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OPTIMIZATION OF ION TRACK CHARACTERISTICS IN A TRACK BIOSENSOR

Abstract. When constructing a computer model of an ion track in a biosensor, it is important to take into account the main structural features of a real track. As now established, the transition from track to sample volume is not abrupt. In the present work, the three layer structure of the inner walls of the track (including Penumbra) is taken into account. It is shown that the passage of a charged liquid through the track depends significantly on the defect structure of this transition layer. Since the profile of the current density flowing through the liquid track depends on the defective structure of the transition layer in the track, it is important to determine the ion bombardment conditions that provide its optimization. Thus, at the first stage of creating a track structure, it is necessary to solve certain problems of radiation physics of the interaction between fast ions and a thin film. In turn, these characteristics of track structure will determine the sensitivity of the biosensor to the detection of contaminants in a particular environment. It is shown that it is important to take into account the specific influence of each of the three-layer boundary layer on the flow of the “carrier” fluid. Carrier liquid means a “pure” substance into which contaminants should be determined. Studies have shown that the optimization of the functioning of a track biosensor is a multi-parameter task, in which several parameters must be varied simultaneously. Therefore, computer simulation makes it possible to be an effective method for optimizing the parameters of a track biosensor. Further studies should be aimed at finding a correlation between the structural features of Penumbra and biosensor parameters. However, this requires a significant improvement in the algorithms and computer model.

Key words: defect structure of track, sensitivity of track biosensor, computer modelling.

INTRODUCTION

The action of a track biosensor is based on the passage of ion flows (in particular, electrolytes) through cylindrical nanopores. These nanopores (nanotracks) are obtained by ion bombardment of thin dielectric films (for example, polymeric ones). When foreign nano-micro-objects enter the liquid flowing through the nanotracks, the profile of the current flowing through the nanotrack changes, which, in principle, makes it possible to identify biological contaminants in the medium.

The main difficulties in improving the parameters of the track biosensor are due to the fact that the processes of migration and diffusion in nanopores differ significantly from these processes in macro-volumes [1; 2]. Attempts to investigate the features of diffusion in nanopores were made long ago in the 20'th century. It has recently been found [3; 4] that these features are largely due to the fact that in nanopores a significant part of diffusing particles interacts with the inner surfaces of nanopores. It is these interactions that determine the features of the passage of ion flows in nanopores, which can improve the parameters of the track biosensor.

A nanotrack in a track biosensor is modeled as a nanocylinder [5]. The model should reflect the real features of the defect structure of the internal surfaces. The presented models provide for the presence of adsorption and scattering centers [6; 7]. The roughness of the inner surface (RIS) significantly affects the movement of the ion flow in the track. In this work, the model is implemented allowing varying the value of RIS.

Computer simulation of the passage of ion flows through nanocylinder allows one to simultaneously check the influence of various factors on the efficiency of the biosensor: the shape of the nanotrack and its diameter, the defective structure of the inner surface of the ratio of the characteristics of the carrier liquid and biological contaminants.

1. SIMULATION OF A REAL STRUCTURE OF THE ION TRACK

A formation of internal surfaces of tracks in a thin film is accompanied by complex defect formation processes and various diffusion-controlled reactions. Experiments show that the track area consists mainly of 3 parts: the inner part (core), a disordered cylindrical layer (Penumbra) and a slightly deformed surrounding volume in the film (Fig. 1).

1.1. SIMULATION OF AN INTERNAL SURFACE OF THE ION TRACK

The track wall consists of ions with identical characteristics, which we called nodal ions (NI). The charge of NI is half that of the ions of the liquid flowing through the track. The construction of the ion track is as follows:

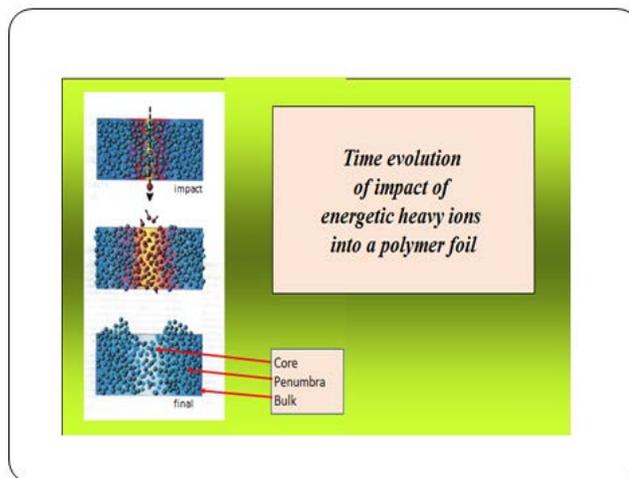


Fig. 1. The real structure of the ion track

1. From the nodal ions, we build the first layer, which is a circle with a diameter equal to the track diameter.
2. Then it's necessary to count the number of layers that we need to build in accordance with the length of the track. We build the required number of layers.
3. The even layers are located relative to the odd ones with an offset of 0,5 of the diameter of the nodal ion, so a dense surface of track (without breaks) is obtained (Fig. 2). Modeling of adsorption centers is described in [3; 8]. Nodal atoms with increased charge are scattering centers.

