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Computer modeling of ion current pulsations in track-containing foils

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ABSTRACT

A phenomenological model for description of ion current pulsations in track-containing foils is proposed. Such structures belong to artificial porous materials having diverse applications. Typically pulsations of the ion current are observed in experiments in which the track-containing polymer foils are embedded in electrolytes, and AC voltage is applied. The proposed model is designed on the base of classical molecular dynamics. The interacting currents in tracks are simulated by two-dimensional system of oscillating model particles located in the nodes of a plane lattice. In the model external discontinuous forces are introduced to simulate an application of AC voltage. Interaction between model particles is varied to clarify its influence on pulsation effect. It is assumed that the average amplitude of oscillations of model particles is proportional to the average amplitude of current oscillations in real track structure. The model describes adequately the main features of the pulsation effect that were found experimentally. The obtained results can be useful for creation and improvement of sensors and other devices of track electronics.

1. Introduction

Porous materials cause a growing interest due to their unique physical properties and diverse practical applications. Many investigations are devoted to their study, fabrication and modification [1–3]. Recent advances in nanosciences and nanotechnologies have made it possible to precisely control the morphology as well as physical and chemical properties of pores in nanoporous materials that make them attractive in particular for regulating and sensing transport at the molecular level.

A particular importance purchased artificial porous materials (APM). These materials open up wide perspectives to create new electronic devices, to solve biological, medical and technical problems. Numerous results showed that APM can be a basis for new destinations in electronics with promising perspectives and points at the emergence of electronic devices with unique properties [4–8].

Upon impact of swift heavy ion beams onto insulating and semiconducting solids continuous zones of radiation damage (the so-called latent ion tracks [9,10]) remain. Such zones in insulating targets can be etched away giving rise to long straight parallel nanopores. Depending on the etching conditions (temperature, concentration, etching time) the resulting pores have a size between a few tens nm and μm. The tracks filling with any type of conducting matter (metallically conducting, ion-conducting or semiconducting, liquid or solid, homogeneous or in form of dispersed nanoparticles) can be considered as conducting nanowires. In general these nanowires are electronically passive elements which are characterized by a positive resistance and/or diode-like characteristics [11]. According to known results [12–17], the main properties of the ion current through tracks depend on the track shapes, mean diameters, and on the host material.

In polymeric membranes embedded in electrolytes, the etched pore walls usually become charged up due to the breaking of polymeric bonds. This effect, in combination with the longitudinal asymmetric shape of conical tracks leads the result that currents running through electrolyte-filled conical etched tracks are rectified by such structures ("etched track diodes") [11]. Under certain conditions it has been possible to tailor the track structures so that they transmit discontinuous, spike-like currents. They can behave like electronically active elements, being characterized by negative differential resistances [18,19].

The proper design of the irradiated polymer foils allows creating structures which exhibit electronic properties that mimic bioelectronics functionalities, as they resemble somewhat biological membranes which also contain a number of parallel

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electrolyte-filled nanopores. In the case of nanometric diameters such nanopores allow the “ultrafiltration” of viruses from liquids, which is usually not possible with conventional filter [20,21].

If a nanopore is in contact with a solution of weakly soluble salt, ionic concentrations inside the pore can increase above the level dictated by the solubility product of this compound so that precipitates form and effectively plug the pore. This phenomenon has recently been observed in conically shaped polymer nanopores as a voltage-induced drop of the transmembrane current [15,22,23].

The effect of current pulsations when ions pass through the tracks is of particular interest [22,24–27]. In microscopic theories of this effect specific factors, such as a formation of precipitates in the process of ion passing through electrolyte filled tracks, is considered. The precipitates are unstable and their formation followed by dissolution that leads to the ion current fluctuations in time. It is reasonable to assume that collective interactions between tracks in electrolytes lead to specific features of current oscillations, as individual tracks do not show this behavior.

To describe the properties of nanopores (in particular the ion transport in tracks) different models and mathematical methods are used. For example, the current through nanotracks is described by stationary Poisson Nernst Planck equations [28,29]. Molecular dynamics simulation is used in [30,31] to describe the ion current rectification.

In the present work we propose a phenomenological model of ion current pulsations in track-containing foils designed on the base of classical molecular dynamics and show that taking into account *only one factor* (the interaction of currents in the system of tracks) causes the emergence of current spikes.

