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EFFECTIVE CONTROLLABILITY OF A COMPOSITE IN STRONG FIELDS

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A method and computer program for numerical solution of the problem of averaging of a nonlinear composite of periodic structure have been developed. The effective dielectric constant and effective coefficient of controllability of a composite of the ferroelectric-dielectric type have been calculated for arbitrary values of the averaged electric field (earlier such calculations were performed only in the approximation of weak fields). It has been established that the phenomenon of the stability of the effective coefficient of the controllability is preserved for arbitrary values of the averaged electric field.

Keywords: *effective controllability, nonlinear composite of periodic structure, effective dielectric constant, effective coefficient of the controllability, gradient method.*

Introduction. The problem of how to calculate averaged characteristics of nonlinear composite materials is being discussed in sufficient depth in the literature on electroceramics in view of the potentially-attractive properties of ferroelectrics in the production of devices that are readjusted by applying a constant voltage (see [1–4]). The characteristic of the nonlinearity of electroceramics is the relative controllability defined as [2] (this article considers composite materials fabricated only from isotropic components)

$$T = \frac{\varepsilon(0) - \varepsilon(E)}{\varepsilon(0)}, \tag{1}$$

where $\varepsilon(E)$ corresponds to the strength of the field $E = |\nabla\varphi|$ applied to the material. Precisely this property is used to devise electric devices with the characteristics controlled by applying a constant voltage.

By this time, the case of small fields, when the function $\varepsilon(E)$ can be approximated by a quadratic function of the form

$$\varepsilon(E) = \varepsilon(0) - \mu E^2 \tag{2}$$

has been studied to a greater or lesser extent.

An analysis of the case of small fields leads to interesting results. For example, it is shown in [2, 5] that a ferroelectric–dielectric composite material may have an effective controllability exceeding by 5–10% that of its photoelectric component (the relative controllability of a dielectric is equal to zero), whereas in [6] it is stated that the excess of the effective controllability over the controllability of a pure dielectric can be considerable (ten times). The conclusions were drawn for weak fields within the framework of Eq. (2); it is obvious that they are inapplicable to arbitrary fields (at least by virtue of the fact that at a high E the dielectric constant, Eq. (2), becomes negative).

It is known from experiments that the function $\varepsilon(E)$ has a form similar to that presented in Fig. 1 (sec [2]). To approximate the graph presented in Fig. 1, we will select the function

$$\varepsilon(E) = \frac{\varepsilon_0 - \varepsilon_\infty}{1 + k|E|^2} + \varepsilon_\infty, \tag{3}$$

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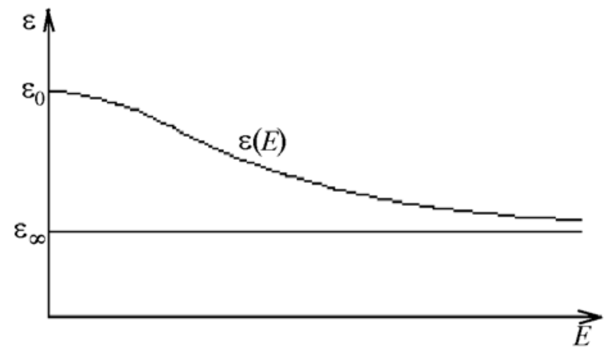

Fig. 1. Dielectric constant of a material ε vs. the electric field strength E.

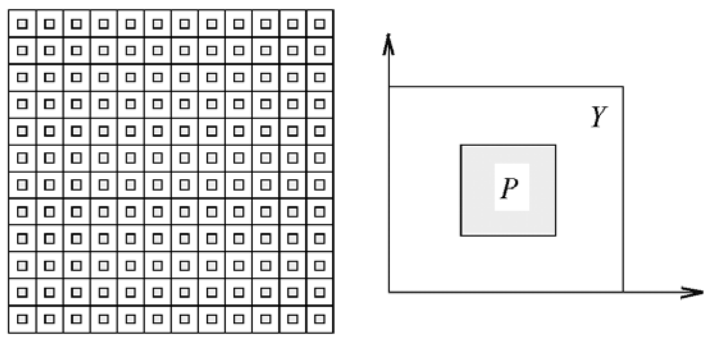

Fig. 2. Composite of periodic structure (to the left) and its elementary cell (to the right).

where ε_0 and ε_∞ are the values of $\varepsilon(E)$ at zero and "at infinity." Expression (3) depicts the characteristic behavior of the function, presented in Fig. 1, in the entire range of E values.

