Sensors

Improvement of new electronic materials using computer modeling

Y.V. Bondaruk[1], T.S. Kavetskyy[2,3*], A.O. Vinkovskaya[1], M. Kushniyazova[4], D.O. Dyachok[1], L.I. Pankiv[2], H.M. Klepach[2], O.R. Mushynska[2], O.V. Zubrytska[2], O.I. Matskiv[2], Y.V. Pavlovskyy[2], S.Y. Voloshanska[2], S.S. Monastyrska[2], L.V. Bodnar[1], A.E. Kiv[1,5]

[1]*South-Ukrainian K.D. Ushynsky National Pedagogical University, 65020 Odesa, Ukraine*
[2]*Drohobych Ivan Franko State Pedagogical University, 82100 Drohobych, Ukraine*
[3]*Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovak Republic*
[4]*Kazakh-British Technical University, 050000 Almaty, Republic of Kazakhstan*
[5]*Ben-Gurion University of the Negev, 84105 Beer-Sheva, Israel*
[*]*Corresponding author e-mail: kavetskyy@yahoo.com*

Abstract. Porous materials occupy an important place among the materials of electronic equipment. Nanopores, which are obtained by ion irradiation of materials, have a complex internal structure that depends on the interaction of fast ions with the substance. Obtaining such structures is important, in particular, in the manufacture of biosensor devices based on them. The most effective methods of studying their properties are computer simulations. However, effective computer models of track structures, necessary for the development and improvement of modern biosensors, are not being created actively enough. The approach proposed here involves a detailed study of the interaction of ion flows with the inner surface of the nanotrack. This approach takes into account the structural features of the inner surface of the track as well as the role of adsorption and scattering centers and other local centers. In the existing approaches, the processes mentioned above are mainly described phenomenologically, which does not indicate the ways of modifying the characteristics of the material that is necessary for the device improvement.

Keywords: nanopores, ion-induced nanotracks, track biosensors.

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1. Introduction

One of the requirements to obtain high sensitivity track biosensors is to use materials that exhibit a high number of identical long and narrow confined pore volumes. This means that porous materials such as filter paper or thin foils cut of wood would be inadequate as their pores are irregularly shaped and interconnected. Furthermore, the randomly varying pore lengths will lead to deviations of the total concentration of deposited enzymes from pore to pore and, hence, to considerable data straggling. Therefore, creating pores by energetic radiation beams is favorable. As the pores produced thermally by intense laser or electron beams have too bad aspect ratios (*i.e.* radius/length) due to their relatively large diameters, they cannot meet the criterion of long narrow confined pore volumes [1–3].

In the process of ion bombardment, various structural defects, scattering centers, *etc*. appear on the inner surfaces of the tracks. As a result, the characteristics of the biosensors utilizing ion bombarded porous materials are determined by a wide range of defects on the inner surfaces of the tracks. In this work, the main attention is paid to the fact that the models developed here reflect as fully as possible the structural features of the inner track surface, which are defined by a fast ion passing through the substance. Since the adsorption centers on the track inner surface have a decisive influence on the liquid flow through the track, different models of the defects on its inner surface have been developed. Moreover, a surface roughness parameter was introduced to simulate the effect of a wide spectrum of defects on the liquid flow through the track. Track biosensors with satisfactory characteristics have already been created [4–9]. The task is to improve significantly their parameters by further studying all the structural characteristics of tracks. It is assumed that new biosensor devices created on the basis of improved track structures will be able to detect extremely small levels of chemical or biological pollution.

2. Individual features of a nanotrack in a porous material

Nanotracks used for creating track biosensors exhibit different performance properties depending on the material where they are formed and ion bombardment conditions. It turned out later that the biosensor sensitivity and reliability depend on the selected mode of operation. This dependence is defined by the structure of adsorption centers on the nanotrack inner walls.

2.1. General characteristics of adsorption centers in a nanotrack

Adsorption centers on the inner surface of a nanotrack can have different structures and different properties. Accordingly, they affect the parameters of the track biosensor in different ways. An important characteristic of an adsorption center is its charge. When a passing ion enters the potential well of the adsorption center, the duration of its stay in the bound state depends on the nature of the interaction of the trapped ion with the ions that form the potential well. At the same time, the life-time of the trapped ion affects the flux density through the nanotrack. Therefore, we previously performed simu-lations of different variants of adsorption centers [10–12].

