# MODELING OF COMPOSITES WITH DIFFERENT PHYSICAL AND GEOMETRICAL CONNECTIVITIES BY EFFECTIVE MODULES AND FINITE ELEMENT METHODS

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Summary The study discusses complex approaches for determination of the effective moduli for multiphase composite materials with different geometrical structures and coupled physical fields. These approaches are based on the effective modulus method for composite materials, computer design of representative volumes with microstructure features and finite element technologies for solution of coupled boundary problems for inhomogeneous representative volumes. The piezoelectric, magnetoelectric, thermoelastic and poroelastic anisotropic composite models are considered. The sets of boundary conditions indicated for these cases permit to define the full assemblies of the effective moduli from quasistatic constitutive equations for active composites. Porous piezoelectric composites are investigated more carefully with hypothesis of the inhomogeneous polarization fields. The efficiency of the proposed models is illustrated by the analysis of hydroacoustic piezoelectric devices and piezogenerators made of porous piezoceramics.

## INTRODUCTION

In the recent years there has been an increased interest in research of composite materials of complex structure that show effective properties for many practical applications. For example, porous piezoelectric composite ceramics have ultra high volume piezosensitivity, low acoustic impedance and expanded passband of frequencies. Therefore, the use of porous piezocomposite materials permits to improve considerably main operating parameters of ultrasonic piezogenerators. Two-phase magnetoelectric composites consisting of piezo- and magnetoactive phases demonstrate the capability to mutual transformation of magnetic and electric fields, even though each single phase does not have such property. Modern magnetoelectric composites have high effectiveness of magnetoelectric transformation, relatively high temperatures of phase transitions and significant technological resources. The problems of determining the effective properties of more traditional composites still remain actual for composites with coupled fields, for example, for thermo- and poroelastic porous bodies, especially when taking in account their microstructure. Theoretical and computer investigations of composite materials of complex structure allow explaining and simulating some of their important characteristics and permit to give predictions on the effectiveness of various relations and couplings of structures of constituent phases.
A number of papers [1-7] develop approach based on the effective modulus method for composite mechanics, computer modeling of representative volumes with regard to their microstructure and finite element technologies for solving coupled physic-mechanical problems for representative volumes of composites with specific boundary conditions. The main ideas of such comprehensive approach can be shown using an example of a porous piezoelectric composite material [1-6].

## MODELLING OF POROUS PIEZOELECTRIC MEDIA BY EFFECTIVE MODULES METHOD

For porous piezocomposite modeling we use the effective modules method and finite element technique in accordance with [1-6]. As usually, we will denote the volume-averaged quantities in the broken brackets as $\langle\ldots\rangle = \frac{1}{\Omega}\int_{\Omega}(\ldots)d\Omega$, where $\Omega$ is the region occupied by the representative volume of porous piezocomposite. For tensors we use the vector-matrix notations. Thus we introduce the strain (pseudo-) vector $\mathbf{S}=\{\varepsilon_{11},\varepsilon_{22},\varepsilon_{33},2\varepsilon_{23},2\varepsilon_{13},2\varepsilon_{12}\}$, the stress (pseudo-) vector $\mathbf{T}=\{\sigma_{11},\sigma_{22},\sigma_{33},\sigma_{23},\sigma_{13},\sigma_{12}\}$, and the dielectric displacement vector $\mathbf{D}$, where $\varepsilon_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ are the components of the strain tensor, $\sigma_{ij}$ are the components of the stress tensor. By the fields functions $\mathbf{u}$ and $\varphi$ one can determine the strain vector $\mathbf{S}$ and the electric fields vector $\mathbf{E}$

$$\mathbf{S} = \mathbf{L}(\nabla)\cdot\mathbf{u}, \qquad \mathbf{E} = -\nabla\varphi, \tag{1}$$

$$\mathbf{L}^*(\nabla) = \begin{bmatrix} \partial_1 & 0 & 0 & 0 & \partial_3 & \partial_2 \\ 0 & \partial_2 & 0 & \partial_3 & 0 & \partial_1 \\ 0 & 0 & \partial_3 & \partial_2 & \partial_1 & 0 \end{bmatrix}, \qquad \nabla = \begin{Bmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{Bmatrix}. \tag{2}$$