The aim of the present work was to obtain averaged characteristics for the case considered and, in particular, to elucidate the properties of the effective controllability of a composite for no small fields.

Statement of the Problem and Numerical Method of Its Solution. We will consider a composite material of periodic structure obtained by repeating an elementary cell Y (Fig. 2).

Let the elementary cell consist of a matrix whose material is a nonlinear ferroelectric containing a centrally located inclusion from a linear dielectric. We will consider the plane problem in which all the quantities depend on the variable $\mathbf{x} = (x, y)$. This problem describes also a three-dimensional composite reinforced by a system of parallel cylinders. Then, in view of the symmetry of the problem, it is sufficient to consider, on an elementary cell, the following problem of electrostatics (the plane statement of the problem is considered):

$$\operatorname{div}\left(\varepsilon\left(\mathbf{x},\ \left|\nabla\varphi(\mathbf{x})\right|\right)\nabla\varphi(\mathbf{x})\right) = 0\,. \tag{4}$$

By virtue of the symmetry the following boundary conditions hold:

$$\left.\frac{\partial\varphi}{\partial n}\right|_{x=0} = \left.\frac{\partial\varphi}{\partial n}\right|_{x=1} = 0\,, \tag{5}$$

$$\varphi\big|_{y=0} = -E/2\,;\quad \varphi\big|_{y=1} = E/2\,. \tag{6}$$

Let the function $\varepsilon(\mathbf{x}, \left|\nabla\varphi(\mathbf{x})\right|)$ have the following form:

$$\varepsilon\left(\mathbf{x},\ |\nabla\varphi(\mathbf{x})|\right)=\begin{cases}1, & \mathbf{x}\in P;\\ \dfrac{\varepsilon_0-\varepsilon_\infty}{1+k|\nabla\varphi|^2}+\varepsilon_\infty, & \mathbf{x}\in Y\setminus P,\end{cases} \tag{7}$$

where P is the internal square of the cell; Y is the entire cell; ε_0 and ε_∞ are the dielectric constants at zero and at infinity. We note that the function $\varepsilon(\mathbf{x},\ |\nabla\varphi(\mathbf{x})|)$ can be multiplied by a constant number without altering the solution of problem (4)–(6). Therefore, assuming the dielectric constant of the linear component equal to unity, we do not limit the generality of the discussion.

Problem (4)–(7) contains $\nabla\varphi$ in the coefficient and, according to the acting classification, is strongly non-linear. Standard packages of programs for solving boundary-value problems do not provide a possibility of solving this type of problems. For example, the ANSYS package makes it possible to solve problems with coefficients that depend on φ but not on $\nabla\varphi$. In this connection the necessity of writing programs for numerical solution of boundary-value problem (4)–(7) arises.

We will find the functional whose minimization corresponds to the solution of problem (4)–(7). We will seek it in the form $\int_Y q(|\nabla\varphi|)d\mathbf{x}$.

Multiplying Eq. (4) by the trial function $-\delta\varphi(\mathbf{x})$ and integrating over the region Y, we obtain

$$-\int_Y \delta\varphi\,\mathrm{div}\left(\varepsilon\left(|\nabla\varphi|\right)\nabla\varphi\right)d\mathbf{x}=\int_Y \varepsilon\left(|\nabla\varphi|\right)\nabla\delta\varphi\nabla\varphi d\mathbf{x}. \tag{8}$$

In Eq. (8) the integral over the boundary $\int_{\partial Y}\varepsilon(|\nabla\varphi|)\delta\varphi\dfrac{\partial\varphi}{\partial n}d\mathbf{x}=0$, since according to (5), at the left and right boundaries of the region $\partial\varphi/\partial n = 0$, whereas on the lower and upper boundaries of the region $\delta\varphi(\mathbf{x}) = 0$ according to (6).

