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*Vasyl Stefanyk Carpathian National University*

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D. Fink[1,2], A.E. Kiv[3,4], T.S. Kavetskyy[3,5,6], D.O. Dyachok[3], Y.V. Bondaruk[3], A.O. Vinkovskaya[3], N.K. Hoivanovych[5], L.I. Pankiv[5], O.V. Zubrytska[5], O.I. Matskiv[5], U.V. Khromiak[7], Y.Y. Pavlyshak[5], Y.V. Pavlovskyy[5], V.M. Senkiv[5], S.S. Monastyrska[5]

# Computer modeling of diffusion processes in porous materials

[1]*Nuclear Physics Institute, Czech Academy of Sciences, Řež, Czech Republic;*
[2]*Universidad Autónoma Metropolitana-Iztapalapa, México, D.F., Mexico;*
[3]*South Ukrainian National Pedagogical University named after K.D. Ushynsky, Odesa, Ukraine, kiv.arnold20@gmail.com;*
[4]*Ben-Gurion University of the Negev, Beer-Sheva, Israel;*
[5]*Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine, kavetskyy@yahoo.com;*
[6]*Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovak Republic;*
[7]*Lviv State University of Life Safety, Lviv, Ukraine*

Track structures belong to nanomaterials. Therefore, when studying such structures, it is important to take into account the general properties of nanomaterials. It is important to predict the structural features of the tracks, the configuration of defects on the inner surfaces of the tracks depending on the characteristics of the fast ions that create them. Using a computer experiment, it is possible to achieve results that are much more difficult to obtain in a conventional laboratory experiment. The formation of a nanotrack with the necessary structural parameters depends not only on ion-stimulated processes, but also on other methods of film processing, in particular chemical etching. Computer modeling of the passage of ion flows through nanotracks allows obtaining results that must be taken into account to improve the quality of modern biosensors. New algorithms and computer programs have been developed to solve these problems.

**Keywords:** porous materials, ion-induced nanotracks, track structures, computer modeling, biosensors.

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## Introduction

Many solid substances in biology, medicine, and technology are porous materials into which impurity solutions can penetrate. Regarding the pore population, a distinction should be made between open and closed pores on the one hand and macroscopic and nanoscopic pores on the other hand. Open pores are accessible from the surface by means of non-diffusive processes of capillary percolation or microcapillary diffusion [1], closed pores, which do not have a direct connection with the outside world, are accessible only by diffusion.

The transition from macroscopic (where fluid dynamics and capillarity are preserved) to nanoscopic (where nanofluidics takes place) pores occurs when the pore radius is close to the Debye length.

In addition to the common methods of measuring porosity, there are also less popular approaches that use adequate tracer solutions that penetrate the pores and thus provide information on the average available pore depth and the average open pore volume at depth. In addition, these methods allow determination of tracer penetration rates (extracted from tracer depth distributions as a function of penetration time), which can provide clues to depth-dependent average pore cross-sectional areas and possible capture centers along the pore wall (see, e.g., earlier study of the penetration of aqueous lithium salt solutions into polymers at ambient temperature and at different pH values [2], as well as the penetration of hot liquid lithium from 770 to 1270 K into glassy polymer carbon [3].

# I. Track structures for biosensors

In biosensors, biological sensory elements interact with the substance under investigation. The signal produced by the interaction of the sensitive element with the substance under investigation is then converted into a signal that can be measured and quantified through a transducer. The signal processing system amplifies the electrical signal and transmits it to the data processor. The development of efficient biosensors with high functionality has led to significant achievements in various scientific fields.

However, the experimental design of biosensors faces difficulties, which in some cases can be overcome with the help of computational methods. Computer modeling can complement or replace classical experimental methods of developing biosensors.

The basis of any track biosensor is the track structure, which, in this particular case, is a polymer film irradiated with fast heavy ions. As a result, there are hidden tracks, which have already been mentioned. The structural disorder along the tracks changes, as well as the entire electronic behavior of the material. The track structure created in this way allows electrolytes to permeate throughout the polymer along the hidden track, thus forming parallel conductive nanowires between the front and back sides of the foil. In this way, irradiated polymer films can exhibit electronic properties that mimic bioelectronic functional features, as they resemble biological membranes that also contain parallel electrolyte-filled nanopores. Carbonaceous accumulations along the hidden tracks act as an obstacle to the smooth passage of the ion current with low-frequency, direct or alternating current. As a result, charges can accumulate so that their electric field exceeds the intensity. In this way, we observe current jumps.

The model particles of the carrier flow are characterized by charges, the interaction of which is described in our work by the shielded Coulomb potential. The progressive movement, which simulates the action of the external field, is superimposed on the chaotic movement of the microparticles in the track. The model assumes the preservation of the density of nanoparticles and the continuous process of particle flow along the track [4].