After the first layer in the nanocylinder wall a layer of Penumbra with a thickness of several nodal ion radii is built (Fig. 1). The closer to the core of the track, the more disordered this layer. This can be achieved by varying the size of the ions that make up the layer. As you move away from the core of the track gradually, Penumbra turns into a normal volume lattice.

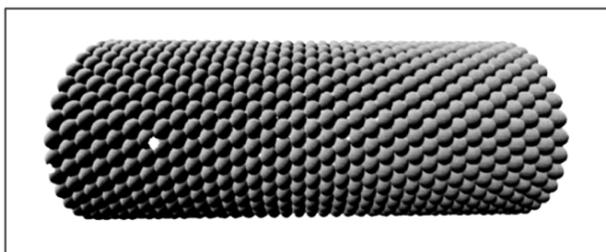


Fig. 2. View of the roughness of the inner surface of the model nanocluster

Thus, the proposed model makes it possible to create conditions for the flow of an ionic liquid through a nanotrack, which reflect the defective structure of the interior of the nanotrack. It should be noted that in some cases it becomes necessary to give the model a conical shape (Fig. 3), which, according to the experimental results, improves the parameters of the biosensor.

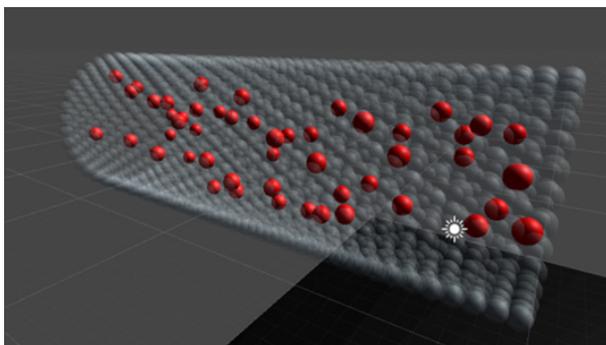


Fig. 3. Conical nanotrack model

It is also important to take into account the specific influence of the three-layer boundary layer (Fig. 1) on the flow of the “carrier” fluid. Carrier liquid (CL) means a “pure” substance into which contaminants (including biological ones) get. During the functioning of the biosensor, there is an influence of Penumbra on the core of the track. There is a certain evolution of this Penumbra and, accordingly, the evolution of the nucleus (Fig. 1). The model should capture and show all these processes: these processes affect the flow of the CL in the track. In the case of a conical track shape, the nature of the influence of Penumbra on the flow of CL through the track changes. Therefore, it is important in the process of computer simulation to find out the possibility of forming such a nucleus and Penumbra that provides an optimal ion current for the track sensitivity. To this end, for different structures of the track walls, we studied the nature of the CL flow through the tracks.

1.2. SIMULATION OF THE ION FLUX THROUGH THE TRACK

Creating an ion flow includes several steps:

1. The track is filled with a certain amount of ions, which provides the required density of the CL. These ions are randomly and evenly distributed along the length of the track. The Random program is used. 2. An array of ions in the CL is given a temperature in accordance with the approach of the molecular dynamics method [9]. All ions in the array are given initial velocities taken from the Maxwell distribution for a specific temperature and using the Random program. The program sets the magnitude and direction of the velocity for each ion. 3. Next, an external force is applied to each ion in the array, which simulates the external applied voltage in the biosensor.

Earlier [6], it was found that the appearance of an extraneous micro-nano-object in the CL is detected in connection with the appearance of negative peaks on the time dependence of the current in the track biosensor. Further studies showed that a change in the current through the tracks when a foreign object enters the CL can also be used when the polluting object is discrete. In this case, a series of peaks appears in the current profile, and their number is proportional to the number of discrete polluting objects (Fig. 4). Modeling of foreign pollution is carried out by changing the basic characteristics (size, mass, charge) of randomly selected ions in the CL.

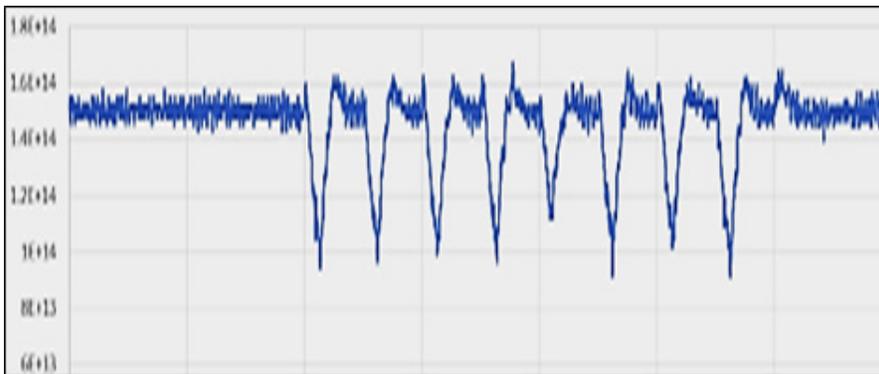


Fig. 4. Negative peaks in the profile of ion current. In general, the number of peaks is proportional to the number of discrete foreign objects in the CL

2. INFLUENCE OF TRACK PARAMETERS ON BIOSENSOR SENSITIVITY

The problem of improving the track biosensor is complicated by the fact that the track characteristics are mutually dependent and difficult to reproduce. For example, adsorption centers significantly affect the sensitivity of the device. However, this effect can be compensated if the exact conditions of penumbra formation are not taken into account when fabricating the track structure. Therefore, model experiments are extremely important. As an example, let us consider the influence of the density of adsorption centers on the sensitivity of a Fig. 5 shows the dependence of the CL current on the concentration of foreign contaminants.

