

## Some computational aspects of homogenization of thermopiezoelectric composites

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On the basis of the paper [1] two topics are discussed. Firstly, exact formulae for the homogenized coefficients of a layered thermopiezoelectric composite are derived. Secondly, by applying the Ritz method, the local problems are solved approximately. Specific cases are also examined and illustrated.

### 1. INTRODUCTION

The first published results on homogenization of piezoelectric composites with periodic structure are due to the second author [2]. This author used the method of  $\Gamma$ -convergence. Next, Bloch expansion techniques were applied in [3] to the dynamic equations. As could be expected, the homogenized coefficients coincide with those derived in [2]. Different techniques of prediction of the effective moduli of piezoelectric composites were used in Refs. [4-13].

Homogenization of the equations of thermoelasticity with periodic coefficients was performed by Francfort [14,15]. Mathematically very elegant setting, without the assumption of periodicity was proposed in [16]. In the last paper, correctors were also introduced and investigated. If the initial conditions for the equations of thermoelasticity are nonhomogeneous, then the initial condition for the temperature of the homogenized system changes, somewhat surprising result. Homogenization of the equations of thermopiezoelectricity with periodic coefficients was performed by us in [1]. The formula for the initial temperature of the homogenized body reduces to that primarily derived by Francfort [14] in the absence of an electric field. Similar phenomenon was observed for the equations of thermodiffusion with not necessarily periodic structure [17].

It is worth noting that piezoelectric and thermopiezoelectric composite materials are receiving interest in the developing field of "smart" materials, cf. also [18,19]. They are also useful in modelling the behaviour of biological materials exhibiting piezo- and pyro-electric effects, cf. [2].

The aim of the present contribution is mainly twofold. Firstly, for a thermopiezoelectric layered composite with a microperiodic structure, analytical formulae for the homogenized coefficients are specified. This is a one-dimensional homogenization and the local problems involve ordinary derivatives only. Secondly, in order to find solutions of the *local* problems, general procedure of applying the Ritz method is outlined and next used in the two-dimensional case. To illustrate our procedure specific cases are solved and the results presented in the form of figures. In particular, we treat a composite made of two phases: quartz and lithium niobate. To make our paper self-contained as far as possible, we provide also the most important results of [1].

We observe that numerical methods for much simpler physical situations were developed in [20-25].

## 2. BASIC EQUATIONS

Let  $\Omega \subset \mathbb{R}^3$  be a bounded, sufficiently regular domain and  $(0, \tau)$  ( $\tau > 0$ ) — a time interval. The elastic, thermoelastic, piezoelectric, dielectric and pyroelectric moduli are denoted by  $c_{ijkl}$ ,  $\gamma_{ij}$ ,  $g_{ijk}$ ,  $\epsilon_{ij}$  and  $\lambda_i$ , respectively, *cf.* [26,27]. Throughout this paper small Latin indices take values 1, 2 and 3. Next,  $k_{ij}$  stands for the heat conductivity,  $\rho$  is the density and  $\beta = \frac{C_e}{T_0}$ ;  $C_e$  is the specific heat at constant strain per unit volume and  $T_0$  is the reference (absolute) temperature. We identify  $\bar{\Omega}$  with the underformed state of the thermopiezoelectric composite with a microperiodic structure. Thus for  $\varepsilon > 0$ , the material functions just introduced are  $\varepsilon Y$ -periodic, where  $Y = (0, Y_1) \times (0, Y_2) \times (0, Y_3)$  is the so-called basic cell, *cf.* [28–31]. More precisely, we write

$$\begin{aligned} c_{ijkl}^\varepsilon(x) &= c_{ijkl} \left( \frac{x}{\varepsilon} \right), & g_{ijk}^\varepsilon(x) &= g_{ijk} \left( \frac{x}{\varepsilon} \right), \\ \epsilon_{ij}^\varepsilon(x) &= \epsilon_{ij} \left( \frac{x}{\varepsilon} \right), & k_{ij}^\varepsilon(x) &= k_{ij} \left( \frac{x}{\varepsilon} \right), & \gamma_{ij}^\varepsilon(x) &= \gamma_{ij} \left( \frac{x}{\varepsilon} \right), \\ \lambda_i^\varepsilon(x) &= \lambda_i \left( \frac{x}{\varepsilon} \right), & \beta^\varepsilon(x) &= \beta \left( \frac{x}{\varepsilon} \right), & \rho^\varepsilon(x) &= \rho \left( \frac{x}{\varepsilon} \right), \end{aligned} \quad (1)$$

where  $x \in \Omega$  and the functions  $c_{ijkl}^\varepsilon$ ,  $g_{ijk}^\varepsilon$ , *etc.* are  $\varepsilon Y$ -periodic, where  $\varepsilon > 0$  is a small parameter.

