



E-ISSN: 2708-454X  
P-ISSN: 2708-4531  
IJRCDS 2022; 3(1): 01-04  
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[www.circuitsjournal.com](http://www.circuitsjournal.com)  
Received: 16-10-2021  
Accepted: 02-12-2021

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## Macroscopic modeling of processes in ferroelectric crystals

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DOI: <https://doi.org/10.22271/27084531.2022.v3.i1a.17>

### Abstract

A general approach to modeling the components of radio electronic equipment based on modern materials of functional microelectronics, in particular, ferroelectric crystals, is considered. A model of a ferroelectric capacitor is presented as a nonlinear inertial element of an electric circuit. The correspondence of the theory to the experimental results is shown.

**Keywords:** Macroscopic modeling, ferroelectric crystals, electric circuit

### Introduction

**Formulation of the problem:** In connection with the ever-increasing requirements for modern radio-electronic equipment, the issue of transition to a modern element base, on the basis of which this equipment is designed, acquires special relevance.

Solving the problem of microminiaturization and improving the technical and economic indicators of radio electronic equipment with a simultaneous expansion of its functionality largely depends on the widespread use in the development of methods and devices of microelectronics.

Great success has been achieved in the creation of integrated circuits, the main elements of which are made in the form of semiconductor structures with different properties. However, the further development of such circuits has a theoretical limit due to the design complexity, reduced reliability, and power consumption.

The problem of overcoming these limitations was the reason for the use of various in nature physical phenomena occurring in artificial and natural environments to create devices, the functions of which are usually implemented using a complex multi-element circuit.

**Characteristics of the investigated element:** The use in engineering practice of properties and phenomena in a solid and, first of all, properties that manifest themselves in the process of converting various types of energy, opens up wide opportunities for creating new devices. In particular, devices and elements based on all kinds of ferroelectrics have recently found wide application; for example, barium titanate ( $\text{BaTiO}_3$ ), triglycine sulfate or lead titanate zirconate. In the general case, a ferroelectric is a nonlinear inertial element. Its nonlinearity is due to the nonlinear nature of the polarization curve, and its inertia is due to the time lag of the induction of the electric field  $D$  from the strength  $E$ .

In the study of these systems, two approaches are possible - microscopic, based on model concepts of the structure of matter, and macroscopic (phenomenological), which describes the phenomena in the most general form, establishing the basic laws of the phenomenon without using model concepts of the structure of matter. It is in this last circumstance that the main merit of phenomenological theories, their general character.

In this work, a generalized approach to the analysis of components and structures based on ferroelectric crystals and films as elements of electrical circuits is briefly outlined.

**Mathematical model of the investigated element:** The main goal of the study is to determine a model (in the general case) of a ferroelectric capacitor, which allows calculating its characteristics as a four-pole. The basic requirements for a mathematical model include the simplicity of expressions, the minimum number of experimentally determined parameters and the accuracy and simplicity of the mathematical apparatus used to solve this model sufficient for practical purposes and tasks.

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When compiling the model, the method of modeling functional elements proposed in the work / 1 / was used. According to this method, all electronic devices, regardless of the type of their internal structure and the complexity of the phenomena that determine the principle of their functioning, are considered from a unified point of view in the sense that the nature of the use of these devices depends on the performance of certain functions by them at the inputs accessible from the outside.

A one-dimensional model of charge transfer  $q$  in a nonlinear inertial system in the form of a balance equation has the form:

$$\frac{dq(t)}{dt} + \frac{1}{\tau_r(q)} q(t - \tau_0(q)) = \sum_{k=1}^n \sigma_k(q) u_k(t), \quad (1)$$

where  $q = \int_V \rho_{av} d\xi$ ,  $\rho_{av}$  — average charge density  $\rho_{av} = 1/V \int_V \rho d\xi$ ;  $\tau_r$  — charge relaxation time;  $\tau_0 = l/V$  — charge transfer time;  $l$  — span length;  $V$  — the drift speed;  $\sigma_k$  — the instantaneous value of the input conductivity of the investigated element;  $u_k$  — the input voltage;  $n$  — the number of inputs.