The variation of the functional $\int_Y q(|\nabla\varphi|)d\mathbf{x}$ has the form

$$\delta\int_Y q\left(|\nabla\varphi|\right)d\mathbf{x}=\int_Y q'\left(|\nabla\varphi|\right)\frac{\nabla\varphi\nabla\delta\varphi}{|\nabla\varphi|}d\mathbf{x}. \tag{9}$$

For the coincidence of the right-hand sides of Eqs. (8) and (9) the following equality should hold:

$$q'\left(|\nabla\varphi|\right)\frac{1}{|\nabla\varphi|}=\varepsilon\left(|\nabla\varphi|\right). \tag{10}$$

Since all the functions in (10) depend only on $|\nabla\varphi|$, to determine $q(z)$ we obtain the equation $q'(z) = \varepsilon(z)z$ ($z \in [0, \infty)$) which for the function (3) acquires the form

$$q'(z)=\left(\frac{\varepsilon_0-\varepsilon_\infty}{1+k|z|^2}+\varepsilon_\infty\right)z.$$

Whence we find

$$q(z)=\frac{\varepsilon_0-\varepsilon_\infty}{2k}\ln(1+kz^2)+\frac{\varepsilon_\infty}{2}z^2.$$

In the region of the linear material $q(z) = z^2/2$. Thus, the sought functional, whose minimization yields the solution of problem (4)–(7), has the form

$$F(\varphi) = \int_P \frac{1}{2}\, |\nabla\varphi(\mathbf{x})|^2\, d\mathbf{x} + \int_{Y\setminus P} \left(\frac{\varepsilon_0 - \varepsilon_\infty}{2k} \ln\left(1 + k\,|\nabla\varphi(\mathbf{x})|\right)^2 + \frac{\varepsilon_\infty}{2}\, |\nabla\varphi(\mathbf{x})|^2 \right) d\mathbf{x}\,. \tag{11}$$

Now we will obtain a discrete approximation for functional (11). For this purpose, we will divide the region Y by a uniform grid $N \times N$ so that the grid lines coincide with the boundaries of the internal square. We will denote $h = 1/N$. The gradients will be approximated by the difference derivatives

$$|\nabla\varphi|^2 = \left(\frac{(\varphi_{i,j+1} - \varphi_{i,j})^2}{h^2} + \frac{(\varphi_{i+1,j} - \varphi_{i,j})^2}{h^2} \right),$$

where $\varphi_{i,j}$ is the value of the sought function at the point with the coordinates $x = ih$, $y = jh$; i, and j change within the range 0, 1, ..., N. Thus, in the discrete problem the integral functional that is to be minimized in solution will be replaced by a nonlinear function of $N^2 - 1$ variables, which has the form

$$\overline{F}(\varphi_{ij}) = \int_P \frac{1}{2}\, |\nabla\varphi|^2\, d\mathbf{x} + \int_{Y\setminus P} \left(\frac{(\varepsilon_0 - \varepsilon_\infty)}{2k} \ln\left(1 + k\,|\nabla\varphi|^2\right) + \frac{1}{2}\,\varepsilon_\infty\, |\nabla\varphi|^2 \right) d\mathbf{x}$$

$$\approx \frac{\varepsilon_0 - \varepsilon_\infty}{2k} \sum_{(ih,jh)\in Y\setminus P} \sum \left(\ln\left(1 + k\left(\frac{(\varphi_{i,j+1} - \varphi_{i,j})^2}{h^2} + \frac{(\varphi_{i+1,j} - \varphi_{i,j})^2}{h^2} \right)\right)\right) h^2$$

$$+ \frac{\varepsilon_\infty}{2} \sum_{(ih,jh)\in Y\setminus P} \sum \left(\frac{(\varphi_{i,j+1} - \varphi_{i,j})^2}{h^2} + \frac{(\varphi_{i+1,j} - \varphi_{i,j})^2}{h^2} \right) h^2$$

$$+ \frac{1}{2} \sum_{(ih,jh)\in P} \sum \left(\frac{(\varphi_{i,j+1} - \varphi_{i,j})^2}{h^2} + \frac{(\varphi_{i+1,j} - \varphi_{i,j})^2}{h^2} \right) h^2\,. \tag{12}$$

The values of the function at the lower and upper boundaries are respectively defined as $-E/2$ and $E/2$. The number of points amounts to $(N+1)^2$, the values of the function at the $2(N+1)$ points of the lower and upper boundaries are found, there are $N^2 - 1$ unknown values of the function.