For a fixed  $\varepsilon > 0$  the basic relations describing a linear, thermopiezoelectric solid with the microperiodic structure are, *cf.* [1,26,27]

### (i) Field equations

$$\begin{aligned} \sigma_{ij,j}^\varepsilon + b_i^\varepsilon &= \rho^\varepsilon \ddot{u}_i^\varepsilon & \text{in } \Omega \times (0, \tau), \\ D_{i,i}^\varepsilon &= 0 & \text{in } \Omega \times (0, \tau). \end{aligned} \quad (2)$$

### (ii) Heat equation

$$s^\varepsilon = (\kappa_{ij}^\varepsilon \theta_{,i}^\varepsilon)_{,j} + r^\varepsilon \quad \text{in } \Omega \times (0, \tau). \quad (3)$$

### (iii) Constitutive equations

$$\begin{aligned} \sigma_{ij}^\varepsilon &= c_{ijkl}^\varepsilon e_{kl}(\mathbf{u}^\varepsilon) - \gamma_{ij}^\varepsilon s^\varepsilon - g_{kij}^\varepsilon E_k(\varphi^\varepsilon), \\ \theta^\varepsilon &= -\gamma_{ij}^\varepsilon e_{ij}(\mathbf{u}^\varepsilon) + \beta^\varepsilon s^\varepsilon - \lambda_i^\varepsilon E_i(\varphi^\varepsilon), \\ D_i^\varepsilon &= g_{ikl}^\varepsilon e_{kl}(\mathbf{u}^\varepsilon) + \lambda_i^\varepsilon s^\varepsilon + \epsilon_{ik}^\varepsilon E_k(\varphi^\varepsilon). \end{aligned} \quad (4)$$

### (iv) Geometrical relations

$$e_{kl}(\mathbf{u}^\varepsilon) = u_{(k,l)}^\varepsilon = \frac{1}{2}(u_{k,l}^\varepsilon + u_{l,k}^\varepsilon), \quad E_k(\varphi^\varepsilon) = -\varphi_{,k}^\varepsilon. \quad (5)$$

Here  $\sigma_{ij}^\varepsilon$ ,  $u_i^\varepsilon$ ,  $b_i^\varepsilon$ ,  $\rho^\varepsilon$ ,  $E_i^\varepsilon$ ,  $D_i^\varepsilon$ ,  $\theta^\varepsilon$  and  $s^\varepsilon$  are the stress tensor, the displacement vector, the body force vector, the mass density, the electric field vector, the electric displacement vector, the relative temperature and the entropy, respectively. Moreover we have  $r^\varepsilon = \frac{R^\varepsilon}{T_0}$ ,  $\kappa_{ij}^\varepsilon = \frac{k_{ij}^\varepsilon}{T_0}$  and  $\beta^\varepsilon = \frac{C_e^\varepsilon}{T_0}$ , where  $R^\varepsilon$  represents heat sources;  $\mathbf{b}^\varepsilon$  and  $r^\varepsilon$  are  $\varepsilon Y$ -periodic.

We note that in our paper [1], the material coefficients appearing in Eqs. (4) were distinguished by a bar.

