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Simulation of The Passage of Ion Flows Through Nanotracks

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Abstract:- *A computer model of a cylindrical nanopore created using the classical method of molecular dynamics is described. The essential element of the model is the potential wells of the adsorption centers on the internal surface of nanopore, the depth of which is determined by the coefficient in Hooke's law. The model describes well experimental features of the passage of ion flows in real nanotracks in modern biosensors.*

Keywords: cylindrical nanopore, ion flows, biosensors.

INTRODUCTION

Migration of charged particles in nanopores had been studied for a long time [1- 7]. In recent years, interest to the problem has increased significantly in connection with the biomedical needs, in particular, with the creation of novel nanobiosensors [8 – 11]. Some mechanisms of the passage of charged liquids through nanopores (such as etched ion tracks [2]) are proposed in [11 - 13]. The revealed experimental regularities are interpreted also on the basis of theoretical concepts described in [13]. However, important experimental dependences meanwhile have not been explained yet. In this paper the developed computer model for the passage of ion flows through cylindrical nanopores that model etched ion tracks in the modern track biosensors is described. The method of classical molecular dynamics (MD) [14 - 16] was used. This model allowed explaining the observed experimental peculiarities on the basis of fairly simple assumptions.

DESCRIPTION OF THE MODEL AND METHODOLOGY

Model particles (MP), corresponding to moving ions inside a nanopore, are represented by point charges, the interaction of which is described by a screened Coulomb potential. A cylinder of a certain diameter and height limits the space within which the MP can move (Figure 1). The translational motion that is caused by the action of the external field is imposed onto the chaotic motion of MP inside the cylinder. The model provides for the preservation of the density of MP and the continuous process of particles flowing through the tube. This is achieved by adding an appropriate number of particles through the "bottom cover" of the cylinder as they exit through the "top cover". On the internal surface the charges are located that simulate its real structure (ionized atoms, broken bonds etc.). In addition, adsorption centers (AC) are modeled on the inner surface. They are holes through which particles can extend beyond the nanocylinder. At the moment of intersection of the surface by MP, the model provides for the inclusion of the Hook's force ($F = -kx$) which tends to push the ion back into the nanocylinder. The depth of the potential well of AC is determined by the value of Hook's coefficient k. To realize the model, we have implemented an application on the C#.Net code [17 - 18] using the abilities of the powerful graphical engine Unity3d [19]. The program has a graphic interface that contains an image of the chaotic motion of particles inside a cylindrical surface and their translational motion under the action of an external force, two windows with program parameters and the information about the selected particles.

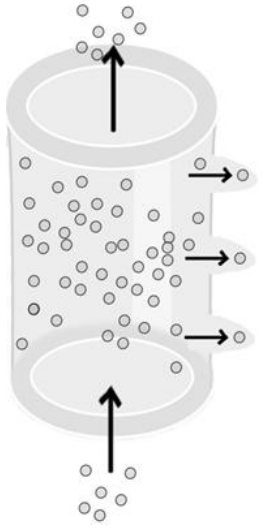

Figure 1. Schematic image of the model; the horizontal arrows indicate the ingression of ions into the potential wells.

The program has two basic sections. The first one is MD that performs all calculations with MP inside the cylindrical surface, and the second one is the above-mentioned Graphics engine that is responsible for rendering the results in real time. As output data, the MD program renders the calculated forces, velocities and coordinates of the MP. By scaling the data, we moved to

higher order values of the calculated quantities. The dimensionless equations were used with parameters of the appropriate order. An optimization algorithm for reducing the number of operators in the program was an important factor that reduced the accumulation of computational errors. As a result, the subtraction error did not exceed 0.1%. In the MD method, the equations of motion for *i*-th particle are [15]:

$$m\frac{d^2\vec{r}_i(t)}{dt^2} = \sum_{i\neq j}^{N-1}\vec{F}(r_{ij}) \qquad (1)$$

$$\vec{F}(r_{ij}) = -\sum\frac{\partial U(\vec{r}_{ij})}{\partial x_i} \qquad (2)$$

where m is the mass of the particle, $\vec{r}_i(t)$ is the radius – vector of i-th particle, r_{ij} is the distance between the particles i and j, $\vec{F}(r_{ij})$ is the force that acts on the i-th particle from the remaining j particles.
The potential energy of the system is:

$$U(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N) = \sum_{i=1}^{N}\sum_{j=1,j>i}^{N}U_{ij}(r_{ij}) \qquad (3)$$

