THE RESEARCH PROCESS OF ACTIVE DIELECTRICS: SYSTEM INTERCONNECTIONS

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Abstract: *Ferroelectric thin films are widely used in devices of micro- and nanoelectronics. In particular, their unique properties (high values of relative permittivity, hysteresis loop, close to rectangular) are connected with the presence of a phase transition leading to a change of the functional dependencies form between the material parameters at temperatures below and above the phase transition temperature. Depending on the purposes of materials research consisting in the analysis of their properties or the materials synthesis with specified characteristics, two tasks can be solved: materials analysis ; controlled synthesis of a material with specified properties.The authors considered the generalized structure of the study process of ferroelectric materials; the interconnection of the parameters of active dielectrics was analyzed. It made it possible to optimize the process of studying the materials used in elements of functional electronics.*

Keywords: ACTIVE DIELECTRIC, PROPERTIES RESEARCH, FUNCTIONAL ELECTRONICS

Ferroelectric thin films find wide application in devices of micro- and nanoelectronics. In particular, their unique properties (high values of relative permittivity, hysteresis loop, close to rectangular) are connected with the presence of a phase transition, leading to changes in functional dependencies between the parameters of the material at temperature below and above the phase transition temperature. Depending on the purposes of materials research consisting in the analysis of their properties or the materials synthesis with specified characteristics, two tasks can be solved:

a) the task of analysis of materials with specific properties, subject to experimental determination. A special case of the problem is the study of a variety of materials to select those properties which have desirable quantitative characteristics;

b) the task of synthesis of materials with the specific properties. The peculiarity of this task is the need to not only measure material properties, but also study ways of their correction under the influence of influencing factors. In turn, the allocation of these tasks leads to the distinction of morphological structures, that is, the relationship of the individual components within the subsystems, at the same time some relations are common in the solution of both objectives, which can be shown using the so-called "tree of problems," used in research organizations structuring [1].

The generalized structure of study process of ferroelectric materials in the solution of the problem of synthesis of materials with specified properties is shown in detail in this article (Fig. 1).

Fig. 1 shows a structure applicable to the study process of the ferroelectrics properties, in general case, the task is the establishment of multiple functions $\{y_1, y_2, \ldots, y_j \ldots, y_k\} \epsilon Y$ of independent variables $\{x_1, x_2, \ldots, x_i \ldots, x_n\} \epsilon X$ such that:

$$y_j = f_j(x_1, x_2, \ldots, x_i, \ldots, x_n).$$

A random process $F(X)$ is given by the set (system) of functions $f_j(x_1, x_2, \ldots, x_i \ldots, x_n)$, where $j = 1, 2, \ldots, k$, each of which hypothetically describes the j-process. Accordingly, the experimental study of ferroelectrics is directed by the multi-factor experiment. Then for each function $f_j(x_1, x_2, \ldots, x_i \ldots, x_n)$ in the presence of q levels of measurement-required number of experiments O_j will be determined by the ratio

$$O_j = q^{i_j} \qquad (1)$$

Where $i_j \epsilon [1, n]$ is the number of arguments – factors, on which the j-function F_j depends, where $j = 1, 2, \ldots, j \ldots, k$.

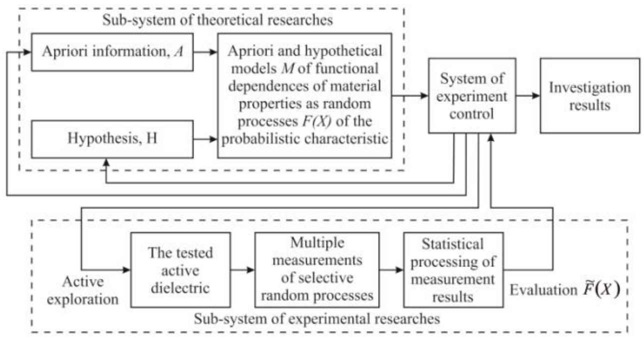

Fig. 1 *Generalized structural scheme of the study process of active dielectrics for solution of tasks of materials synthesis*

