**NUMERICAL SIMULATION OF HYSTERESIS IN FERROELECTRIC MATERIALS USING THE JILES-ATHERTON METHOD**

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Ferroelectrics, crystalline dielectrics that have spontaneous polarization in a certain temperature range, which changes significantly under the influence of external impact. Electrical properties are in many ways similar to the magnetic properties of ferromagnets (hence the name ferroelectrics, accepted in foreign literature). Among the most studied and used in practice are barium titanate, Rochelle salt (which gave the name to the entire group of crystals), triglycine sulfate, and so on [1; 2].

The relevance of this topic is aimed at creating a tool that will allow a more profound and accurate analysis of the electrophysical properties of ferroelectric materials, which is important for their application in various technological areas, such as memory devices, sensors and actuators. The unique properties of ferroelectrics allow the development of more efficient and reliable systems, which is especially important in the context of rapid technological progress and growing requirements for the functionality and durability of materials.

The purpose of the work is to carry out a software implementation of numerical modeling of ferroelectric hysteresis using the Jiles-Atherton theory.

**Material and methods.** The material of the study is ferroelectrics, as well as the main electrophysical properties of ferroelectric materials. The work is based on analytical and experimental research methods, as well as numerical modeling, which is a software implementation for analyzing ferroelectric hysteresis in order to study its properties and behavior.

**Results and their discussion.** Currently, there are a number of problems associated with the modeling of ferroelectrics, including difficulties in describing nonlinear dynamic processes such as hysteresis, as well as in determining phenomenological parameters that require calibration.

Let us consider the theory of the Jiles-Atherton (*JA*) model for modeling the dependence of polarization on the electric field strength of ferroelectrics. The Jiles-Atherton model is traditionally used to describe magnetic materials. An adapted version of constructing a hysteresis loop model for an inhomogeneous ferroelectric, such as barium titanate ($BaTiO_3$), is a more complex task than for magnetic materials, since it is necessary to take into account the features of ferroelectric behavior, such as the nonlinear relationship between polarization and electric field [3].

The basic idea of the Jiles-Atherton model is that the total polarization $P$ of a ferroelectric is considered as the sum of three components:

- hysteresis-free polarization $P_{an}$;
- reversible (reversible) polarization $P_{rev}$;
- irreversible (non-reversible) polarization $P_{irr}$.

The polarization $P$ of a ferroelectric located in an external electric field with strength E depends on the magnitude of the equivalent internal field $E_e$, equal to (see formula 1):

$$E_e = E + \alpha P, \quad (1)$$

where $\alpha$ is a coefficient that takes into account the effect of the interaction of the external electric field with the internal one created by the polarization of the material $P$.

The magnitude of the anhysteresis-free polarization $P_{an}$ is written as a function (see equation 2):

$$P_{an} = P_s \cdot f\left(E_e\right), \quad (2)$$

where $P_s$ is the saturation polarization, and $f(E_e)$ is some function equal to zero when $Ee$=0 and to one when $E_e$ tends to infinity. In this model, $f(E_e)$ is often chosen as the hyperbolic tangent (see equation 3):

$$f\left(E_e\right) = \tanh\left(\frac{E_e}{a}\right), \quad (3)$$

where $a$ is a parameter that determines the shape of the polarization curve.

For reversible and irreversible polarization we can write (see equations 4 and 5):

$$P_{rev} = c \cdot \left( P_{an} - P_{irr} \right) \tag{4}$$

$$P = P_{irr} + P_{rev} \tag{5}$$

The differential equation for irreversible polarization (see equation 6):

$$\frac{dP_{irr}}{dE} = \frac{1}{k \cdot (1-c)} \left[ \frac{dP_{an}}{dE} - k \cdot \left| \frac{dP_{irr}}{dE} \right| \cdot \left( P_{an} - P_{irr} \right) \right], \tag{6}$$

where k is a coefficient related to the coercive force.

The differential equation for polarization can be written in the following form (see equation 7):

$$\frac{dP}{dE} = \frac{\alpha}{A} \left( E - \frac{P}{\chi} \right) + \beta, \tag{7}$$

where $E$ is the external electric field, $P$ – polarization, $\alpha$, $\beta$ – model parameters, $\chi$ – dielectric susceptibility, $A$ – coercive voltage.

The advantages of using the Jiles-Atherton model include:

- accuracy: the model allows accurate prediction of the behavior of ferroelectrics under various conditions;
- flexibility: the model can be adapted to different types of materials and conditions;
- numerical methods: the use of efficient numerical methods, such as the Runge-Kutta method, to solve complex differential equations [4].

However, despite its advantages, the Jiles-Atherton model has some limitations. For example, the accuracy of the model depends heavily on the correct choice of the parameters $\alpha$, $P_s$, $a$, $c$, and $k$. In addition, the model can be complicated by adding additional physical effects, such as temperature dependence or the influence of mechanical stresses.

**Conclusion.** As a result of the conducted study, the method of numerical modeling of hysteresis for ferroelectric materials was thoroughly investigated, analyzed and tested using the adapted theoretical Jiles-Atherton model. It was found that the Jiles-Atherton model is a powerful tool for modeling and analyzing complex hysteresis phenomena in ferroelectric materials. The main components of the model include anhysteresis-free polarization $P_{an}$, reversible polarization $P_{rev}$, and irreversible polarization $P_{irr}$. These components allow more accurate description of the behavior of material polarization under conditions of an alternating external electric field [5].

If we analyze the results of the obtained model, we can draw some conclusions:

1) for more accurate modeling of hysteresis, it is recommended to carefully check and refine the implementation of the Jiles-Atherton model, including all the necessary nonlinear dependencies;

2) conduct a more detailed analysis of the model parameters, possibly using optimization methods to find suitable values;

3) increase the number of cycles and the amplitude of the electric field change for a more obvious manifestation of hysteresis effects;

4) conduct testing of the numerical method, varying the integration step and other parameters to ensure the accuracy and stability of the solution.

5) It should be noted that the Jiles-Atherton model opens up opportunities for further research and development in the field of modeling and analysis of complex hysteresis phenomena in ferroelectric materials.

1. Characteristics of some ferroelectrics. – URL: https://www.booksite.ru/fulltext/1/001/008/100/712.htm – (date of access: 05.11.2024).

2. Phase transitions in ferroelectrics with distributed polarization caused by a regular change in composition: Agreement with BRFFR No. F08R-110 dated April 1. 2008: research report (conclusion) / scientific. hands V. N. Shut; [performed by: V. N. Shut, I. F. Kashevich, S. E. Mozzharov, Yu. A. Shienok]; Ministry of Education of the Republic of Belarus, VSU named after P.M. Masherov. – Vitebsk, 2010. – 46 p – URL: https://rep.vsu.by/handle/123456789/24873 – (date of access: 05.11.2024).

3. Method for correcting the shape of the magnetization curve in the Jiles-Atherton model of a ferromagnetic core. – URL: http://sgma.alpha-design.ru/MMORPH/N-40-html/katkova/katkova.htm (date of access: 05.11.2024).

4. Runge-Kutta 4th Order Method to Solve Differential Equation. – URL: https://www.geeksforgeeks.org/runge-kutta-4th-order-method-solve-differential-equation/ (date of access: 05.11.2024).

5. Simplification of the Jiles-Atherton model for simulating soft magnetic materials in Spice simulators. – URL: https://valvolodin.narod.ru/articles/simple_model_JA.pdf (date of access: 05.11.2024).