The screened Coulomb potential is U_{ij} = exp (- α r_{ij}) /r_{ij}. The pair interaction approximation between MP was used. In accordance with the Verlet algorithm [15], the position of the particles and their velocities at each time step are determined by the relationships:

$$\vec{r}_i^{\,n} = \vec{r}_i^{\,n-1} + \Delta t\vec{v}_i^{\,n-1} + \frac{(\Delta t)^2}{2m}\vec{F}_i^{\,n-1}$$
$$\vec{v}_i^{\,n} = \vec{v}_i^{\,n-1} + \frac{\Delta t}{2m}(\vec{F}_i^{\,n} + \vec{F}_i^{\,n-1}) \qquad (4)$$
$$\vec{F}_i^{\,n} = -\sum_{j,j\neq i}^{N}\frac{\partial U_{ij}^{n}}{\partial x_i}, \qquad (5)$$

where i is the particle's number, n is the number of the integration step, Δt is the value of the integration step.

Taking into account the external force, F_{ex} (the electric voltage applied to the nanopore) the resulting force acting on the MP is:

$$\vec{F}(r_{ij}) = -\sum\frac{\partial U(\vec{r}_{ij})}{\partial x_i} + Fex \qquad (6)$$

RESULTS AND DISCUSSION

According to our assumptions, several significant factors influence the passage of ionic fluxes through cylindrical nanopores. The first of these is connected with the interaction of charged particles with the internal surface of the nanopores. Depending on the diameter of the cylindrical pore, a different proportion of migrating particles interact with the surface of nanopore. For a sufficiently large diameter, some of the ions can pass through the nanocylinder without interacting with the surface at all. Those particles that interact with the surface during the passage of a cylindrical pore are subject to elastic scattering on the surface and are captured by the AC. Depending on the energy of the adsorption (the depth of the potential wells of AC), the migrating particles spend different times in the adsorbed state, which affects the rate of passage of ions (particle flux) through the nanochannels. When studying this case with our model, the usual exponential dependence of the average ion lifetime in the potential well of AC on the depth of the well is obtained (Figure 2). The simulation showed that the decrease in the ion flux is proportional to the surface density of AC on the inner surface of the nanocylinder (Figure 3).

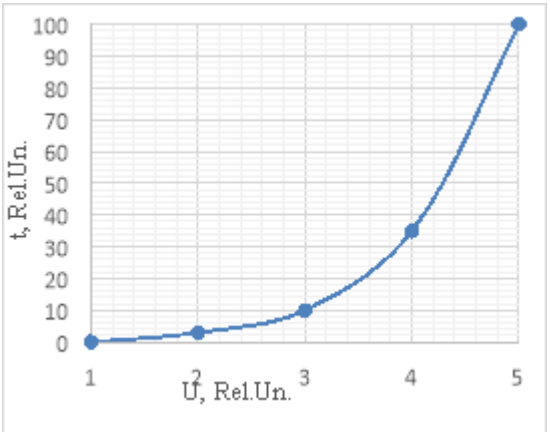

Figure 2. Dependence of the location time of MP in AC on the depth of AC

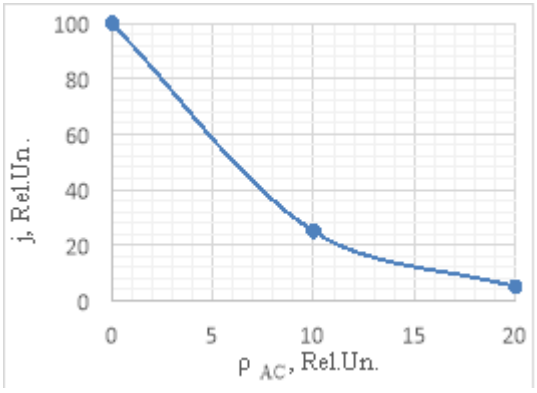

Figure 3. Dependence of the ion current on the surface density of AC

Therefore, it was necessary to find out in the model, how the proportion of particles interacting with the surface depends on the diameter of the nanocylinder. The program can trace the passage of all particles through

the nanocylinder and calculate the fraction of particles from the total flow interacting with the surface of the nanopore (N/N_0). Figure 4 shows the fraction of ions interacting with the surface relative to the total number of ions at a given time, in dependence on the diameter of nanocylinder. It can be seen that with an increase in the diameter of the nanocylinder, the N/N_0 ratio decreases, and with a decrease in the diameter, N/N_0 tends to unity, which means that almost all ions in the last case interact with the surface. Based on Figure 4, we can interpret Figure 5. With decreasing nanocylinder diameter, first a horizontal part of the curve is observed when $N/N_0 \ll 1$. The lower horizontal section of the curve corresponds to the condition $N/N_0 \approx 1$. The decrease in flux between the horizontal sections of the curve corresponds to a gradual increase in the ratio N/N_0.