The tensors of material functions satisfy the usual symmetry conditions

$$c_{ijmn}^\varepsilon = c_{mnij}^\varepsilon = c_{ijnm}^\varepsilon = c_{jimn}^\varepsilon,$$

$$\gamma_{ij}^\varepsilon = \gamma_{ji}^\varepsilon, \quad g_{kij}^\varepsilon = g_{kji}^\varepsilon, \quad \epsilon_{ij}^\varepsilon = \epsilon_{ji}^\varepsilon.$$

We make the following assumption: there exists a constant  $\alpha > 0$  such that for almost every  $x \in \Omega$ , the following conditions are satisfied

$$\begin{aligned} c_{ijmn}^\varepsilon(x) e_{ij} e_{mn} &\geq \alpha |e|^2, & \gamma_{ij}^\varepsilon(x) a_i a_j &\geq \alpha |a|^2, \\ \kappa_{ij}^\varepsilon(x) a_i a_j &\geq \alpha |a|^2, & \epsilon_{ij}^\varepsilon(x) a_i a_j &\geq \alpha |a|^2, \end{aligned} \quad (6)$$

for each  $e \in \mathbb{E}_s^3$  and each  $a \in \mathbb{R}^3$ ; here  $\mathbb{E}_s^3$  is the space of symmetric  $3 \times 3$  matrices.

Substituting (4) into Eqs. (2) and (3) we obtain ( $\epsilon > 0$  and fixed):

$$\begin{aligned} (c_{ijmn}^\varepsilon u_{m,n}^\varepsilon - \gamma_{ij}^\varepsilon s^\varepsilon + g_{kij}^\varepsilon \varphi_{,k}^\varepsilon)_{,j} + b_i^\varepsilon &= \rho^\varepsilon \ddot{u}_i^\varepsilon, \\ (g_{imn}^\varepsilon u_{m,n}^\varepsilon + \lambda_i^\varepsilon s^\varepsilon - \epsilon_{ik}^\varepsilon \varphi_{,k}^\varepsilon)_{,i} &= 0, \\ s^\varepsilon &= [\kappa_{ij}^\varepsilon (-\gamma_{mn}^\varepsilon u_{m,n}^\varepsilon + \beta^\varepsilon s^\varepsilon + \lambda_k^\varepsilon \varphi_{,k}^\varepsilon)_{,i}]_{,j} + r^\varepsilon. \end{aligned} \quad (7)$$

Obviously,  $u^\varepsilon$ ,  $s^\varepsilon$ ,  $\varphi^\varepsilon$ ,  $b^\varepsilon$ , and  $r^\varepsilon$  are functions of  $x \in \Omega$  and  $t \in (0, \tau)$ .

Equations (7) represent the system of equations for finding  $u^\varepsilon$ ,  $\varphi^\varepsilon$  and  $s^\varepsilon$ . It has to be completed by the boundary and initial conditions. We assume the *homogeneous boundary conditions*:

$$u^\varepsilon(x, t) = 0, \quad \theta^\varepsilon(x, t) = 0, \quad \varphi^\varepsilon(x, t) = 0 \quad (8)$$

for  $x \in \partial\Omega$  and  $t \in [0, \tau]$ ;  $\partial\Omega$  stands for the boundary of  $\Omega$ .

The *initial conditions* are

$$\begin{aligned} u^\varepsilon(x, 0) &= \mathbf{U}(x), & \dot{u}^\varepsilon(x, 0) &= \mathbf{V}(x), \\ \theta^\varepsilon(x, 0) &= T(x), & \varphi^\varepsilon(x, 0) &= F(x). \end{aligned} \quad (9)$$

The functions  $\mathbf{U}$ ,  $\mathbf{V}$ ,  $T$  and  $F$  are prescribed.

Under physically reasonable assumptions, a solution  $(u^\varepsilon, \varphi^\varepsilon, s^\varepsilon)$  to the initial-boundary value problem just formulated exists and is unique.

### 3. HOMOGENIZATION

In order to find the effective or macroscopic coefficients we employed the method of two-scale asymptotic expansions, cf. [29, 30]. In our case we make the following *Ansatz*

$$\begin{aligned} u^\varepsilon(x, t) &= u^0(x, y, t) + \varepsilon u^1(x, y, t) + \varepsilon^2 u^2(x, y, t) + \dots \\ \varphi^\varepsilon(x, t) &= \varphi^0(x, y, t) + \varepsilon \varphi^1(x, y, t) + \varepsilon^2 \varphi^2(x, y, t) + \dots \\ s^\varepsilon(x, t) &= s^0(x, y, t) + \varepsilon s^1(x, y, t) + \varepsilon^2 s^2(x, y, t) + \dots \end{aligned} \quad (10)$$