Due to the fact that a comprehensive study of material is not limited by the study of the reaction of one parameter of a set $\{y_1, y_2, \ldots, y_j \ldots, y_k\} \epsilon Y$, in general, the number of experiments is determined by the sum of O_Σ:

$$O_\Sigma = \sum_{j=1}^{k} O_j \qquad (2)$$

Here it is assumed that on the basis of the analysis of a priori information from set A is known, from which specific factors X_{ij} from the set X (i.e. $X_{ij} \subset X$) depends each function y_j. In the case when a priori information is not enough to highlight the set X_{ij}, to obtain the reliable information about the properties of the test material, you need an experimental study of the functions y_j depending on all possible factors n. In this case, the expression (1) due to the fact that $i_j = n$ it always takes the form:

$$O_1 = O_2 = \ldots = O_j = \ldots = O_k = q^n.$$

Accordingly, the expression (2) is also transformed:

$$O_\Sigma = kq^n.$$

In general, when you want the behavior of multiple measurements, the value q takes into account the number of measurements at each level.

It should be noted that (2) gives an inflated number of experiments in case of intensive parameters – factors of the set X serve as arguments of several functions. Look at the example of ferroelectric materials having pronounced piezoelectric properties. Analysis of a number of scientific works and results of modern researches shows that practical interest for materials of this class is the study of the dependencies the following extensive parameters: the polarization P and the mechanical deformation x from strain X, electric field E, temperature T, frequency f. In addition, the presence of the inverse piezoelectric effect causes the necessity of measurement of the dependency of E and X (in this case, they characterize intrinsic properties of a ferroelectric, they are extensive parameters) on intensive parameters – effects. These dependencies can be represented as a family of univariate functions under fixed parameters denoted by the subscript indices

$$P(X)\big|_{E,T,f}\ ,\ P(E)\big|_{X,T,f}\ ,\ P(T)\big|_{X,E,f}\ ,$$
$$P(f)\big|_{E,X,T}\ ,\ P(x)\big|_{X,E,T,f}\ ;$$

$$x(X)\big|_{E,P,T,f}\ ,\ x(E)\big|_{X,P,T,f}\ ,\ x(P)\big|_{X,E,T,f}\ ,$$
$$x(T)\big|_{X,E,P,f}\ ,\ x(f)\big|_{X,E,P,T}\ ;\ E(x)\big|_{X,T,f}\ ;\ X(P)\big|_{E,T,f}\ .$$

The totality of the single-factor dependencies on a particular extensive parameter carries information equivalent to the corresponding multivariate dependencies:

$$\begin{gathered} P(X,E,T,f,x);\ x(X,E,T,P,f) \\ E(x,X,T,f);\ X(P,E,T,f) \end{gathered}. \quad (3)$$

If the factors are x and P, it has the reverse effect. Identifying each of the four types of experiments depending on ordinate indices $j = 1\ldots4$ and that $i_1 = i_2 = 5$, $i_3 = i_4 = 4$, according to (2) we determine that in this case the number of experiments:

$$O_{\Sigma} = q_1^5 + q_2^5 + q_3^4 + q_4^4\,.$$

The analysis of a set of dependencies (3) can detect the redundancy of its member functions. Since constants of the inverse piezoelectric effect are equal to the corresponding constant direct effect, the dependency $E(x,X,T,f)$ is duplicated by dependency $P(X,E,T,f,x)$ and the dependency $X(P,E,T,f)$ by $x(X,E,T,P,f)$. Given the above, we imagine (3) to be an equivalent set from the point of view of the amount of information about the material properties:

$$P(X,E,T,f,x),\ x(X,E,T,P,f).$$

In this case, the number of measuring operations will be reduced to

$$O'_{\Sigma} = q_1^5 + q_2^5\,.$$

Before measuring, the drawing up of the apriori model *M* of the process *Y = F(X)*, which is a set of functional dependencies $\{y_j\}$. Then the initial model *M* represents a mapping of apriori and hypothetical ideas about the properties of the test material in the form of some blurred region, such that with some probability the actual process *Y = F(X)* belongs to the blurred area. This probability, in its turn, is an assessment of the adequacy of the original model.