Charges simulating the real structure of the track (ionized atoms, broken bonds, etc.) are located on the inner surface of the track. In addition, adsorption centers (AC) are modeled on the inner surfaces. They act as "holes" through which the model particles (MP) can cross the boundary of the surface of the nanocylinder. At the moment when the copper particle crosses the surface of the track, it is assumed that the Hooke force ($F = -kx$) is activated, which tends to push the ion back into the nanocylinder [5].

The role of AC in the passage of liquids through nanotracks has been studied in detail. It was found that the location of the AC on the track walls significantly affects the diffusion processes in the track (Fig. 1).

Those particles that interact with the surface during passage through the cylindrical pore undergo elastic scattering on the surface and are captured by adsorption centers. Depending on the adsorption energy (the depth of the AC potential wells), the migrating particles spend different times in the adsorbed state, which affects the rate of passage of ions (the flow of particles) through the nanochannels. Using the computer model, the exponential dependence of the average lifetime of ions in the AC potential well on the depth of the well was obtained [6].

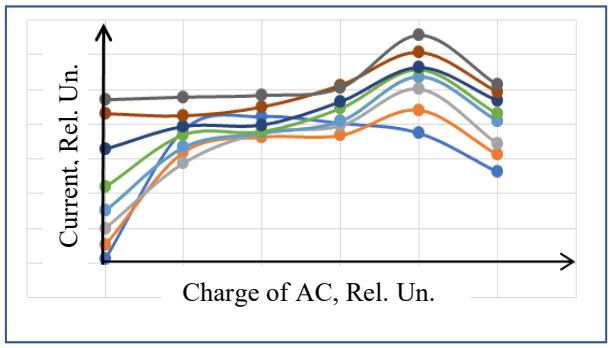


**Fig. 1.** The dependence of the model particles flow on the amount of charge of the AC under the condition of uneven distribution of AC on the internal surface of the track.

It was found that the charge of MP in the flow influences on the dependence of the flow density on the diameter of the track [7]. The result is shown in Fig. 2.

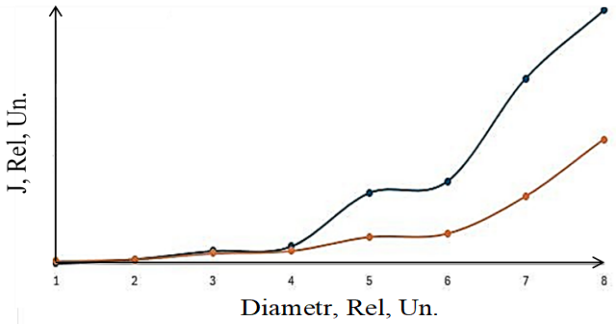


**Fig. 2.** Influence of the charge of model particles in the flow on the dependence of the flow density on the diameter of the track. The lower curve (red) corresponds to a smaller particle charge.

Fig. 3 shows the dependence of the model particle flow on the adsorption center charge. Different curves correspond to different applied voltages. It is evident from figure that at sufficiently low initial voltages, the charge of the adsorption center has a noticeable effect on the main flow. Thus, we conclude that the correlation of different device parameters at once affects the sensor sensitivity.

# II. Desorption from porous materials

An additional method for studying diffusion in track structures is to measure the desorption of various markers from the bulk of the material [8, 9]. The comparison of the desorption cross-sections from different porous materials shows that the desorption of Li or B markers from the tracks proceeds rather slowly as compared with the desorption from the other examined porous materials (thought to be a free volume effect). However, the cross-section values of desorption from tracks of Li and B are roughly the same comparable in size with the cross-

section values of the desorption cross-sections for C and P.

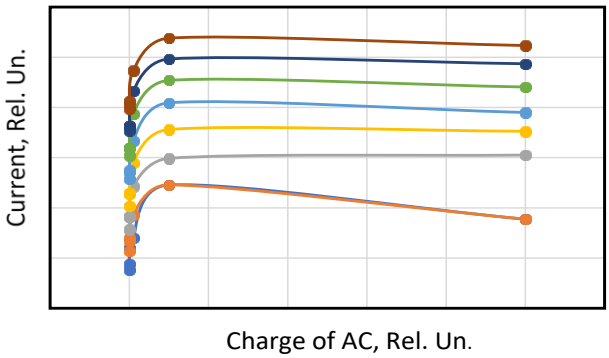


**Fig. 3.** Dependence of current density on the adsorption centers charge.

It was established that the markers are bound much stronger to the polymeric tracks perhaps due to the abundance of radiation-induced trapping centers (radicals, dangling bonds…) to which the markers have considerable affinity. It could, however, also point at a geometrical similarity of desorption from both pore surfaces in C or P on the one hand, and of the free volume elements within the tracks on the other hand. These elements are thought to be very narrow, their dimensions never exceeding the radiation track core diameters which range between typically ~5 and 10 nm. These arguments are applicable also to the two other marker species Li and B in the track desorption case. On the one hand, the amazing similarity of the desorption curves may be the result of both ions suffering from the same geometrical confinement within the radiation track cores. On the other hand, both markers could be bound with similar strength to the tracks, and finally one might recall that coupled diffusion of anions and cations (here: Li and B, respectively) in solvents for maintaining overall charge neutrality leads to comparable mobility within the tracks, hence to comparable desorption curves (Fig. 4).