2. Overview of known experimental results

For ion current pulsations in track-containing foils the following features may be noted [32,33]:

- Spike emission depends on the amplitude and frequency of the applied voltage.

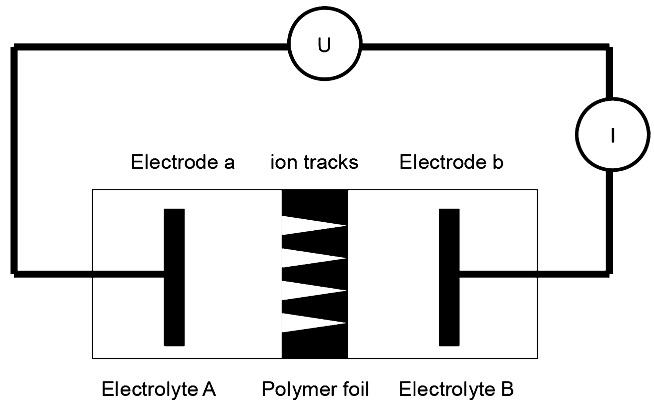

Fig. 1. Principle arrangement of experimental setup to study current spike emission in ion track-containing foils embedded in electrolytes (current/voltage measurements).

- The high ion track density (higher than some threshold density) is necessary to obtain the effect of current spikes.
- Current spikes preferentially occur at pronounced, rather equidistant applied voltages.
- Maximal spike heights do not seem to be affected markedly by the frequency of the applied voltage.
- Current spike spectra are not always reproducible though their principle features remain the same.
- Current spike emission appears to vanish rapidly with frequency of applied voltage decrease which indicates the existence of a threshold frequency for spike emission.

3. The model

The model describes the ion current pulsations in the track-containing polymer foils embedded in electrolyte. A schematic representation of such structure can be seen in Fig. 1. A polymer foil with ion tracks is embedded in electrolyte. In the case of biosensor device different types of electrolytes can be used to

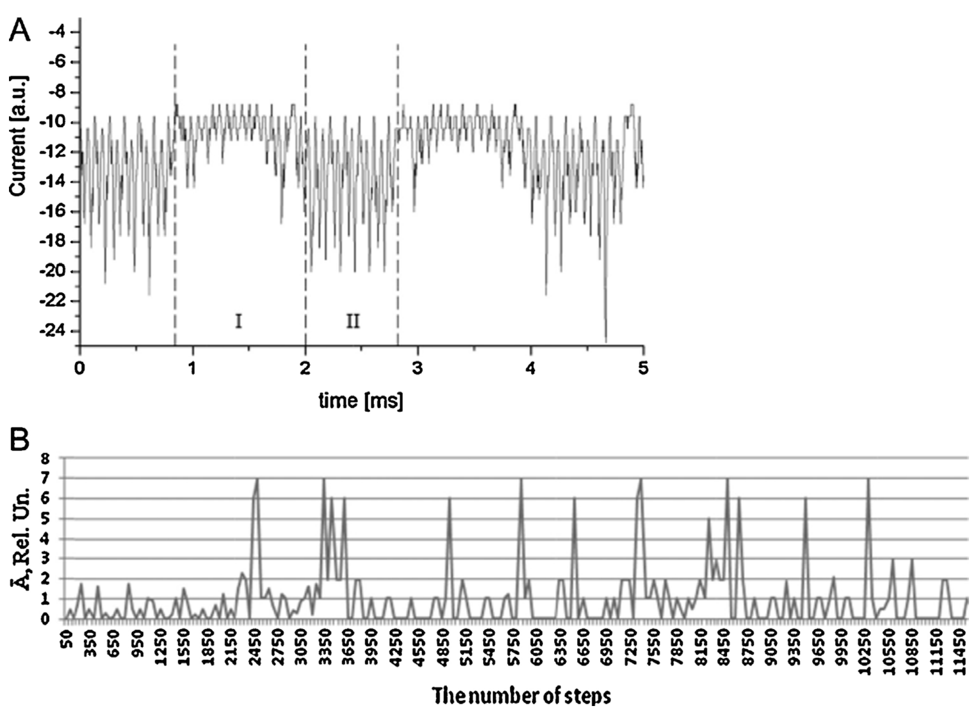

Fig. 2. Current spikes in conditions of real experiment [32]. Region I corresponds to regular oscillations, region II corresponds to current spikes (a). Illustration of model spikes in the model experiment. At the horizontal axis is the average amplitude of MP oscillations (b).