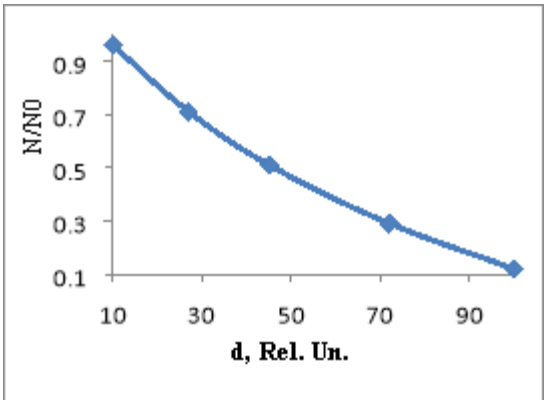

Figure 4. Dependence of the proportion of MP interacting with the surface, on the diameter of the nanocylinder

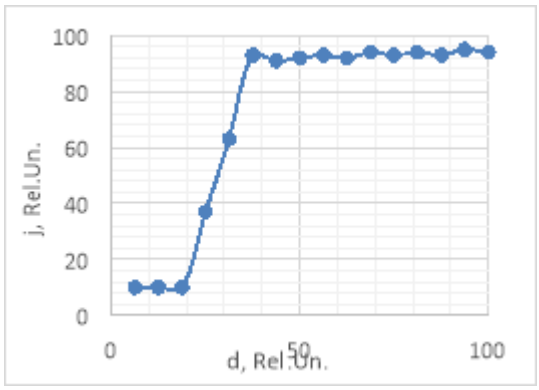

Figure 5. Dependence of the ion current in nanocylinder on its diameter

Figure 5 is similar to Figure 6 (Figure 6 in the experimental work [13]). So the proposed model complements the explanation of the dependence of the sensor current on the radius on sensor tracks given in [13]. Apparently, the N/N_0 relation largely determines the nature of the dependence in Figure 6, although the factors considered in [13] play their role depending on the actual conditions of the creation of the nano-track and the specific film material.

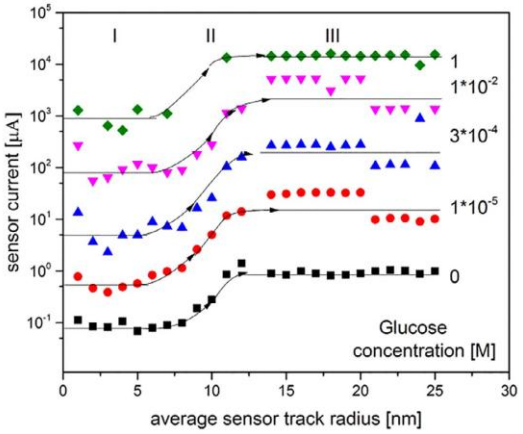

Figure 6. The recorded sensor current as a function of sensor radius, r_{sensor} for different concentrations of glucose [13]

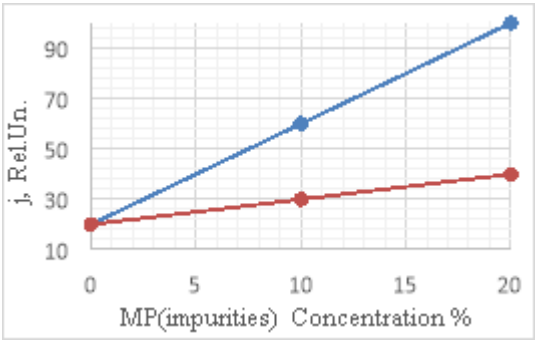

Figure 7. Dependence of the ion current in nanocylinder on the concentration of "impurities". The red line corresponds to a higher density of AC.

The work also demonstrated the possibility of studying the sensoric characteristics of the model. A certain fraction of "impurities" was introduced into the composition of MP. This was achieved by such a way that for some part of the MP in the interaction potential between "impurities" and between "impurities" and the particles of the main flow, the constant screening in the screened Coulomb potential was changed. Then the dependence of the flux of MP on the "impurity" concentration was found. As one can see in Figure 7, there is a direct proportionality between the flux of MP and the concentration of "impurities" , which is important for scaling sensor readings (see for example [16]).

CONCLUSION

Using the classical method of MD, a cylindrical nanopore model was created and the passage of ionic fluxes

through such a pore was simulated. It was found that the important factor determining the magnitude of the ion flux are the density of the adsorption centers on the inner surface of the nanocylinder and its diameter. The magnitude of the ion flux is significantly affected by the density of AC and the binding energy of ions in AC. It is shown how the proposed model can be used to simulate the characteristics of real biosensor, the detection of specific foreign agents in the composition of a given ionic liquid.

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