We will seek the solution of the nonlinear problem

$$\overline{F}(\varphi_{ij}) \to \min$$

numerically by the gradient method. Let expression (12) assign the functional $\overline{F}(\varphi_{ij})$. The initial value of the sought function φ_{ij}^0 will be assigned in the form of a linear function and such that $\varphi_{ij}^0 = -E/2$ at $j = 0$ and $\varphi_{ij}^0 = E/2$ at $j = N$. We will find the value of the functional $\overline{F}(\varphi_{ij}^0)$. We will assign the following quantities: δ is the accuracy with which the gradient is determined, and α is the coefficient of the descent step in the direction of the functional derivative. The gradient taken with the opposite sign indicates the direction over which the functional decreases its value. However, if the magnitude of the descent cannot be determined, there may be outskirts where the functional decreases its value. If the norm of the gradient $\|\nabla\overline{F}(\varphi_{ij})\| \le \delta$, then φ_{ij} is the solution sought. If not, we seek an intermediate solution φ'_{ij} so that

$$\varphi'_{ij} = \varphi_{ij} - \alpha\nabla\overline{F}(\varphi_{ij})\,, \quad \overline{F}(\varphi'_{ij}) < \overline{F}(\varphi_{ij})\,. \tag{13}$$

The value of α is determined so that it can be at the point where condition (13) is valid. If (13) is not fulfilled, then at each subsequent step α is decreased twice until it becomes valid.

Testing of the Program. Prior to the use of the program for calculations it should be tested on problems with known solutions.

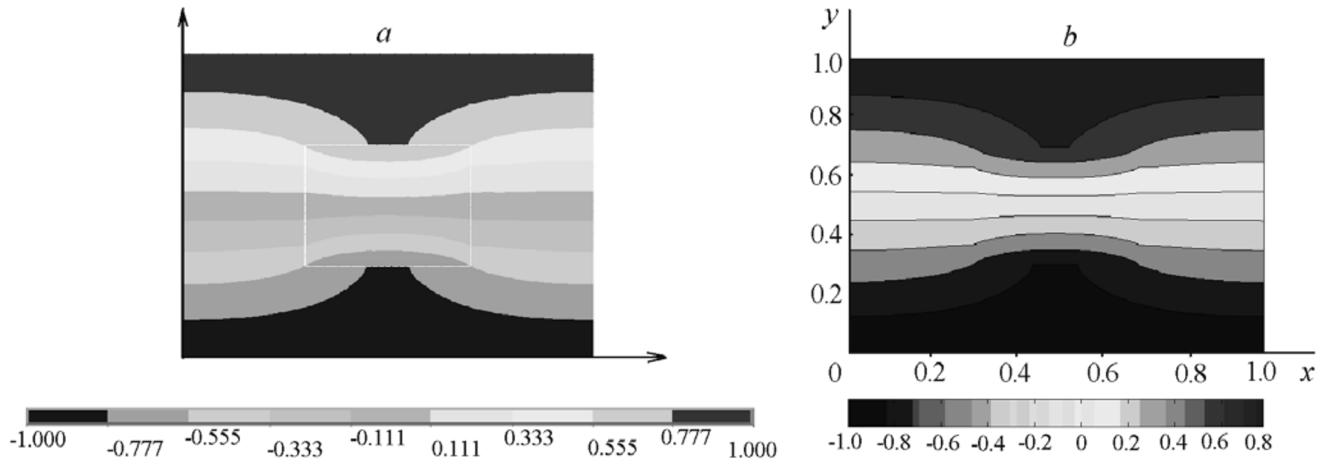

Fig. 3. Potential $\varphi(x, y)$ calculated with the aid of ANSYS (a) and of the written program (b). φ, kV; x, y, mm.

