

## Modeling processes for the protection of bacteria

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### Abstract

Bacteria are a common cause of the disease. The goal was modelling nanostructures for diagnostics of bacteria. They were used biophysical techniques, tracking electronics, computer simulation. As a result of the model received nanobiosensors based tracking technology for fast and accurate identification of bacteria.

*Keywords:* bacteria, protection, modelling processes, biophysical technique, simulation

### 1 Introduction

Infectious diseases are threats to human life. Medical technologies should facilitate the accurate and rapid detection of bacteria to prevent outbreaks of bacterial diseases. It is known that track devices are used to create a number of biological sensors that can identify bacteria [1, 2]. The technology of ion tracks is based on a unique phenomenon - the effect of heavy ions on the substance leads to the formation of narrow and extended regions of radiation damage (with diameters of ~ 5-10 nm, lengths from 30 to 300 microns), which are called tracks. A feature of track membranes, in particular track membranes is the high adsorption of a number of biologically important molecules, including bacteria.

The aim of the study was to study and simulate nanostructures with predetermined properties for bacterial diagnostics.

**Materials and methods of research:** Physical methods of research (working with heavy metal ions using a nuclear gun), biophysical methods (optical methods), biological methods (microscopy) and biochemical methods (spectrometry) were used by standard methods. When creating tracks, standard methods of track electronics were used [2, 3].

The study of multifunctional nanostructures was carried out in NNLOT KazNU named after al-Farabi and in research laboratories of universities. Quanta 3D 200i Multifunction

Scanning Electron Microscope with Integrated Focused Ion Beam, Energy Dispersive Spectrometer and Crystallographic Analysis for the Diagnosis and Investigation of Polymer with Tracks, Microscope LeicaDM6000 M, a motorized digital material science microscope with a separate CTR6000 control unit and a tripod built in a tripod Leica Screen, with halogen illuminators of 100 W and memorization of 2 positions for the study of bacteria.

The method of molecular dynamics was applied, in which the time evolution of a system of interacting atoms or particles is monitored by the integration of their equations of motion. To describe the motion of atoms or particles, classical mechanics was used. In the simulation, the forces of interatomic interaction were represented in the form of classical potential forces (as the gradient of the potential energy of the system). The sets of configurations obtained during the calculations were distributed in accordance with some statistical distribution function, for example, corresponding to a microcanonical distribution [4, 5].

To develop the model, classical molecular dynamics with the Verlet algorithm was used [6]. We used the C#.Net application with the Unity3d graphics engine. The research work was carried out within the framework of the grant of the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan on the topic "Designing and creating nanostructures for the detection of bacteria (NANOBAC) and therapeutic interventions" (No.

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## 2 Results and discussion

One of the main reasons for the high sorption capacity of track membranes, in particular with respect to proteins, is the method of obtaining membranes. When the film was irradiated with accelerated charged particles and subsequent physicochemical treatment on its surface, and especially on the inner surface of the pores, various peroxide compounds and groups possessing an affinity for the electron or proton were formed. The number of such functional groups was large, since an ester group is present in each monomer unit, which is the basis for their formation upon irradiation and physicochemical treatment of the film. They dissociated in neutral and alkaline solutions, which led to the appearance of a "net" of negative charges on the surface of the membrane itself, and especially on the inner surface of the pores. Functional groups were able to form a donor-acceptor bond with the corresponding groups of proteins or enzymes, ensuring their strong bond with the membrane and, accordingly, increasing sorption. Therefore, during the filtration or concentration of various biological media adsorption of biological agents took place. The unique optical, electronic and magnetic properties of track devices were used by us to create nanobiosensors that will be able to detect bacterial infections more accurately and quickly than existing methods. Ionic tracks containing thin polymer films immersed in suitable electrolytes were used by us as substrates for constructing nanobiosensors that use the bioreaction principle  $x + y \rightarrow Z$ , where X is an analyte, the Y and Z agent is the reaction product. This is achieved by using a set (usually 10 6 ... 9 cm) of parallel etched tracks (each of them corresponds to a specific biological agent) in a thin polymer film. Ion-track technology based on the deposition of various materials into channels of track membranes presents ample opportunities for the modification of materials in biomedicine, in micro- or nanotechnologies, and in this connection can become one of the technologies that integrates nanostructural engineering. Prospects for the development of the obtained technology are associated not only with the realization of the possibility of forming ion tracks in various materials, but also with the obtaining of nanostructures of an even smaller diameter in order to study the role of the size factor in various physicochemical and mechanical properties [7]. With the help of ion track technology, a multitude of multilayer nanostructures with alternating layers of parallel nanodiodes can be produced in the substrate substance [8, 9, 10]. Biomass cells associated with patterns on both surfaces of the substrate will be able to maintain certain direct links to each other through the track structures. Molecular mechanisms of cellular adhesion with a substrate are studied using data on their spatial arrangement, joint localization and activation of adhesion receptors and associated structural and signaling proteins, such as paxillin, talin, vinculina and focal adhesion kinases [9, 10]. Such a nanoplatform can be used to identify microorganisms.