2.2. Dependence of the kinetics of current flow through the nanotrack on the characteristics of adsorption centers

The studies [12] have shown that adsorption centers on the nanotrack walls play a decisive role for optimizing the biosensor parameters. Two modifications of adsorption centers were investigated, namely with inelastic and elastic interaction of trapped ions with the atoms of the potential well. Moreover, the cases of statistically uniform and non-uniform distribution of adsorption centers over the inner surface of the nanotrack were studied.

In the case of inelastic interaction between the trapped ion and the walls of the adsorption center as well as uniform distribution of these centers over the wall surface, an ohmic dependence of the current through the nanotrack on the applied voltage is observed. This option enables obtaining the best biosensor parameters (Fig. 1).

However, such nanotracks can hardly be obtained by ion bombardment. The adsorption centers formed in this way provide mostly elastic interaction of the trapped ions with the center walls. In this case, a non-ohmic dependence of the current through the nanotrack on the applied voltage is obtained (Fig. 2). Thus, computer simulation makes it possible to find the ways to improve the microscopic parameters of nanotracks.

There are two ways to influence the defect structure of nanotracks. The first way takes into account the interaction mechanisms of fast ions with the film material during track formation. The second way implies development of special chemical etching methods for finalizing track formation after the ion bombardment. In both cases, dedicated studies are required.

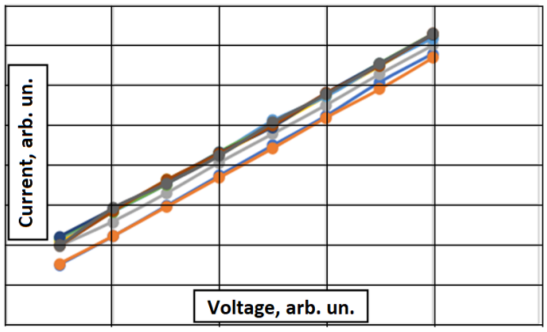

Fig. 1. Current density of model particles *vs* external voltage. Different curves correspond to different values of the initial external voltage. The voltage was increased in the same way in all the cases during subsequent measurements. In this case, inelastic interaction of model particles with adsorption centers was specified, and there was a uniform distribution of adsorption centers on the internal surfaces of the track.

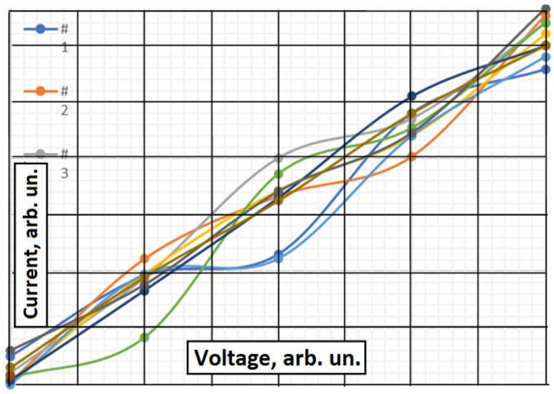

Fig. 2. Current density of model particles *vs* external voltage. Different curves correspond to different values of the initial external voltage. The voltage was increased in the same way in all the cases during subsequent measurements. Here, the case when elastic interaction of the trapped ions with adsorption center walls was specified. In this case, a non-ohmic dependence of the current through the nanotrack on the applied voltage is obtained.

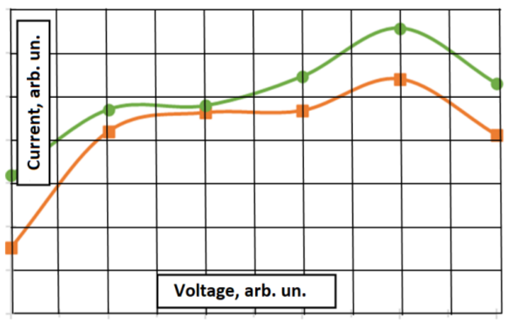

Fig. 3. Current density of model particles *vs* external voltage. Different curves correspond to different values of the initial external voltage. The voltage was increased in the same way in all the cases during subsequent measurements. Figure shows the passage of model particles through the nanotrack in the case of the *Gaussian* distribution of adsorption centers on the nanotrack walls.

