# Generalized model of pulsating track device N Mykytenko<sup>1</sup>, D Fink<sup>2, 3</sup>, A Kiv<sup>1, 2\*</sup>

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## Abstract

A model for description and study of pulsating track-based devices is developed. The track electronics opens up perspectives for solving new scientific and technical problems. The successful solution of these problems requires an elucidation of the mechanisms of the functioning of track-based devices. In this paper, the nature of the pulsating behaviour of electric parameters of track devices is clarified using a specially developed model based on classical Molecular Dynamics. It is demonstrated that the model describes adequately the main features of pulsations in track devices that were established experimentally.

Keywords: track electronics, current pulsations, molecular dynamics

#### **1** Introduction

Nowadays nanotechnologies develop into various directions and nanostructures have numerous application scopes. Among the new areas of nanoelectronics, which have recently been widely developed, there is also the ion track electronics. It refers to new directions with promising perspectives and points at the emergence of electronic devices with unique properties not previously known in traditional electronics. This may open new possibilities of solving problems in the electronics industry [1-4]. In particular, track devices are used for creation of novel biological sensors, which can identify many biological objects [5-8]. Figure 1 shows the principle setup to the corresponding experimental arrangements.



FIGURE 1 Principle arrangement of experimental setup to study current spike emission from ion track-containing foils embedded in electrolytes via current/voltage measurements

Track devices are complex systems with a set of parameters that depend on the sizes and shapes of tracks,

their density, electronic structure of the inner surface of tracks, on the features of the film surface and so on. In experimental works of both S. Ziwy et al. and D. Fink et al. the effect of current spikes was found and studied for ions passing through electrolyte-filled individual etched [9] and multiple thin latent [10] and etched [11] ion tracks in polymers and other materials [12]. Later this effect was studied in a much more regular and controlled way than ever before [13]. In [14] a model of the pulsating track devices was proposed based on ideas of the theory of neural networks.

The operation of the track-device is determined by many microscopic processes, the simultaneous description of which is a difficult task. Therefore, a phenomenological description of such devices is an important stage in the clarification of the main principles of their functioning. In this paper, we report the results of creation and study of generalized phenomenological model of pulsating track device.

#### 2 The model

A physical model not necessarily has a superficial resemblance to a real object, which has to be studied. A model should reflect the basic properties of the real object and the features of its behaviour. In the present paper, we envisage to investigate the pulsating behaviour of electrical parameters of track-based devices. In the case of pulsating track, devices the following main features are observed [13, 14]:

 Spikes emitted from latent or funnel-type tracks in polymers embedded in suitable electrolytes often show another peculiarity, which was hitherto

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unknown. Between both track types, a principle difference as concerns the spike emission does not exist.

- The spike emission depends on the amplitude and frequency of the applied voltage.
- The maximum spike heights do not seem to be affected markedly by the frequency of the applied voltage.
- The high ion track density is necessary to obtain the effect of spikes. This is caused by some specific interaction between tracks, mechanism of which has to be clarified.
- The spikes preferentially occur at pronounced, rather equidistant voltages.
- The spike spectra are not always reproducible though their principle features remain the same.
- With frequency decrease spike emission appears to vanish rapidly which indicates the existence of a threshold frequency for spike emission.

To develop a model we used a classical Molecular Dynamics (MD) with a Verlet algorithm [15, 16]. The model is a 3D space lattice, each node of which corresponds to an individual track in the track device, Figure 2.



FIGURE 2 Correspondence between individual track and MP

The density of nodes is proportional to the density of tracks. Each node is a potential well, in which one or more so called model particles (MP) can be placed. Thus,

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in fact the model resembles a regular crystal lattice. Because the geometry of the model lattice is irrelevant, we use a simple cubic geometry. The lattice has a temperature, which is introduced in accordance with a conventional MD method [17]. The particles oscillate in the lattice nodes according to the introduced temperature. We suggest that the current value in the track device is proportional to the average amplitude of the oscillations of MP. The application of a sinusoidal voltage is modelled by the action of external forces (EF) introduced in the model, which at certain time intervals "nudge" the particles in the nodes. The directions of the action of EF are determined by the random function. We can vary the value and the frequency of the EF action, thus simulating the change of the applied voltage. The interaction of particles in the nodes is described by a potential of the most general form (Lenard-Jones) [18, 19].

The potential parameters, the particles mass and temperature are chosen so as to make the model stable and allow carrying out a computer experiment.

We performed a computer experiment to check how the developed model reflects the main properties of pulsations in the track device. In computer experiment, it has been seen that with the increase of the absolute value of EF the average amplitude of MP oscillations increases. However, from time to time the mean amplitude of MP oscillations increases dramatically, Figure 3. This situation corresponds to the occurrence of the current spike in the track device, Figure 4. Visualization of the situation in Figures 3a,b shows that the observed MP oscillations spikes correspond to the cases when sufficient amounts of MP move simultaneously for a large distance from their nodes as a result of their interaction and return back after a short time. The conditions of such "model spike" are determined by the parameters of the interaction potential between MP, the action of EF and the temperature of MP. The temperature of the MP describes the fluctuating nature of the excited states of the MP. Below in Table 1 the correspondence between the model characteristics and the characteristics of the real track devices is shown.