It can be seen that with an increase in the density of adsorption centers (yellow line), their influence on the ion current increases sharply. Current changes caused by the presence of contaminants will also be greater.

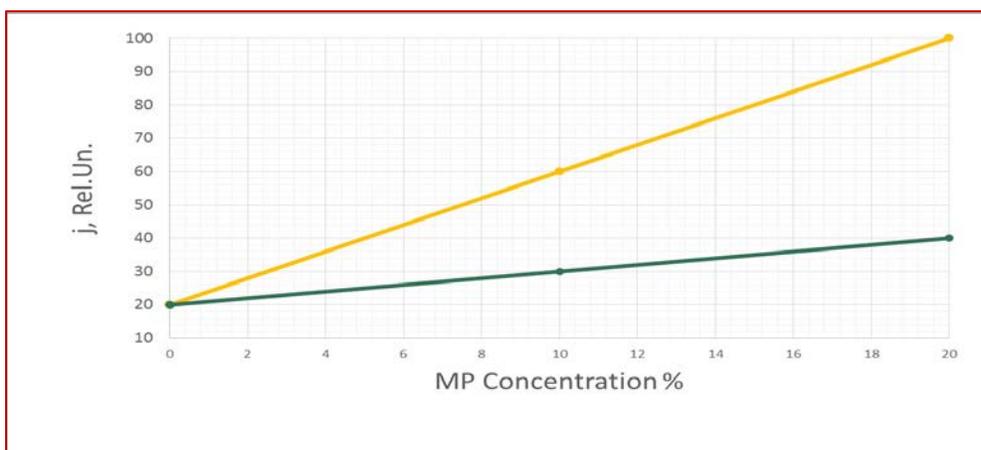


Fig. 5. Dependence of the CL current on the concentration of mixed products (MP). Yellow line corresponds to larger concentration of adsorption centers

DISCUSSION AND CONCLUSION

The article shows that despite the fact that the track biosensor operation scheme is quite simple, the creation of a high-quality device requires optimization of a large number of track structure parameters. The operation of a track biosensor is based on the migration of liquids and gases in nanopores. Migration and diffusion of a substance in nanopores does not proceed in accordance with the usual Fick laws and requires a special study. It has been established that the interaction of a diffusant with the inner surfaces of a nanopore plays a decisive role when considering diffusion in nanopores. To improve the parameters of the track biosensor, the main task is to find ways to control the passage of CL through the tracks. The solution of this problem is connected with the directed creation of local centers on the inner surfaces of tracks and the corresponding defective structure of Penumbra.

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АНОТАЦІЯ

ОПТИМІЗАЦІЯ ТРЕКОВИХ ХАРАКТЕРИСТИК ІОНІВ У ТРЕКОВОМУ БІОСЕНСОРІ

При побудові комп'ютерної моделі іонного треку в біосенсорі важливо враховувати основні структурні особливості реального треку. Як тепер установлено, перехід від треку до об'єму зразка не є різким. У цій роботі враховано тришарову структуру внутрішніх стінок треку (включаючи Penumbra). Показано, що проходження зарядженої рідини через трек істотно залежить від дефектної структури цього перехідного шару. Оскільки профіль густини струму, що протікає через рідинний трек, залежить від дефектної структури перехідного шару у треку, важливо визначити умови іонного бомбардування, які забезпечують його оптимізацію. Таким чином, на першому етапі створення трекової структури необхідно вирішити певні задачі радіаційної фізики взаємодії швидких іонів з тонкою плівкою. У свою чергу, ці характеристики структури треку визначатимуть чутливість біосенсора до виявлення забруднень у конкретному середовищі. Показано, що важливо враховувати специфіку впливу кожного з тришарових пограничних шарів на протіканні «носій» рідина. Рідина-носій означає «чисту» речовину, в якій слід визначати забруднення. Дослідження показали, що оптимізація функціонування трекового біосенсора є багатопараметричною задачею, в якій необхідно змінювати декілька параметрів одночасно. Таким чином, комп'ютерне моделювання дає можливість бути ефективним методом оптимізації параметрів трекового біосенсора. Подальші дослідження мають бути спрямовані на виявлення кореляції між структурними особливостями Penumbra та параметрами біосенсора. Однак це потребує значного вдосконалення алгоритмів і комп'ютерної моделі.

Ключові слова: дефектна структура треку, чутливість трекового біосенсора, комп'ютерне моделювання.