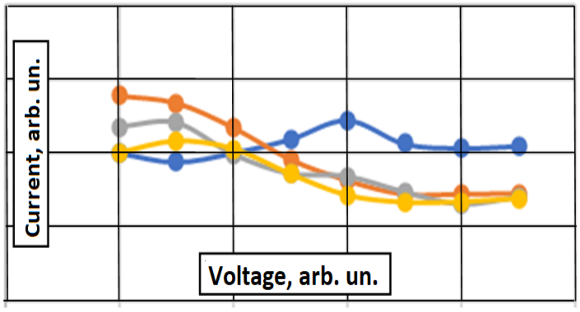

Fig. 4. Current density of model particles *vs* external voltage. Different curves correspond to different values of the initial external voltage. The voltage was increased in the same way in all the cases during subsequent measurements. Figure shows the passage of model particles through the nanotrack in the case of the *non-Gaussian* distribution of adsorption centers on the nanotrack walls.

Previously, the significance of the adsorption center charge on the role of the center for optimizing the track parameters was found [1, 13]. In this work, the role of the adsorption center charge was studied in detail. It was found in particular that the influence of the adsorption center charge on the passage of model particles through the nanotrack depends on the spatial distribution of these centers on the nanotrack walls (Figs. 3 and 4).

3. Discussion of results and conclusion

The performed studies show that optimization of track biosensor characteristics is a multi-parameter problem, solution of which requires first of all development of the methods for obtaining track materials with a given defect structure. Since simultaneous variation of different characteristics is necessary to find the desired track structure, creation of computer models is the most effective approach. The obtained results point to the need to form a certain set of local centers on the nanotrack inner walls. However, implementation of this task involves solving specific problems of radiation physics, in particular, the problem related to passing fast ions through the matter, as well as problems associated with chemical etching mechanisms.

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Authors and CV

Yurii Bondaruk, PhD student at the South-Ukrainian K.D. Ushynsky National Pedagogical University. Author of 7 publications. The area of his research interests is physical properties of nanomaterials.
E-mail: bondaruk@windowslive.com, https://orcid.org/0000-0003-4231-1416

Taras Kavetskyy, PhD, Associate Professor, Head of Laboratory and Senior Researcher at the Drohobych Ivan Franko State Pedagogical University as well as Visiting Researcher at the Institute of Physics, Slovak Academy of Sciences, Bratislava. Author of more than 400 publications. The area of his research interests is physical properties of nanomaterials. https://orcid.org/0000-0002-4782-1602

Alina Vinkovskaya, PhD student at the South-Ukrainian K.D. Ushynsky National Pedagogical University. Author of 9 publications. The area of her research interests is physical properties of nanomaterials.
E-mail: alina.vinkovskaya@gmail.com

Mariya Kushniyazova, PhD student at the Kazakh-British Technical University. Author of 2 publications. The area of her research interests is physical properties of nanomaterials.

E-mail: kshnmariya@gmail.com

Dmytro Dyachok, PhD, Associate Professor, Head of Department at the South-Ukrainian K.D. Ushynsky National Pedagogical University. Author of more than 30 publications. The area of his research interests is physical properties of nanomaterials.
E-mail: dyachok13@gmail.com, https://orcid.org/0000-0002-9036-1138

Lyudmyla Pankiv, PhD, Associate Professor and Senior Researcher at the Drohobych Ivan Franko State Pedagogical University. Author of more than 40 publications. The area of her research interests is physical properties of nanomaterials.
E-mail: lyuda_pankiv@ukr.net, https://orcid.org/0000-0002-4918-2138

Halyna Klepach, PhD, Associate Professor at the Drohobych Ivan Franko State Pedagogical University. Author of more than 180 publications. The area of her research interests is structural properties of biomaterials.
E-mail: h.klepach@ddpu.edu.ua, https://orcid.org/0000-0003-0784-8373

Oksana Mushynska, PhD student at the Drohobych Ivan Franko State Pedagogical University. Author of 8 publications. The area of her research interests is physical properties of nanomaterials.
E-mail: nokr@ukr.net, https://orcid.org/0000-0003-1804-2615

Oksana Zubrytska, PhD student at the Drohobych Ivan Franko State Pedagogical University. Author of 5 publications. The area of her research interests is physical properties of nanomaterials.
E-mail: oksanazubrytska23.02@gmail.com

Oles Matskiv, PhD student at the Drohobych Ivan Franko State Pedagogical University. Author of 14 publications. The area of his research interests is physical properties of nanomaterials.