In concordance with constitutive equations for static case we will introduce the moduli of piezoelectric medium

$$\mathbf{T} = \mathbf{c}^E\cdot\mathbf{S} - \mathbf{e}^*\cdot\mathbf{E}, \qquad \mathbf{D} = \mathbf{e}\cdot\mathbf{S} + \boldsymbol{\varepsilon}^S\cdot\mathbf{E}. \qquad 3)$$

Here $\mathbf{c}^E$ is the $6\times 6$ matrix of elastic stiffness moduli at constant electric field, $\mathbf{e}$ is the $3\times 6$ matrix of piezoelectric moduli; $\boldsymbol{\varepsilon}^S$ is the $3\times 3$ matrix of dielectric permittivity moduli at constant mechanical strain. For inhomogeneous body these moduli will be functions of coordinates $\mathbf{x}$: $\mathbf{c}^E=\mathbf{c}^E(\mathbf{x})$; $\mathbf{e}=\mathbf{e}(\mathbf{x})$; $\boldsymbol{\varepsilon}^S=\boldsymbol{\varepsilon}^S(\mathbf{x})$. We will determine the effective moduli $\mathbf{c}^{Eeff}$, $\mathbf{e}^{eff}$, $\boldsymbol{\varepsilon}^{Seff}$ by the following technique [2–6]. We consider the static piezoelectric problem for representative volume $\Omega$:

$$\mathbf{L}^*(\nabla)\cdot\mathbf{T}=0\,,\qquad \nabla\cdot\mathbf{D}=0\,,\qquad \mathbf{x}\in\Omega\,; \tag{4}$$

$$\mathbf{u}=\mathbf{x}\cdot\boldsymbol{\varepsilon}_0\,,\qquad \varphi=-\mathbf{x}\cdot\mathbf{E}_0\,,\qquad \mathbf{x}\in\Gamma=\partial\Omega\,. \tag{5}$$

We call the problem (1)–(5) the $u\varphi$-problem and denote the solution of this problem by $\mathbf{u}^{u\varphi}$, $\varphi^{u\varphi}$. From the obtained solution we find $\mathbf{S}^{u\varphi}=\mathbf{S}(\mathbf{u}^{u\varphi})$, $\mathbf{E}^{u\varphi}=\mathbf{E}(\varphi^{u\varphi})$, $\mathbf{T}^{u\varphi}=\mathbf{T}(\mathbf{u}^{u\varphi},\varphi^{u\varphi})$ and $\mathbf{D}^{u\varphi}=\mathbf{D}(\mathbf{u}^{u\varphi},\varphi^{u\varphi})$.
From the set of solutions of these problems it is possible to define all effective moduli of porous piezocomposites. For example, piezoceramic, homogeneously polarized along the axis $x_3$, is anisotropic material of crystallographic class 6*mm* and have 10 independent moduli (5 elastic, 3 piezoelectric and 2 dielectric moduli). Thus, for all piezoceramic moduli determination it is enough to consider five various $u\varphi$-problems with different boundary conditions in (5). So we have the following problems and the formulae for calculation a full set of the effective moduli of porous piezoceramic:

I-$u\varphi$. $\boldsymbol{\varepsilon}_0=\varepsilon_0\mathbf{e}_1\mathbf{e}_1$, $\mathbf{E}_0=0$ $\Rightarrow$ $c_{1j}^{E\,\mathrm{eff},u\varphi}=\left\langle\sigma_{jj}^{u\varphi}\right\rangle/\varepsilon_0$; $j=1,2,3$; $e_{31}^{\mathrm{eff},u\varphi}=\left\langle D_3^{u\varphi}\right\rangle/\varepsilon_0$.