In form, the equation of the proposed model is a nonlinear homogeneous differential equation of the first order with a deviating argument. The solution of this equation in the above form is possible only by numerical methods. To obtain an analytical solution (in the linear approximation), it is necessary to use various types of asymptotic solutions and their approximations.

We use the approximation  $\tau_r = \text{const}$  and  $\tau_0 = \text{const}$ . The latter is valid for sufficient values of the bias voltage  $U_0$  determining the field at which the charge drift velocity reaches the saturation value, i.e.,  $V = \text{const}$ .

In this case, the nonlinearity will be concentrated in the dependence  $\sigma(q)$  and the model equation will take the form

$$\frac{dq(t)}{dt} + \frac{1}{\tau_r} q(t - \tau_0) = \sum_{k=1}^n \sigma_k(q) u_k(t) \quad (2)$$

Equation (2) can be analytically solved using the small parameter method [4]. In this case, the parameter  $\varepsilon$  is introduced into the equation and the expansion in terms of the parameter  $q$  and  $\sigma(q)$  is performed. If the parameter  $\varepsilon$  is introduced into the equation and for  $n = 1$ , the equation takes the form

$$\frac{dq(t)}{dt} + \frac{1}{\tau_r} q(t - \tau_0) = \sigma(q)(U_0 + \varepsilon U(t)) \quad (3)$$

We will seek a solution to (2.5) in the form  $q = q(t, \varepsilon)$

$$q = q(t, \varepsilon) = \sum_k q_k(t) \varepsilon^k \quad (4)$$

Upon satisfaction of the condition

$$q|_{t=0} = q(t, \varepsilon)|_{t=0} = q_0 \quad (5)$$

Suppose that in a neighborhood of the point  $q_0$   $\sigma(q)$  can be expanded in a Taylor series

$$\sigma(q) = \sum_n \frac{\sigma^{(n)}(q_0)}{n!} (q - q_0)^n \quad (6)$$

In turn

$$\frac{dq}{dt} = \sum_k \frac{dq_k}{dt} \varepsilon^k \quad (7)$$

Substituting (4), (6), and (7) into (3), we obtain

$$\sum_k \left( \frac{dq_k(t)}{dt} + \frac{1}{\tau_r} q_k(t - \tau_0) \right) \varepsilon^k = (U_0 + \varepsilon U(t)) \sum_n \frac{\sigma^{(n)}(q_0)}{n!} \left( \sum_k q_k(t) \varepsilon^k \right)^n \quad (8)$$

As a result of solving (8), we obtain a system of linear differential equations.

Let us select from (8) the equation of the first approximation:

$$\frac{dq_1(t)}{dt} + \frac{1}{\tau_r} q_1(t - \tau_0) - \frac{1}{\tau_r} \left. \frac{d\sigma_i}{di} \right|_{I_0} U_0 q_1(t) = \sigma_0 U_m \sin(\omega t) \tag{9}$$

Taking into account external influence, type  $u(t) = U_0 + U_m(t)$ , select from (8) the equation of the second approximation:

$$\frac{dq_2(t)}{dt} + \frac{1}{\tau_r} q_2(t - \tau_0) - \frac{d\sigma}{dq} \Big|_{q_0} U_0 q_2(t) - \frac{1}{2} \frac{d^2\sigma}{dq^2} \Big|_{q_0} U_0 q_1^2(t) = \frac{d\sigma}{dq} \Big|_{q_0} q_1(t) U_m \sin(\omega t) \tag{10}$$

Analytical equations of higher degrees of approximation are even more cumbersome expressions.

When describing the dynamic characteristics of myocardial fiber, equation (1) allows one to determine only one component of the total current - the conduction current  $i_n = \sigma(q)[U_0 + U(t)]$ .

The second component is the displacement current, which is set by the type of nonlinear capacitance of the ferroelectric:  $i_C = C(q_C) \cdot (dU(t)/dt)$ .

The ferroelectric is characterized by the ambiguity of dependence  $\sigma(q)$ , that in the presence of a delay  $\tau_0$  leads to relaxation oscillations in the regime of a given displacement  $U_0(I_0)$ .