The method of molecular dynamics allowed to find instantaneous values of microscopic quantities of the system, such as coordinates and particle velocities. With the help of microscopic quantities, instantaneous values of the macroscopic quantities of the system were computed: energy, total momentum, moment of inertia [5]. We carried out a simulation to check how the developed model will reflect the basic properties of pulsations in the track instrument. A computer experiment showed that with an increase in the absolute value of the external force, the average amplitude of oscillations of model particles increases. However, from time to time the average amplitude of oscillations of model particles increases very sharply (Figure 1). This corresponds to the appearance of current surges in the track instrument (Figure 2). As can be seen from Figures 1 and 2, observed oscillation jumps of model particles correspond to those cases when a sufficiently large number of model particles, as a result of their interaction with each other, move simultaneously at a large distance from their nodal centers, and then return in a short time. The conditions of such a model pulse are determined by the parameters of the interaction potential between model particles, the action of external force and temperature.

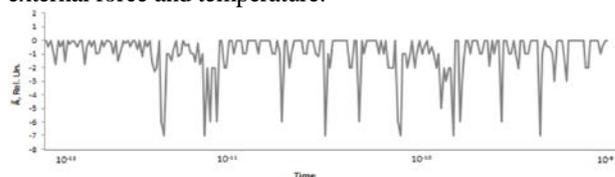


FIGURE 1 Impulses of the model in a computer experiment. On the horizontal axis - computer time in seconds. On the vertical axis - the average amplitude of oscillations of model particles

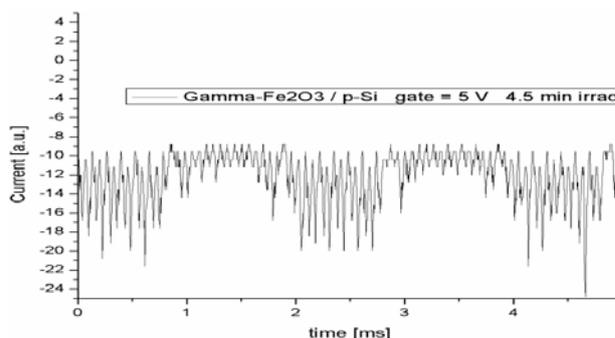


FIGURE 2 Current pulses in a real experiment with a track instrument

When creating the model, we based on the fact that for different forms of tracks (latent, funnel-shaped) and for different materials of films, the basic properties of current pulses remain the same. So there was an idea of creating a generalized phenomenological model. We needed a model that would reflect the basic characteristics of real track instruments.

## 3 Conclusions

Thus, as a result of the work, a model of a nanobiosensor working on the basis of track technology has been developed, which is applicable for rapid and accurate detection of bacteria in biological media.

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