where  $y = \frac{x}{\varepsilon}$ . The functions  $u^0(x, \cdot, t)$ ,  $u^1(x, \cdot, t)$ ,  $\dots$ ,  $\varphi^0(x, \cdot, t)$ ,  $\varphi^1(x, \cdot, t)$ ,  $\dots$ ,  $s^0(x, \cdot, t)$ ,  $s^1(x, \cdot, t)$ , etc., are  $Y$ -periodic. The main steps of the asymptotic analysis are outlined in the paper [1]. We

shall now provide those results which are essential for our subsequent considerations. For a function  $f \in L^1(Y)$  we set

$$\langle f \rangle = \frac{1}{|Y|} \int_Y f(y) dy.$$

The homogenized form of Eqs. (3) and (7)<sub>1,2</sub> is

$$\begin{aligned} \langle \rho \rangle \frac{\partial^2 u_i^0}{\partial t^2} &= c_{ijmn}^h \frac{\partial^2 u_m^0}{\partial x_j \partial x_n} + g_{kij}^h \frac{\partial^2 \Phi^0}{\partial x_j \partial x_k} - \gamma_{ij}^h \frac{\partial \theta^h}{\partial x_j} + \langle b_i \rangle, \\ \frac{\partial}{\partial t} \langle s^0 \rangle &= \kappa_{ij}^h \frac{\partial^2 \theta^h}{\partial x_j \partial x_i} + \langle r \rangle, \\ g_{ikj}^h \frac{\partial^2 u_k^0}{\partial x_j \partial x_i} - \epsilon_{ij}^h \frac{\partial^2 \Phi^0}{\partial x_j \partial x_i} + \lambda_i^h \frac{\partial \theta^h}{\partial x_i} &= 0. \end{aligned} \quad (11)$$

We observe that the displacement field  $u^0(x, t)$  and electric potential field  $\Phi^0(x, t)$  do not depend on the local variable  $y \in Y$ . The entropy of the homogenized thermopiezoelectric solid is the average of  $s^0(x, y, t)$  over  $Y$  and thus it is equal to  $\langle s^0(x, y, t) \rangle = \frac{1}{|Y|} \int_Y s^0(x, y, t) dy$ . The physical interpretation of  $\theta^h(x, t)$  is readily inferred from (11); it is the temperature field of the homogenized body.

The effective coefficients are given by the following expressions:

$$\begin{aligned} c_{ijmn}^h &= \left\langle c_{ijmn} + c_{ijpq} \frac{\partial \chi_p^{(mn)}}{\partial y_q} + g_{pij} \frac{\partial \theta^{(mn)}}{\partial y_p} \right\rangle, \\ g_{kij}^h &= \left\langle g_{kij} + c_{ijmn} \frac{\partial \Phi_m^{(k)}}{\partial y_n} + g_{mij} \frac{\partial R^{(k)}}{\partial y_m} \right\rangle, \\ \gamma_{ij}^h &= \left\langle \gamma_{ij} - c_{ijpq} \frac{\partial \Gamma_p}{\partial y_q} - g_{kij} \frac{\partial Q}{\partial y_k} \right\rangle, \\ \kappa_{ij}^h &= \left\langle \kappa_{ij} + \kappa_{ik} \frac{\partial \Theta_j}{\partial y_k} \right\rangle, \\ \epsilon_{im}^h &= \left\langle \epsilon_{im} - g_{ipq} \frac{\partial \Phi_p^{(m)}}{\partial y_q} + \epsilon_{ik} \frac{\partial R^{(m)}}{\partial y_k} \right\rangle, \\ \lambda_i^h &= \left\langle \lambda_i - \epsilon_{ik} \frac{\partial Q}{\partial y_k} + g_{ipq} \frac{\partial \Gamma_p}{\partial y_q} \right\rangle, \\ \beta^h &= \left\langle \beta + \gamma_{pq} \frac{\partial \Gamma_p}{\partial y_q} + \lambda_k \frac{\partial Q}{\partial y_k} \right\rangle \end{aligned} \quad (12)$$

where the *local* functions  $\chi_i^{(mn)}$ ,  $\theta^{(mn)}$ ,  $\Phi_i^{(m)}$ ,  $\Gamma_i$ ,  $R^{(m)}$ ,  $Q$  and  $\Theta_i$  are  $Y$ -periodic. They are solutions to the *local* problems which will now be formulated.