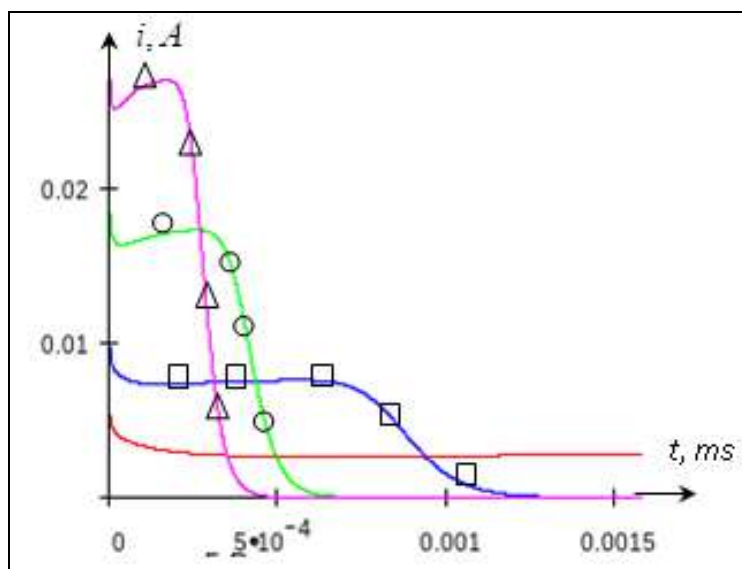
We propose an analysis of the relaxation oscillations, given according to the model described above.

Given the ambiguity of the addition  $\sigma(q)$  and assuming  $\tau_0 = \text{const}$ , we represent the model as:

$$\begin{cases} \frac{dq(t)}{dt} + \frac{1}{\tau_r(q)} q(t - \tau_0) = \sigma U_0 \\ G(q, \sigma) = 0 \end{cases} \tag{11}$$

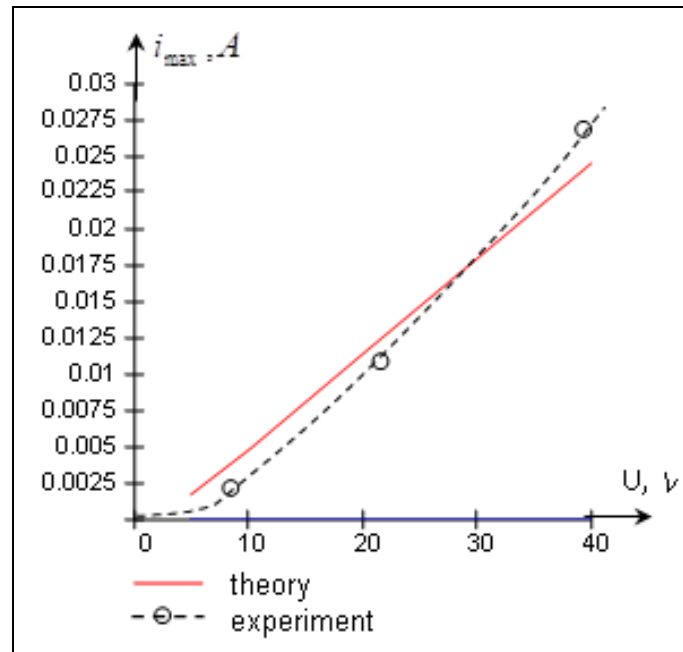
**Results:** The model is analyzed numerically. Addition  $\tau_r(q)$  was given in the form  $\tau_r(q) = \frac{\tau_{r0}}{1 + (q/q_0)^4}$ .

Solving the equation of the model by the Runge-Kutta method of the 4th order, we find under the input action the form of the Heaviside function  $u(t) = U \cdot 1(t)$ , where  $U$  is the signal amplitude, the displacement current (Fig. 1).



**Fig 1:** Output current pulses at input amplitudes of 5V(□), 10V(○), 20V(Δ) and 30V(·).

Figure 2 shows the maximum bias current versus input voltage.



**Fig 2:** Dependence of the maximum amplitudes of the output signals on the input voltage.

### Conclusions

It can be seen from the results of the studies that the form of relaxation oscillations obtained by the proposed model is in qualitative agreement with the experimental results.

Thus, the use of the proposed model of charge transfer allows one to obtain important dynamic characteristics of the element under study by simple methods, while ensuring the adequacy of the results of experimental studies.

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