Methods of experimental study of field dependencies of ferroelectric materials are showed in the work [2], in [3] – the modeling of temperature dependences of the parameters of ferroelectrics with phase transition of the second kind, the explanation of the discrepancies of the results of experiment and theoretical calculations derived from the theory of Landau-Ginzburg-Devonshire is given. In this regard, the methodical error caused by the difference of the dielectric constant of the ferroelectric, measured in adiabatic conditions and calculated in isothermal conditions is appreciated.

The following are some aspects of modeling of the field dependences of the ferroelectrics parameters on the basis of thermodynamic theory. Use the expression for the dependence of polarization *P* on electric field *E*:

$$P = \frac{E\varepsilon_0}{\chi^x}\left(1 - \frac{(\varepsilon_0 E)^2 \xi_{11}}{(\chi^x)^3} - \frac{(\varepsilon_0 E)^4 \zeta_{111}}{(\chi^x)^5}\right), \quad (4)$$

where the coefficients χ^x, ξ_{11}, ζ_{111}, can be determined experimentally, based on their physical meanings. For example, according to [4] the coefficients ξ_{11} and ζ_{111} are calculated by the experimentally obtained dependence *P(E)* by solving the system of equations:

$$\begin{cases} P_0^2 = \dfrac{3}{4}\left(-\dfrac{\xi_{11}}{\varsigma_{111}}\right) \\ \chi_0^x = \dfrac{3}{16}\dfrac{(\xi_{11})^2}{\varsigma_{111}} \end{cases}, \quad (5)$$

where P_0, χ_0^x – values of the spontaneous polarization and inverse dielectric susceptibility at the Curie temperature.

The expression (4) is used to model the main loop of the dependence polarization *P(E)* (Fig. 2).

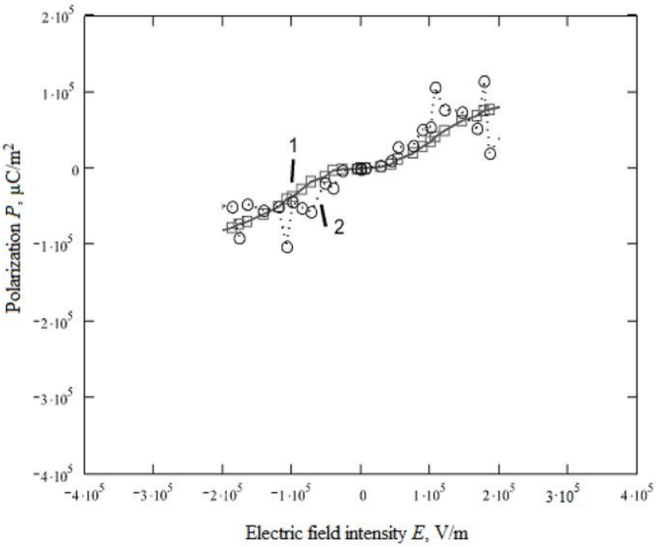

Fig. 2 *Basic curve of polarization: 1 – experimental; 2 – simulated based on the thermodynamic theory*

The results of the experiment coincide with theoretical values only in a narrow range of small applied fields (in the range from 100 kV/m to 100 kV/m). With increasing field on module the experimental curve deviates significantly from the theoretical one. A similar result was observed, for example, in [4] modeling dependencies $\varepsilon(E)$.

The reason of this discrepancy is that in the result of applying the DC field in the crystal charged layers located near the electrodes spatially appear. This in turn reduces the dielectric constant measured in the equilibrium state.

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