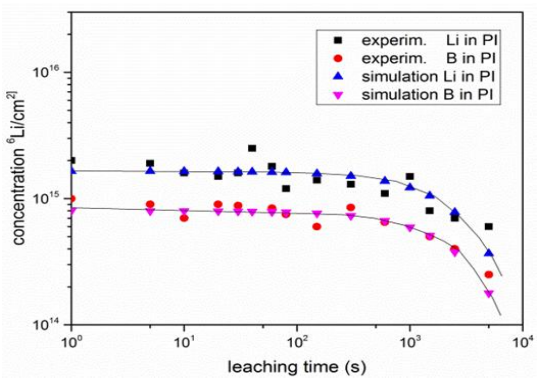


**Fig. 4.** Total Li and B contents in 3.5 GeV Bi-irradiated ion tracks, after leaching the sample in water.

## Conclusion

The study showed that, of all the local centers on the track walls, the adsorption centers have a decisive influence on the passage of the ionic liquid through the track. When creating ion-induced tracks for the biosensor it is important to take into account the correlation of all characteristics of track. The passage of various ions in tracks depends on the conditions under which they are created, namely, the mass and energy of the ions creating the tracks. These factors determine the spectrum of structural defects on the inner surface of the track. Therefore, a thorough study of the characteristics of adsorption sites on the track walls is essential.

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***Fink D.*** – D.Sc. in Physics, Professor;
***Kiv A.E.*** – D.Sc. in Physics and Mathematics, Professor;
***Kavetskyy T.S.*** – PhD in Physics and Mathematics, Associate Professor;
***Dyachok D.O.*** – PhD in Physics and Mathematics, Associate Professor;
***Bondaruk Y.V.*** – PhD student;
***Vinkovskaya A.O.*** – PhD student;
***Hoivanovych N.K.*** – PhD in Biology, Associate Professor;
***Pankiv L.I.*** – PhD in Physics and Mathematics;
***Zubrytska O.V.*** – PhD student;
***Matskiv O.I.*** – PhD student;
***Khromiak U.V.*** – PhD in Engineering;
***Pavlyshak Y.Y.*** – PhD in Biology, Associate Professor;
***Pavlovskyy Y.V.*** – PhD in Physics and Mathematics, Associate Professor;
***Senkiv V.M.*** – PhD in Engineering, Associate Professor;
***Monastyrska S.S.*** – PhD in Biology, Associate Professor.

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Д. Фінк[1,2], А.Ю. Ків[3,4], Т.С. Кавецький[3,5,6], Д.О. Дячок[3], Ю.В. Бондарук[3], А.О. Вінковська[3], Н.К. Гойванович[5], Л.І. Паньків[5], О.В. Зубрицька[5], О.І. Мацьків[5], У.В. Хром'як[7], Я.Я. Павлишак[5], Ю.В. Павловський[5], В.М. Сеньків[5], С.С. Монастирська[5]

# Комп'ютерне моделювання дифузійних властивостей у пористих матеріалах

*[1]Інститут ядерної фізики Чеської академії наук, Ржеж, Чеська Республіка;*
*[2]Державний університет в Мехіко, Мехіко, Мексика;*
*[3]Південноукраїнський національний педагогічний університет імені К.Д. Ушинського, Одеса, Україна, kiv.arnold20@gmail.com;*
*[4]Негевський університет Бен-Гуріона, Беер-Шева, Ізраїль;*
*[5]Дрогобицький державний педагогічний університет імені Івана Франка, Дрогобич, Україна, kavetskyy@yahoo.com;*
*[6]Інститут фізики Словацької академії наук, Братислава, Словаччина;*
*[7]Львівський державний університет безпеки життєдіяльності, Львів, Україна*

Трекові конструкції відносяться до наноматеріалів. Тому при дослідженні таких структур важливо враховувати загальні властивості наноматеріалів. Важливо передбачити структурні особливості треків, конфігурації дефектів на внутрішніх поверхнях треків залежно від характеристик швидких іонів, які їх створюють. За допомогою комп'ютерного експерименту можна досягти результатів, які набагато складніше отримати у звичайному лабораторному досліді. Формування нанотреку з необхідними структурними параметрами залежить не тільки від іонно-стимульованих процесів, а й від інших способів обробки плівки, зокрема хімічного травлення. Комп'ютерне моделювання проходження іонних потоків через нанотреки дозволяє отримати результати, які необхідно враховувати для підвищення якості сучасних біосенсорів. Для вирішення цих проблем розроблено нові алгоритми та комп'ютерні програми.

**Ключові слова:** пористі матеріали, іонно-індуковані нанотреки, трекові структури, комп'ютерне моделювання, біосенсори.