Let us assume that the periodic material functions  $c_{ijkl}(y)$ ,  $g_{ijk}(y)$ , etc. are of class  $L^\infty(Y)$ . Such case includes layered thermopiezoelectric materials. We set

$$H_{\text{per}}(Y) = \{v \in H^1(Y) \mid v \text{ takes equal values on opposite sides of } Y\}, \quad (13)$$

$$H_{\text{per}}(Y, \mathbb{R}^3) = \{\mathbf{v} = (v_i) \mid v_i \in H_{\text{per}}(Y), \quad i = 1, 2, 3\}. \quad (14)$$

The unknown periodic local functions entering Eqs. (12) are solutions to the following local problems.



**Problem P<sub>loc</sub><sup>1</sup>**

Find  $\chi_i^{(mn)} \in H_{\text{per}}(Y)$  and  $\theta^{(mn)} \in H_{\text{per}}(Y)$  such that

$$\int_Y [c_{ijmn}(y) + c_{ijpq}(y)e_{pq}^y(\chi^{(mn)}) + g_{kij}(y) \frac{\partial \theta^{(mn)}}{\partial y_k}] e_{ij}^y(\mathbf{v}) dy = 0 \quad \forall \mathbf{v} \in H_{\text{per}}(Y, \mathbb{R}^3),$$

$$\int_Y \left[ g_{imn}(y) + g_{ipq}(y)e_{pq}^y(\chi^{(mn)}) - \epsilon_{ik}(y) \frac{\partial \theta^{(mn)}}{\partial y_k} \right] \frac{\partial w}{\partial y_i} dy = 0 \quad \forall w \in H_{\text{per}}(Y).$$

**Problem P<sub>loc</sub><sup>2</sup>**

Find  $\Phi_i^{(m)} \in H_{\text{per}}(Y)$  and  $R^{(m)} \in H_{\text{per}}(Y)$  such that

$$\int_Y \left[ g_{mij}(y) + g_{kij}(y) \frac{\partial R^{(m)}}{\partial y_k} + c_{ijpq}(y)e_{pq}^y(\Phi^{(m)}) \right] e_{ij}^y(\mathbf{v}) dy = 0 \quad \forall \mathbf{v} \in H_{\text{per}}(Y, \mathbb{R}^3),$$

$$\int_Y \left[ \epsilon_{im}(y) + \epsilon_{ik} \frac{\partial R^{(m)}}{\partial y_k} - g_{ipq}e_{pq}^y(\Phi^{(m)}) \right] \frac{\partial w}{\partial y_i} dy = 0 \quad \forall w \in H_{\text{per}}(Y).$$

**Problem P<sub>loc</sub><sup>3</sup>**

Find  $\Gamma_i \in H_{\text{per}}(Y)$  and  $Q \in H_{\text{per}}(Y)$  such that

$$\int_Y \left[ \gamma_{ij}(y) - c_{ijpq}(y)e_{pq}^y(\Gamma) - g_{kij}(y) \frac{\partial Q}{\partial y_k} \right] e_{ij}^y(\mathbf{v}) dy = 0 \quad \forall \mathbf{v} \in H_{\text{per}}(Y, \mathbb{R}^3),$$

$$\int_Y \left[ \lambda_i(y) + g_{ipq}(y)e_{pq}^y(\Gamma) - \epsilon_{ik} \frac{\partial Q}{\partial y_k} \right] \frac{\partial w}{\partial y_i} dy = 0 \quad \forall w \in H_{\text{per}}(Y),$$

where

$$e_{ij}^y(\mathbf{v}) = \frac{1}{2} \left( \frac{\partial v_i}{\partial y_j} + \frac{\partial v_j}{\partial y_i} \right).$$