FIGURE 3a Illustration of model spikes in the model experiment. At the vertical axis is the average amplitude of MP oscillations. At the horizontal axis is the computer time in seconds



FIGURE 3b Current spikes in conditions of real experiment with track device [12]

TABLE 1 Correspondence between the model characteristics and the characteristics of the real track device

Device characteristics	Model characteristics
Average spike height	Average amplitude of MP oscillations
Value of applied voltage	Value of EF
Frequency of applied voltage	Frequency of EF action
Time interval between current spikes	Time interval between MP oscillations spikes
Areal density of tracks	Spatial density of nodes

To realize the model we have implemented an application on C# .Net [20, 21] using abilities of powerful graphical engine Unity3d [22]. The program has a graphic interface that contains in the screen modelling lattice elements, two windows with program parameters and the information about the selected particles.

The program has two basic classes. The first one is MD that performs all calculations with MP located in the nodes and interacting by Lenard-Jones potential, and the second one is the Graphics that is responsible for rendering the results in real time. As the output data, MD program calculates forces, velocities and coordinates of MP. By scaling the data, we moved to higher order values of 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 [4].

#### **3** Results and discussion

Creating the model, we proceeded from the fact that in the cases of different forms of tracks (latent or funneltype tracks) and different materials of films the main features of current spikes are the same. Thus, the idea of creating a phenomenological generalized model arose. It was necessary to create a model that would reflect the main features of the real track device. Computer experiment with the developed model led to the results shown in Figures 3a, 4a, 5a, 6 and 7. The corresponding experimental results are presented in Figure 3b, 4b and 5b.



FIGURE 4a Dependence of the average amplitude,  $\bar{A}$  of MP oscillations on the value of EF.

In Figure 3a we see that the model provides a good qualitative picture of current peaks observed in the real

track device (Figure 3b). The dependence of the average amplitude  $\overline{A}$  of MP oscillations on the value of EF is displayed in Figure 4a. This dependence is in good agreement with the dependence of the average spike height on the value of applied voltage (Figure 4b).



FIGURE 4b Dependence of the average spike height on the value of the applied voltage [13].

In Figure 5a the dependence of the average amplitude  $\bar{A}$  of MP oscillations on the frequency of EF is shown.



FIGURE 5a Dependence of the average amplitude,  $\bar{A}$  of MP oscillations on the frequency of EF.

The corresponding dependence of the average spike height on the frequency of applied voltage is presented in Figure 5b.



FIGURE 5b. Dependence on the average spike height on the frequency of applied voltage. Points: measurements, line: drawn to guide the eye [13].

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We explain the dependence in the Figure 5b by a "memory effect" which manifests itself in the mechanism of spikes formation: each next spike "remembers" the information about previous spikes. As a result of this effect according to the model there is some optimum frequency of the external exciting factor that provides a maximum average spike height. In the case of our model it means that at higher frequencies of the EF action the model lattice is too disordered after the previous spikes, and the conditions for the synchronization of individual spikes are not favourable. On the other hand, at too low frequencies the model lattice is completely restored after the previous spikes ("forget about the previous spikes"), and thus it hinders the formation of new integrated spike. By the way, the "memory effect" can explain the experimental showing the results that spikes preferentially occur at pronounced, rather equidistant voltages. Preparation of each subsequent spike depends on the system state after the previous spikes, which may be different. The "memory effect" can be also a reason of the fact that the spike spectra are not always reproducible. The influence of previous spikes on the next spike is not the same. The computer experiment with our model shows that the dependence of the maximum value of spike height on the frequency of EF is weak, Figure 6.



FIGURE 6 Dependence of the maximum value,  $A_{max}$  of spike height on the frequency of EF.

We revealed that this dependence is determined by the potential of MP interaction. At the same potential, the maximum value of spike height changes weakly. However, for other potentials this maximum value is already different. It means that that for different types of tracks or different materials we can expect different maximum values of spike height.

Figure 7 explains the necessity of a sufficiently large density of MP (and accordingly tracks) to obtain the spike effect. The dependence in this Figure is strong enough. At too small densities of MP the mean time distance between spikes becomes so large that we simply do not see them any longer.



FIGURE 7 Dependence of the mean time interval,  $\Delta$ S between spikes on the density of MP.

#### 4 Conclusions

A computer experiment with the developed model of the pulsating track device showed that the model reflects the main features of the behaviour of such devices. The important result is that the behaviour of the model "device" essentially depends on the potential of MP interaction. The experimental results show that for different types of track-based devices the pulsating effect is determined significantly by the mean distance between tracks (the areal density). We also proceeded from the experimental fact that there are common properties of pulsating track-based devices independent on the materials and physical characteristics of tracks. As a result, the developed model reveals all main features of the real pulsating track devices.

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