Testing on a linear problem and comparison with the solutions obtained with the aid of ANSYS. A written program must solve linear problems. In this connection the first series of tests consisted in a comparison of the solutions of the linear problems obtained with the aid of a written program and the ANSYS program. Precisely with the aid of the written program the linear problem (4)–(7) was solved, where the function $\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|)$ has the following form:

$$\varepsilon\left(\mathbf{x}, |\nabla\varphi(\mathbf{x})|\right) = \begin{cases} a_1, & \mathbf{x} \in P; \\ a_2, & \mathbf{x} \in Y \setminus P. \end{cases} \tag{14}$$

The size of the periodicity cell was equal to 1×1, with the size of an inclusion amounting to 0.4×0.4. Voltages $-E/2$ and $E/2$ are applied to the upper and lower faces of the elementary cell; this corresponds to a mean field of strength E. The coincidence of the solutions of the linear problem with the aid of the written program and ANSYS program was satisfactory. As an example, Fig. 3 presents the solution of the problem for $a_1 = 1$ and $a_2 = 100$ at $E = 2.0$, with the size of the inclusion being equal to 0.4×0.4; the potential $\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|)$ takes the values given in (14).

Solution of the problem at a high value of the external field. Exact solutions of a nonlinear problem such as (4)–(7) for the region of the type of a "rectangle with an inclusion" are unknown to the present authors. There are strong grounds for believing that they are nonexistent at present. For Eq. (4) one can obtain solutions of axisymmetric problems in a more or less explicit form. However axisymmetric solutions cannot be used as test ones for periodic problems. The problem considered can be test by means of solving a nonlinear problem with the exit to the solution of a linear problem (the latter can be obtained). Note that with increase in the mean voltage applied to a specimen one may expect an increase in the local field. If we consider Eq. (7), we will see that with increase in the field strength the value of the coefficient $\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|)$ approaches ε_∞, i.e., with increase in voltage the problem passes a nonlinear regime, and at high enough E reaches a linear regime whose parameters are known and are assigned by the function

$$\varepsilon(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in P; \\ \varepsilon_\infty, & \mathbf{x} \in Y \setminus P, \end{cases} \tag{15}$$

for which problem (4)–(6) can be solved. Precisely this "exit to a linear problem" at a high voltage will be used by us as a test problem.

We will solve the problem for the first limiting case where $E = 20.0$ and $k = 0.5$. Test solutions allow us to assume that the strength of the local field $|\nabla\varphi|$ is not smaller than E. Then, at the indicated E and k