Moreover,  $\Theta = (\Theta_i)$  is a solution to the following

**Problem P<sub>loc</sub><sup>4</sup>**

Find  $\Theta_i \in H_{\text{per}}(Y)$  such that

$$\int_Y \left[ \kappa_{ik}(y) + \kappa_{ij}(y) \frac{\partial \Theta_k}{\partial y_j} \right] \frac{\partial v_k}{\partial y_i} dy = 0 \quad \forall \mathbf{v} \in H_{\text{per}}(Y, \mathbb{R}^3).$$

**Remark 3.1**

In fact, the two-scale asymptotic method leads directly to the strong formulation of the local problems. Consequently, the material functions involved have to be more regular, at least of class  $C^1(Y)$ . However, the point of departure can be the weak (variational) form of system (7). Then the local problems are given above.

**Remark 3.2**

Having in mind specific problems, for instance layered materials, it is convenient to introduce the following notation:

$$c_{ijmn} = c_{ijmn}, \quad \chi_m^{(ij)} = \chi_m^{(ij)},$$

$$c_{4jmn} = g_{jmn}, \quad \chi_m^{(i4)} = \Phi_m^{(i)},$$

$$c_{4j4n} = -\epsilon_{jn}, \quad \chi_4^{(ij)} = \theta^{(ij)},$$

$$c_{ij44} = -\gamma_{ij}, \quad \chi_4^{(4i)} = R^{(i)},$$

$$c_{4j44} = \lambda_j, \quad \chi_k^{(44)} = \Gamma_k,$$

$$c_{4444} = \beta(y), \quad \chi_4^{(44)} = Q,$$

where  $\alpha, \beta, \gamma = 1, 2, 3, 4$  and  $i, j, k, m, n = 1, 2, 3$ .

Then the strong formulation of the local problems  $P_{\text{loc}}^i$  ( $i = 1, 2, 3$ ) reduces to finding  $Y$ -periodic functions  $\chi_\gamma^{(\alpha\beta)}$  satisfying the relation

$$\frac{\partial}{\partial y_i} \left[ c_{\alpha i \gamma n} \frac{\partial \chi_\gamma^{(\mu\nu)}}{\partial y_n} \right] = -\frac{\partial}{\partial y_i} c_{\alpha i \mu \nu}, \quad (15)$$

and the homogenized (effective) moduli are

$$c_{\alpha\beta\mu\nu}^h = \langle c_{\alpha\beta\mu\nu} \rangle + \left\langle c_{\alpha\beta\gamma n} \frac{\partial \chi_\gamma^{(\mu\nu)}}{\partial y_n} \right\rangle. \quad (16)$$

Thus the effective thermopiezoelectric coefficients are completely described by  $c_{\alpha\beta\mu\nu}^h$  and  $\kappa_{ij}^h$ .

**4. MICROPERIODIC LAYERED COMPOSITE**

Now the basic cell reduces to an interval, say  $(0,1)$ , cf. Fig. 1. We assume that the material coefficients of such a composite are piecewise constant; for the lamination in the direction  $y_3$  they are

$$c_{\alpha\beta\mu\nu}(y) = \begin{cases} c_{\alpha\beta\mu\nu}^{(1)} & \text{for } y_3 \in (0, \xi), \\ c_{\alpha\beta\mu\nu}^{(2)} & \text{for } y_3 \in (\xi, 1). \end{cases}$$

Thus the composite is made of two materials. After lengthy, though simple calculations the local functions can be found in a closed form; they are piecewise linear, cf. [17]; moreover

$$c_{\alpha\beta\mu\nu}^h = \langle c_{\alpha\beta\mu\nu} \rangle - \xi(1-\xi)(\tilde{B}^{-1})^{\kappa\lambda} \llbracket c_{\lambda 3 \alpha \beta} \rrbracket \llbracket c_{\mu \nu \kappa 3} \rrbracket, \quad (17)$$

where

$$\langle c_{\alpha\beta\mu\nu} \rangle = \xi c_{\alpha\beta\mu\nu}^{(1)} + (1-\xi) c_{\alpha\beta\mu\nu}^{(2)},$$

and

$$\llbracket c_{\alpha\beta\mu\nu} \rrbracket = c_{\alpha\beta\mu\nu}^{(2)} - c_{\alpha\beta\mu\nu}^{(1)},$$

$$\llbracket \tilde{B}_{\alpha\beta} \rrbracket = \llbracket \xi c_{\alpha 3 \beta 3}^{(2)} + (1-\xi) c_{\alpha 3 \beta 3}^{(1)} \rrbracket.$$

