# Computer model of track biosensor

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**Abstract.** Being based on the known model of a cylindrical nanopore created using the classical method of molecular dynamics, we have studied the patterns of electrolyte flow passing through a nanocylinder, which is used to simulate an ion-induced track in a thin film. In this study, the nanotrack model takes into account the defect structure of the nanotracks inner surface. A model of a structural defect, which is an adsorption center for model particles passing through a nanocylinder, has been described. It was revealed the sensitivity of the electrolyte flux density to its composition, which is explained by interaction of particles passing through the nanocylinder with structural defects of its inner surface. This effect enables to create a biosensor system for detecting the low concentration of impurities of various types in liquid.

**Keywords:** nanopore, ion-induced nanotrack, track biosensor.

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## 1. Introduction

Porous materials have numerous applications. Concerning the pore peculiarities, it is possible to distinguish, on the one hand, between open and closed pores, and on the other hand, between macroscopic and nanoscopic pores. Open pores can be obtained by using non-diffusive processes (as for example, by ion implantation) [1]. Closed pores can be obtained only by using the diffusion processes [2, 3]. The transition from macroscopic to nanoscopic pores takes place, when the pore radius is of a similar magnitude to the Debye length.

Artificial porous materials, for example the so-called track structures, are widely used to create biosensors. Track biosensors have broad prospects for the use. Therefore, the mechanisms of their functioning are being comprehensively studied [4–6]. The work [7] describes a computer model of such a biosensor. It is shown in this work that the passage of an ionic liquid through a nanotrack has its specifics. For example, a significant dependence of the current density on the diameter of the nanocylinder is observed. This effect of ion current pulsation in a cylindrical nanopore is explained in [8]. A comparison with experimental results is also given there. It was found that the current ripple depends significantly on the track density and arises as a result of interaction between currents in different tracks. Some anomalies in the current pulsations that can be seen in Fig. 1 are caused by fluctuations in the density of ion flow. These fluctuations in the flux density are revealed in a model in which there are adsorption centers on the inner surface of the track. At large capture cross sections, several nanoparticles are accumulated by adsorption centers simultaneously, which then detach, causing current fluctuations.

## 2. Adsorption center model

In the work [7], the mechanism of the effect associated with adsorption centers (AC) on the ion flux passing through the nanocylinder is described. But detailed characteristics of adsorption centers, which can significantly affect the passage of liquids and gases through a nanopore, were not considered. The features of the influence of adsorption centers on the passage of nanoparticles through nanotracks are especially important in the case of using track structures as the basis for creating biosensors. When considering AC, it is necessary to take into account not only the depth of the potential well, on which the “delay time” of a migrating particle depends, but also the probability of the particle being “captured” by the adsorption center.

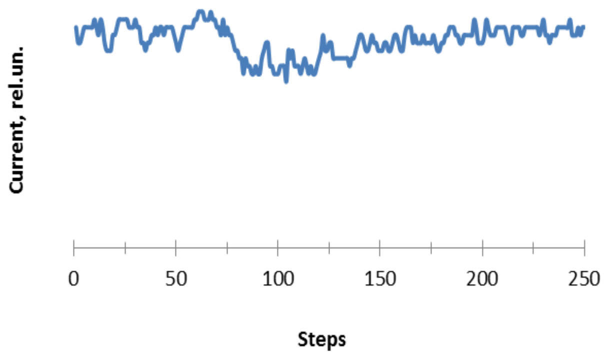


**Fig. 1.** Behavior of the current density of model nanoparticles through a nanocylinder in the model with adsorption centers.

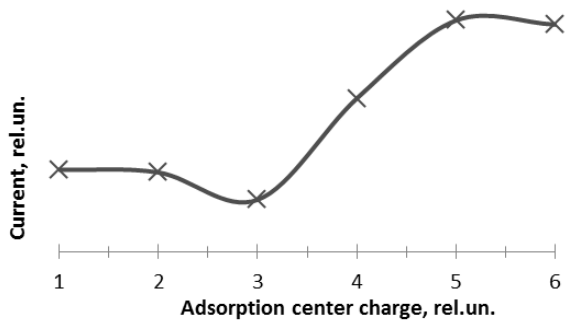


**Fig. 2.** Dependence of the current density inherent to nanoparticles through a nanocylinder on the charge of adsorption centers.