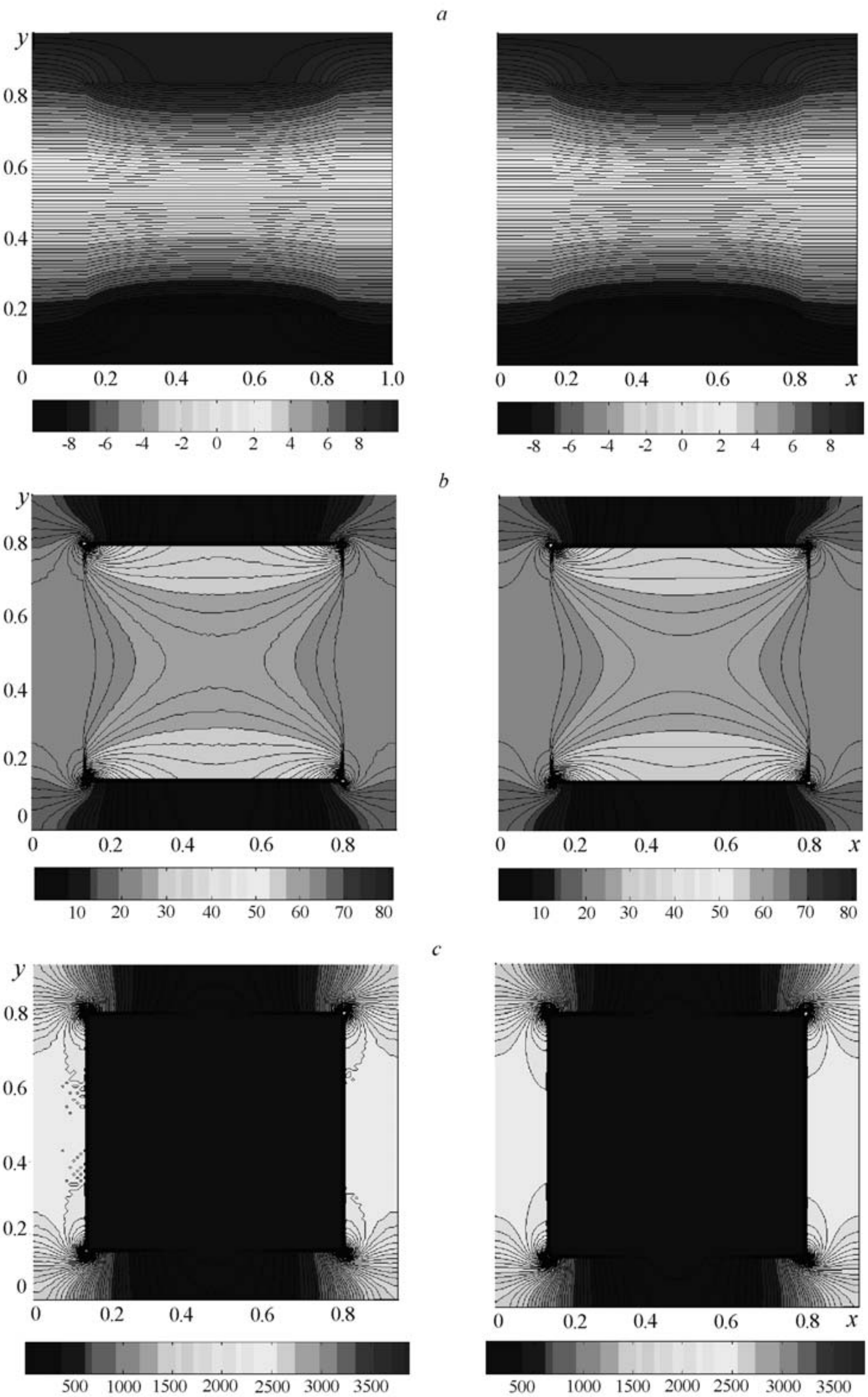

Fig. 4. Solution of the nonlinear (to the left) and linear (to the right) problems at E = 20 kV/cm: a) potential $\varphi(x, y)$, kV; b) gradient $|\nabla\varphi(x, y)|$, kV/cm; c) flux of the gradient $\varepsilon(\mathbf{x}, |\nabla\varphi(\mathbf{x})|)\nabla\varphi(\mathbf{x})$, KC/cm^2. ($\mathbf{x} = (x, y)$). x, y, mm.

$$\frac{\varepsilon_0-\varepsilon_\infty}{1+k\left|\nabla\varphi\right|^2}+\varepsilon_\infty \approx \varepsilon_\infty .$$

TABLE 1. The Values of $\varepsilon_{\text{eff}}(E)$ Calculated with the Use of Various Programs

Programs	E	
	0.2	14
Dielectric constant of an inclusion	150	100
ANSYS	50.08	33.7
Written program	49.77	33.79

