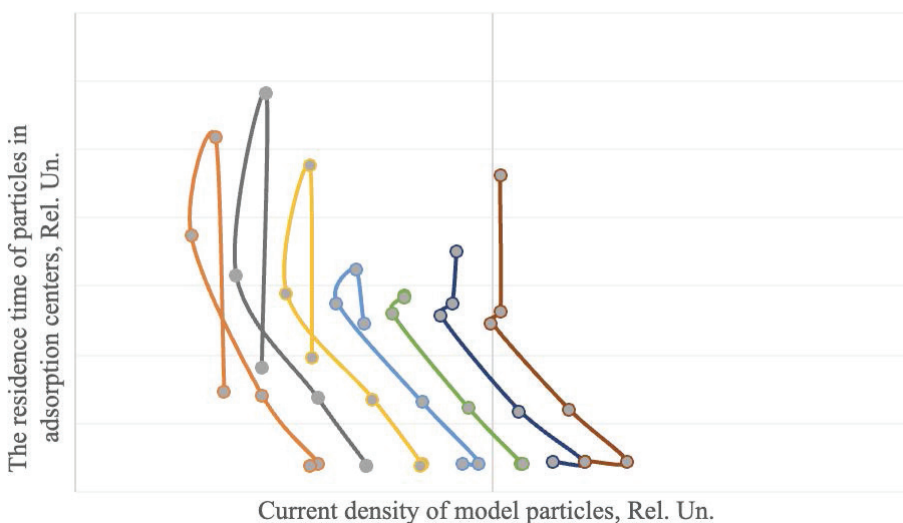


Fig. 5. The dependence of the residence time of particles in adsorption centers on the flow. Curves of different colors correspond to different values of the initial external voltage. The increase in voltage during subsequent measurements was carried out in the same way in all cases

DISCUSSION AND CONCLUSION

The problems of creating new sensory devices have now acquired particular urgency. These should be devices with a sufficiently high sensitivity and cost-effective. In particular, a large number of biosensors for various purposes have been created. The use of computer simulation methods significantly reduces the cost of developing and creating new sensor devices. Computer simulation has made it possible to obtain important results without costly experiments. In this work, it has been established that, regardless of the design features of a track biosensor, its effective application is possible only under a certain operating mode.

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