Modeling of the electromagnetic and elastic properties of composite materials

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Abstract. In this paper, we consider the solution of the problem of the theory of piezoelectricity. The effective elastic, piezoelectric, and dielectric characteristics are calculated for a two-layer composite with a volume concentration of layers of 50%. The corresponding characteristics are calculated for a two-layer material with an orthogonal-reinforced structure. For the numerical solution of the problem, the conjugate gradient method for solving systems of algebraic equations was used. The results were visualized using a software package developed at Bauman Moscow state technical University. The paper presents the distribution of the stress field $\sigma_{ij}$ and the vector $d_i$ in problems $L_r$ and $L_{pq}$.

1. Introduction

The Electromagnetically elastic properties and tools for their study are described in [1-24]. Many areas of production and industry have special requirements for the properties and characteristics of the materials used, such as engineering, shipbuilding, aviation, space industries, construction and others. The interest in creating new modeling methods is growing, as more and more new, modern computer technology provides more and more opportunities to obtain faster and more accurate results [9]. Significant opportunities for creating such solution techniques are offered by the method of asymptotic averaging (MAO), or the method of homogenization. In this paper, we propose the use of this method in the simulation of composite materials with piezoelastic properties [8]. The solution to this problem is based on such phenomena as the piezoelectric effect (direct and inverse). When mechanical stress is applied to some crystals, an electric moment arises [7]. This phenomenon is the essence of the direct piezoelectric effect. In [10], such quantities as the piezoelectric moduli are determined similarly, and it is also shown that these characteristics are components of the third-rank tensor $\varepsilon_{ijkl}$. Most of the theoretical assumptions of this work are based on the definitions and conclusions described and obtained in [1].

2. Mathematical statement of the problem

We need to simulate a composite material with more effective piezoelasticity characteristics. Based on this, in the course of this work, a software package was implemented that made it possible to calculate the effective characteristics of the piezoelastic tensor of various composite materials, depending on the class of their symmetry.
We shall denote the cell periodicity for the task piezoelectricity - $V_{\xi}$. Suppose PL consists of $N$ phases $V_{\alpha} = 1, \ldots, N$. We introduce the parameter $k = \frac{l}{L}$ — a small parameter (under the assumption, $k \ll 1$), where $l$ is the characteristic size of the periodicity cell, and $L$ is the characteristic linear size of the composite material as a whole [2].

We pose the problem of piezoelectricity, with the introduction of Cartesian coordinates ($x^i$), as well as global ($\xi = \frac{x^i}{L}$) and local ($\zeta = \frac{x^i}{k}$) coordinates, and also assume that contact on the interface $\Sigma_{\alpha\beta}$ between the components of the material is ideal:

\[
\sigma_{ij} = 0; \quad (1)
\]
\[-d_{ij} + \rho_e = 0; \quad (2)
\]
\[\sigma_{ij} = C_{ijkl} e_{kl} + v_{ijkl} e_{k}; \quad (3)
\]
\[\epsilon_{ij} = \frac{1}{2}(u_{ij} + u_{ji}); \quad (4)
\]
\[d_i = v_{ij} e_{ij} - 3v_{ik} e_k; \quad (5)
\]
\[\epsilon_c = \varphi_k; \quad (6)
\]
\[[u_i] = 0, [\sigma_{ij}] n_j = 0 \text{ on } \Sigma_{ij}; \quad (7)
\]
\[[\varphi] = 0, [d_i] n_i = 0 \text{ on } \Sigma_{ij}; \quad (8)
\]
\[\sigma_{ij} n_j \big|_{\Sigma} = S_i; \quad (9)
\]
\[d_i n_i \big|_{\Sigma} = d_m. \quad (10)
\]

In the system of equations (1) - (10): (1) is the equilibrium equation, (2) is the Gauss equation, (3) is the elasticity relation taking into account the effect of piezoelectricity, (4) is the Cauchy relation, (5) is the electrical relation with taking into account the inverse piezoelectric effect, (6) is the expression for the electric potential, (7) is the condition of the ideal mechanical effect at the interface of the components, (8) is the ratio of the ideal electrical contact at the interface of the components of the material, (9) is the kinematic and static conditions on the external surfaces, (10) - electrical conditions at the boundaries;

3. Problem Solving method

We write the system of equations 1-10 in the form of two systems: a system of local equilibrium equations and a system of averaged equilibrium equations [13].