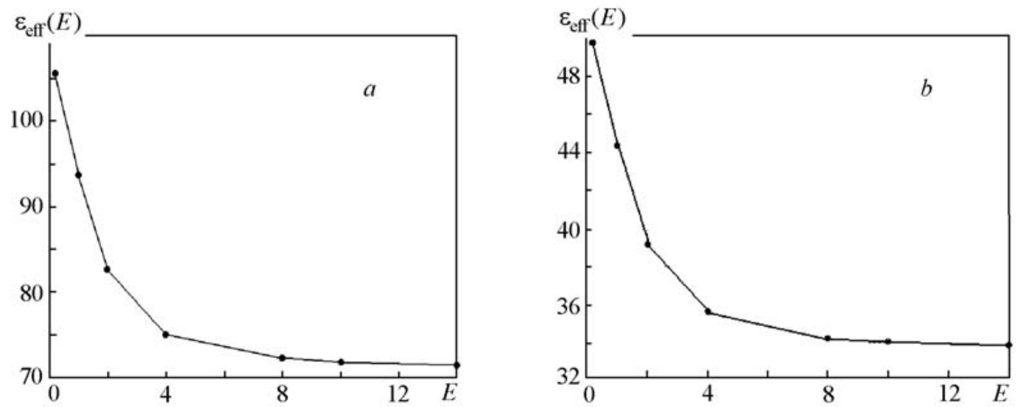

Fig. 5. Effective dielectric constant of a composite as a function of the averaged electric field strength (a, volume content of inclusions 0.16; b, 0.49), the values of the function found at E = 0.1, 1, 2, 4, 8, 10, and 14 kV/cm, designated by points on the graph.

The problem was solved at $\varepsilon_0 = 150$ and $\varepsilon_\infty = 100$. The solutions obtained (potentials and the associated electric field strengths and flows) of the linear and nonlinear problems presented in Fig. 4 practically coincide. The time of their solution differed by 30–50%. The other limiting case is the small field. At $k = 0.5$ and $E = 1$

$$\frac{\varepsilon_0 - \varepsilon_\infty}{1 + k\left|\nabla\varphi\right|^2} + \varepsilon_\infty \approx \varepsilon_0 \,,$$

and the solution of the nonlinear problem must be close to the solution of the linear problem at

$$\varepsilon(\mathbf{x}) = \begin{cases} 1\,, & \mathbf{x} \in P\,; \\ 150\,, & \mathbf{x} \in Y \setminus P\,. \end{cases} \tag{16}$$

The effective dielectric constant of the composite can be defined as [6]

$$\varepsilon_{\text{eff}}(E) = \frac{1}{E^2\left|Y\right|} \int_Y \varepsilon\left(\left|\nabla\varphi\right|\right) \nabla\varphi^2 d\mathbf{x} \tag{17}$$

(as noted, E corresponds to the strength of an averaged electric field). Equation (17) corresponds to the theory of averaging [7, 8].

We will give the value of the effective dielectric constant calculated with the aid of the written program and the ANSYS package (see Table 1). As noted, based on physical notions, the properties of a nonlinear composite at small E must be close to the properties of a linear composite with the dielectric constant of the inclusion equal to 150, whereas the properties of a nonlinear composite at high E must be close to the properties of a linear composite with the dielectric constant of the inclusion equal to 100.

Solutions were obtained for potentials, associate gradients, and the fluxes of gradients for high values of E, E = 20, for linear and nonlinear problems. Having compared the left and the right sides of Fig. 4, we see that they coincide qualitatively.

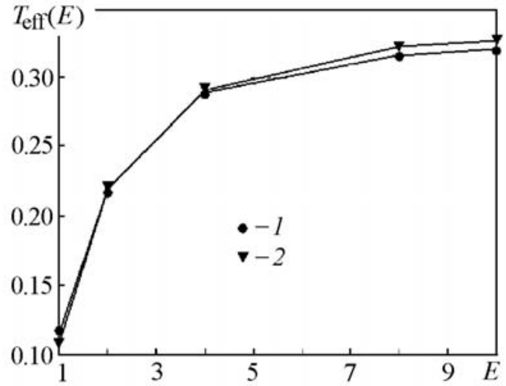

Fig. 6. Coefficients of the controllability of the ferroelectric–dielectric composite (1) and of a homogeneous ferroelectric (2).

For the problem considered, the calculation was carried out for δ = 0.00001, α = 0.0012, N = 100, ε_0 = 50, and ε_∞ = 100. We considered the case where the fraction of the inclusion amounted to 49% of the overall size of the cell. The strength of the averaged electric field E changed from 1.0 to 20.0. Here δ is the accuracy of determination of the gradient (in an ideal case the gradient at the point of a minimum must be equal to zero). The step of the descent α over the gradient was selected experimentally, since it was necessary to attain stability in the convergence of the method. At high values of α the convergence of the method was disturbed. High values of N prolonged the execution time of the problem.