When modeling the AC, the probability of particle capture was varied by changing the charge of the AC. It turned out that the current density of model particles through the nanocylinder depends on the AC charge, and this dependence is different, when the applied voltage changes. It was revealed that, in the case of not too high voltages, it turns out that this dependence is non-monotonic (Fig. 2).

### 3. Passage of inhomogeneous flows through a nanocylinder

We found that the current density of nanoparticles through a nanotrack depends on the composition of the flow. This fact is used to create a biosensor detecting certain harmful impurities. The passage of an ion flow through a cylindrical nanopore was studied using the computer model described in [7]. But in that work the effect of AC at the surface of nanotrack on the current density was not accounted. Now it was done.

The average density of model particles in the volume of the nanocylinder is kept constant. At a stationary flow, there were 10000 model particles in the nanocylinder. All particles in the flow had a charge +1. But several ions have another charge (+2), which were considered as foreign impurities. It turned out that, when including these foreign particles (impurities), the change of the current density occurs (Fig. 3), which enables to reveal the presence of harmful impurities in a liquid medium.

### 4. Discussion

The scheme of the track biosensor at first glance seems to be simple. However, to create a biosensor with high sensitivity and high reliability, it is necessary to solve a set of problems to ensure the optimal parameters of the device. The quality of the track biosensor depends mainly on the correct interpretation of the change in the current density of the ionic liquid flow within the track.

Track structures are usually obtained by ion bombardment of thin dielectric films and subsequent annealing-etching procedures [4, 9].

It has long been ascertained that diffusion processes in porous materials have distinctive features in comparison with the laws of ordinary diffusion [10].

In Ref. [7], the dependence of ionic liquid current in a nanocylinder on the track diameter was discussed. In this work, it has been ascertained that the passage of charged nanoparticles through a nanocylinder significantly depends on the presence of AC on the inner surface of the track. A specific model of AC has been considered. But it should be taken into account that under real conditions, adsorption centers appear as certain defective formations in the process of ion bombardment. Therefore, their structure and properties are defined by the mechanisms of radiation defect formation and features of the film material. In addition, in the process of ion bombardment, other structural defects appear at the inner surfaces of tracks, such as various scattering centers. As a result, biosensor characteristics can be masked by other effects. Nevertheless, track biosensors with acceptable characteristics have already been created [11, 12].

The challenge is to significantly improve their parameters by further studying all the factors that determine their optimal performance.

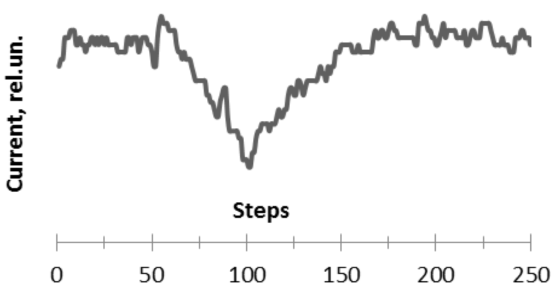


**Fig. 3.** Behavior of the current density in the case of the introduction 0.1% of foreign model particles.

## 5. Conclusion

A computer experiment has shown the promise of creating highly sensitive biosensors based on the passage of ionic liquids through cylindrical nanopores.


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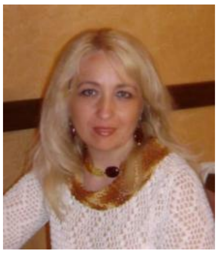

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**Briukhovetska I.V.:** validation, formal analysis
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**Комп'ютерна модель трекового біосенсора**

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**Анотація.** На основі відомої моделі циліндричної нанопори, створеної за допомогою класичного методу молекулярної динаміки, досліджено закономірності проходження потоку електроліту крізь наноциліндр, який використовується для моделювання іонно-індукованого треку в тонкій плівці. У цьому дослідженні модель нанотреків враховує структуру дефектів внутрішньої поверхні нанотреків. Описано модель структурного дефекту, який є центром адсорбції модельних частинок, що проходять крізь наноциліндр. Виявлено чутливість густини потоку електроліту до його складу, що пояснюється взаємодією частинок, які проходять крізь наноциліндр, зі структурними дефектами його внутрішньої поверхні. Цей ефект дозволяє створити біосенсорну систему для детектування низьких концентрацій різного типу домішок у рідині.

**Ключові слова:** нанопора, іонно-індукований нанотрек, трековий біосенсор.