II-$u\varphi$. $\boldsymbol{\varepsilon}_0=\varepsilon_0\mathbf{e}_3\mathbf{e}_3$, $\mathbf{E}_0=0$ $\Rightarrow$ $c_{33}^{E\,\mathrm{eff},u\varphi}=\left\langle\sigma_{33}^{u\varphi}\right\rangle/\varepsilon_0$; $e_{33}^{\mathrm{eff},u\varphi}=\left\langle D_3^{u\varphi}\right\rangle/\varepsilon_0$; $c_{13}^{E\,\mathrm{eff},u\varphi}=\left\langle\sigma_{11}^{u\varphi}\right\rangle/\varepsilon_0=\left\langle\sigma_{22}^{u\varphi}\right\rangle/\varepsilon_0$.

III-$u\varphi$. $\boldsymbol{\varepsilon}_0=\varepsilon_0(\mathbf{e}_2\mathbf{e}_3+\mathbf{e}_3\mathbf{e}_2)$, $\mathbf{E}_0=0$ $\Rightarrow$ $c_{44}^{E\,\mathrm{eff},u\varphi}=\left\langle\sigma_{23}^{u\varphi}\right\rangle/(2\varepsilon_0)$; $e_{15}^{\mathrm{eff},u\varphi}=\left\langle D_2^{u\varphi}\right\rangle/(2\varepsilon_0)$.

IV-$u\varphi$. $\boldsymbol{\varepsilon}_0=0$, $\mathbf{E}_0=E_0\mathbf{e}_1$ $\Rightarrow$ $e_{15}^{\mathrm{eff},u\varphi}=-\left\langle\sigma_{13}^{u\varphi}\right\rangle/E_0$; $\varepsilon_{11}^{S\,\mathrm{eff},u\varphi}=\left\langle D_1^{u\varphi}\right\rangle/E_0$.

V-$u\varphi$. $\boldsymbol{\varepsilon}_0=0$, $\mathbf{E}_0=E_0\mathbf{e}_3$ $\Rightarrow$ $e_{31}^{\mathrm{eff},u\varphi}=-\left\langle\sigma_{11}^{u\varphi}\right\rangle/E_0=-\left\langle\sigma_{22}^{u\varphi}\right\rangle/E_0$; $e_{33}^{\mathrm{eff},u\varphi}=-\left\langle\sigma_{33}^{u\varphi}\right\rangle/E_0$; $\varepsilon_{33}^{S\,\mathrm{eff},u\varphi}=\left\langle D_3^{u\varphi}\right\rangle/E_0$.

Then, for the modeling of porous piezoceramics with 3-0 and 3-3 connectivities we consider the representative volumes having skeleton structure and apply the finite element (FE) technique for solution of problems (1)–(5) for inhomogeneous media. We develop FE models of high-porous ceramics (with open and closed types of pores) using the new cluster models, based on the percolation theory and assuming the heterogeneity of the polarization vector for a variety of piezoelectric finite elements [6]. Here, for taking into consideration inhomogeneous or incomplete ceramics polarization we perform the preliminary modeling of polarization process. To determine the zones that have different polarization we execute the finite element calculations of the electrostatic problem. The results of FEM modeling were compared with the experimental dates for different porous ceramics in the relative porosity range of 0-70 %. We note that for modeling porous material the calculation of inhomogeneous ceramics polarization is very important.

## FINITE ELEMENT ANALYSIS OF PIEZOELCTRIC DEVICES WITH POROUS PIEZOCERAMICS

The methods of the finite element simulation and corresponding computer programs were developed for the computation of composite piezoelectric devices, including the elements of porous or polycrystalline piezomaterials and loaded on the acoustic media, sensors and actuators, piezogeneratiors for the sources of renewed energy with piezoelements made of piezocomposite materials. Based on the results of the computer design, a broadband hydroacoustic piezoelectric transducer with multi-electrode coating was designed and its characteristics were investigated and improved.

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