\[
\frac{\partial}{\partial x^i} \{\sigma^\alpha_{ij}(\bar{x},\xi)\} = 0
\]
\[
\frac{\partial}{\partial \xi^i} \{\sigma^\alpha_{ij}(\bar{x},\xi)\} = 0
\]
\[
\cdots
\]
\[
\frac{\partial}{\partial \xi^i} \{\sigma^\alpha_{ij}(\bar{x},\xi)\} = 0
\]
\[
\frac{\partial}{\partial x} i(x, \xi) = 0 \\
\frac{\partial}{\partial x} j(x, \xi) = 0 \\
\vdots \\
\frac{\partial}{\partial x} n(x, \xi) = 0
\]

We will solve this problem on a periodicity cell. B Udum assume that the periodicity cell is divided into \( N \) parts, and each part is assigned its number \( \alpha \). The task can be divided into 9 separate tasks \([12, 13]\): 6 tasks of type \( \text{“} L_{pq} \text{”} \) and 3 tasks of type \( \text{“} L_{r} \text{”} \):

\[
\text{“} L_{pq} \text{”}: \begin{cases}
\sigma^{(0)}_{i(j,pq)} = 0; \\
\sigma^{(0)}_{j(i,pq)} = C_{ijkl} e^{(0)}_{k(i,pq)} + V_{ij} e^{(0)}_{j(i,pq)}; \\
e^{(0)}_{k(i,pq)} = \frac{1}{2} \left( U_{k(i,pq)} + U_{j(i,pq)} \right).
\end{cases}
\]

\[
\text{“} L_{r} \text{”}: \begin{cases}
\sigma^{(0)}_{i(j,r)} = 0; \\
\sigma^{(0)}_{j(i,r)} = C_{ijkl} e^{(0)}_{k(i,r)} + V_{ij} e^{(0)}_{j(i,r)}; \\
e^{(0)}_{k(i,r)} = \frac{1}{2} \left( U_{k(i,r)} + U_{j(i,r)} \right).
\end{cases}
\]

The variational formulation for problems \( L_{pq} \) has the form:

\[
\delta e^T \sigma dV = \delta U^T \delta d \Sigma \cdot \int \delta e^T d dV = 0
\]

The variational formulation of the problem is formulated in the same form \( L_{r} \).

We will approximate the displacements \( \bar{U} \) and electric potential in finite elements by linear coordinate functions:

\[
\bar{U} = \Phi \bar{q}, \quad \varphi = \bar{\varphi} \bar{r}.
\]

In formulas (15) \( \bar{q} \) and \( \bar{r} \) are the coordinate columns of displacements and electric potentials at the nodes of finite elements. \( \Phi \) and \( \bar{\varphi} \bar{r} \) are the matrix and column of form functions. Then from (14) we obtain the final resolving system of linear algebraic equations [19]:

\[
\bar{K} \bar{q} = \bar{f}
\]

where

\[
\bar{K} = \bar{B}^T \bar{C} \bar{B} dV,
\]
\[
\tilde{C} = \begin{pmatrix} \bar{C} \\ \bar{V} \end{pmatrix}, \quad \tilde{B} = \begin{pmatrix} \bar{B} & 0 \\ 0 & \bar{B} \end{pmatrix}, \quad \bar{B} = \tilde{D} \bar{D}, \quad \bar{B}_r = \bar{D} \bar{F}.
\]

\[
\tilde{q} = \begin{pmatrix} \bar{q} \\ \bar{y} \end{pmatrix}, \quad \tilde{f} = \begin{pmatrix} \bar{f} \\ \bar{F} \end{pmatrix}.
\]

4. Results of a numerical solution

For the test calculation, tourmaline was used, which represents the B- rhombohedral symmetry class according to the classification [20].

We show for this problem also the distribution of the stress tensor field for some problems \( L_{pq} \). Figure 1 shows the distribution \( \sigma_{11} \) in the problem \( L_{11} \) for \( \bar{e} = 0 \).

![Figure 1. Distribution \( \sigma_{11} \), GPa, in the task problem \( L_{11} \)](image)

The distribution \( \bar{q} \) in the task \( L_{1} \) is presented in Figure 2.
Similarly, the values of the desired effective characteristics for composite materials whose components belong to other symmetry groups can be obtained. To do this, you only need to specify the matrix form of their constants - elastic, piezoelectric and dielectric [21].

5. Conclusions
In this work, a method for finding the effective characteristics of a composite material was presented and implemented.

The theoretical basis of the method is given. A software package has been developed that provides the calculation of the desired characteristics.

For the numerical solution of the problem, the conjugate gradient method for solving systems of algebraic equations was used.

The test problem of the theory of piezoelectricity for a single-layer material is solved, on the basis of the results of which it is concluded that the presented method is working.

The effective elastic, piezoelectric, and dielectric characteristics are calculated for a two-layer composite with a volume concentration of layers of 50%. The results of this calculation well satisfy the analytical results, taking into account the computational error.

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