E-mail: omatckiv@gmail.com

Yuriy Pavlovskyy, PhD, Associate Professor at the Drohobych Ivan Franko State Pedagogical University. Author of more than 150 publications. The area of his research interests is physical properties of nanomaterials.
E-mail: yu_pavlovskyy@ukr.net, https://orcid.org/0000-0002-8194-6820

Svitlana Voloshanska, PhD, Associate Professor at the Drohobych Ivan Franko State Pedagogical University. Author of more than 230 publications. The area of her research interests is structural properties of biomaterials. https://orcid.org/0000-0003-4589-6376
E-mail: svitlana.voloshanska@gmail.com

Svitlana Monastyrska, PhD, Associate Professor at the Drohobych Ivan Franko State Pedagogical University. Author of more than 200 publications. The area of her research interests is structural properties of biomaterials. https://orcid.org/ 0000-0001-8529-800X
E-mail: svitlana.monastyrska@gmail.com

Liliia Bodnar, PhD, Associate Professor at the South-Ukrainian K.D. Ushynsky National Pedagogical University. Author of more than 70 publications. The area of her research interests is physical properties of nanomaterials.
E-mail: bodnarl79@pdpu.edu.ua

Arnold Kiv, DSc, Professor at the South-Ukrainian K.D. Ushynsky National Pedagogical University and Visiting Professor at the Ben-Gurion University of the Negev. Author of more than 400 publications. The area of his research interests is physical properties of nanomaterials.
E-mail: kiv.arnold20@gmail.com,
https://orcid.org/0000-0002-0991-2343

Authors' contributions

Bondaruk Y.V.: methodology, investigation, data curation.
Kavetskyy T.S.: conceptualization, investigation, writing – original draft, project administration.
Vinkovskaya A.O.: investigation, formal analysis.
Kushniyazova M.: investigation, formal analysis.
Dyachok D.O.: validation, formal analysis.
Pankiv L.I.: validation, formal analysis.
Klepach H.M.: validation, formal analysis.
Mushynska O.R.: investigation, formal analysis.
Zubrytska O.V.: investigation, formal analysis.
Matskiv O.I.: investigation, formal analysis.
Pavlovskyy Y.V.: visualization, resources.
Voloshanska S.Y.: visualization, resources.
Monastyrska S.S.: visualization, resources.
Bodnar L.V.: writing – review & editing, resources.
Kiv A.E.: conceptualization, writing – original draft, supervision, project administration.

Удосконалення нових електронних матеріалів за допомогою комп'ютерного моделювання

Ю.В. Бондарук, Т.С. Кавецький, А.О. Вінковская, М. Кушніязова, Д.О. Дячок, Л.І. Паньків, Г.М. Клепач, О.Р. Мушинська, О.В. Зубрицька, О.І. Мацьків, Ю.В. Павловський, С.Я. Волошанська, С.С. Монастирська, Л.В. Боднар, А.Ю. Ків

Анотація. Важливе місце серед матеріалів електронної техніки займають пористі матеріали. Нанопори, які отримують іонним опроміненням матеріалів, мають складну внутрішню структуру, що залежить від взаємодії швидких іонів з речовиною. Отримання таких структур важливе, зокрема, при виготовленні на їх основі біосенсорних пристроїв. Найбільш ефективними методами їх дослідження є комп'ютерне моделювання. Однак створення ефективних комп'ютерних моделей трекових структур, необхідних для розробки та вдосконалення сучасних біосенсорів, ведеться недостатньо активно. Запропонований підхід передбачає детальне дослідження взаємодії потоків іонів з внутрішньою поверхнею нанотреку. Такий підхід враховує структурні особливості внутрішньої поверхні треку, роль центрів адсорбції та розсіювання та інших локальних центрів. В існуючих підходах переважно використовується феноменологічний опис цих процесів, який не вказує на шляхи зміни характеристик матеріалу, необхідні для вдосконалення пристрою.

Ключові слова: нанопори, іонно-індуковані нанотреки, трекові біосенсори.