Effective Characteristics of a Nonlinear Composite in a Strong Electric Field. The presented results of testing allow us to conclude that the written program solves numerically the nonlinear problem (4)–(7) with high accuracy in the entire range of applied voltages. After this, it is possible to use the written program to calculate the effective dielectric constant and effective controllability of a composite in strong fields. Precisely the investigation of these characteristics for the case of strong fields was the aim of the present work. For this purpose, problem (4)–(7) was solved at E = 0.1, 1, 2, 4, 8, 10, and 14 kV/cm. In plotting the graphs the values of the functions at these points were taken. Note that the operating strengths of an electric field for real analogs of the materials considered attain several tens (sometimes up to 100) of kilowatts per centimeter (see, e.g., [2]). In the calculations carried out, relative values are used, which does not limit the generality of consideration. It may be regarded that in the foregoing examples kilowatts per centimeter is the unit of field strength.

Effective Dielectric Constant of a Nonlinear Composite. A graph of the function $\varepsilon(E)$ is presented in Fig. 5. At the boundaries of the interval (at E = 1 and 14) the calculated values of the effective dielectric constant coincide with the values obtained from the solution of the linear problem (on the basis of both the program developed and the ANSYS package) at values of the dielectric constant of the matrix 150 and 100. In the calculation the size of the cell has periodicity 1 × 1. Figure 5a presents data for an inclusion of size 0.4 × 0.4 (the volume fraction of inclusions is equal to 0.16), and Fig. 5b of size 0.7 × 0.7 (the volume fraction of inclusions is equal to 0.49). As is seen from Fig. 5, the effective dielectric constant of a composite with a volume content of inclusions equal to 0.16 is almost two times higher than the effective dielectric constant of a composite with a volume content of inclusions equal to 0.49. Such results correspond to the well-known indices for linear composites.

Effective Controllability of a Composite. The effective coefficient of controllability of a composite material can be found using the formula

$$T_{\text{eff}}(E) = \frac{\varepsilon_{\text{eff}}(0) - \varepsilon_{\text{eff}}(E)}{\varepsilon_{\text{eff}}(0)}\,.$$

The values of the effective coefficient of controllability for a composite material with a cell of periodicity 1 × 1 for inclusions of size 0.7 × 0.7 are presented in Fig. 6. For comparison the effective coefficient of controllability for a homogeneous nonlinear material of the matrix is given.

The calculations of the effective coefficient of controllability for a composite material with an inclusion of size 0.4×0.4 yielded results practically coinciding with the values of the effective coefficient of controllability for a composite material with an inclusion of size 0.7×0.7.

Conclusions. The numerical results obtained indicate that the earlier detected (for small field [2, 3]) effect of stability of the controllability coefficient on introduction of linear inclusions into a nonlinear material persists also for strong fields. At the same time, the effect of a considerable increase in the controllability coefficient of a composite possible for weak fields [6] becomes impossible for strong ones. Thus, the possibilities offered by composition technologies for designing nonlinear materials with assigned effective characteristics depend substantially on the characteristics of the field in which a composite will operate.

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NOTATION

a_1, a_2, constants; E, electric field strength; $\overline{F}$, functional; h, step of division of an elementary cell; k, coefficient in the formula that approximates the dependence of the dielectric constant of a photoelectric on the voltage applied for the case of fields of arbitrary strength; N, size of the grid; P, inclusion; q, function; T, relative controllability; $\mathbf{x}$, spatial variable; x, y, coordinates; Y, periodicity cell; z, variable; α, step of decent in the gradient method; δ, accuracy of determination of the gradient; $\varepsilon(E)$, dielectric constant of a material; ε_0, ε_∞, vales of $\varepsilon(E)$ at zero and "at infinity;" μ, coefficient in the formula that approximates the dependence of the dielectric constant of a ferroelectric on the applied voltage for the case of small fields; φ, electric field potential; $\varphi^0_{i,j}$, $\varphi'_{i,j}$, and $\varphi_{i,j}$, the values of the sought function at the point with the coordinates $x = ih$, $y = jh$; $\nabla\varphi$, gradient of φ. Subscript: eff, effective.

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