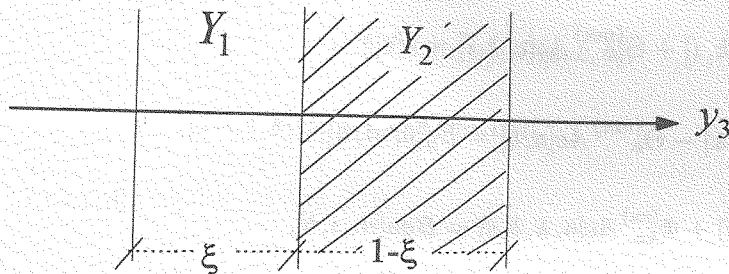


Fig. 1. Layered composite: basic cell;  $Y_1$  — material with coefficients  $c_{\alpha\beta\gamma\delta}^{(1)}$  and  $\kappa_{\alpha\beta}^{(1)}$ ;  $Y_2$  — material with coefficients  $c_{\alpha\beta\gamma\delta}^{(2)}$  and  $\kappa_{\alpha\beta}^{(2)}$

These coefficients have to be completed by the heat conductivity  $\kappa_{ij}$ , which is also piecewise constant. Homogenized heat conductivity coefficient reads

$$\kappa_{ij}^h = \langle \kappa_{ij} \rangle - \xi(1 - \xi) \widetilde{K}^{-1} [\kappa_{i3}] [\kappa_{j3}], \quad (18)$$

where

$$\widetilde{K} = \xi \kappa_{33}^{(2)} + (1 - \xi) \kappa_{33}^{(1)}.$$

## 5. RITZ METHOD

To find the effective coefficients one has to solve primarily the local problems. The Ritz method offers a possibility of determination of the local functions in an approximate manner. Below, we apply this method to our thermopiezoelectric problem.

### 5.1. General case

We shall be looking for an approximate solution of the local problems by the Ritz method. Accordingly, we take

$$\begin{aligned} \chi_k^{(mn)} &= \chi_{ka}^{(mn)} \phi^a(y), & \theta^{(mn)} &= \Theta_a^{(mn)} \phi^a(y), \\ R^{(m)} &= R_a^{(m)} \phi^a(y), & \Phi_k^{(m)} &= \Phi_{ka}^{(m)} \phi^a(y), \\ \Gamma_k &= \Gamma_{ka} \phi^a(y), & Q &= Q_a \phi^a(y). \end{aligned} \quad (19)$$

Here  $\phi^a(y)$ ,  $a = 1, 2, \dots, \tilde{a}$  (the base functions) are prescribed  $Y$ -periodic functions and  $\chi_{ka}^{(mn)}$ ,  $\Theta_a^{(mn)}$ ,  $R_a^{(m)}$ ,  $\Phi_{ka}^{(m)}$ ,  $\Gamma_{ka}$ ,  $Q_a$  are unknown constants. Obviously, the summation convention still applies.

The local problems  $P_{loc}^i$  ( $i=1,2,3$ ) should now be satisfied for test functions of the form

$$v_i = v_{ia} \phi^a(y), \quad w = w_a \phi^a(y). \quad (20)$$

To determine the unknown constants one has to solve the following algebraic equations:

$$\begin{aligned}
 \chi_{ka}^{(mn)} Ac[a, b, k, i] + \Theta_a^{(mn)} Ag[a, b, i] &= Bc[b, i, m, n], \\
 \chi_{ka}^{(mn)} Ag[b, a, k] - \Theta_a^{(mn)} Ae[a, b] &= Bg[b, m, n], \\
 R_a^{(m)} Ag[a, b, i] + \Phi_{ka}^{(m)} Ac[a, k, b, i] &= Bga[m, i, b], \\
 R_a^{(m)} Ae[a, b] - \Phi_{ka}^{(m)} Ag[b, a, k] &= Be[b, m], \\
 \Gamma_{ka} Ac[a, k, b, i] + Q_a Ag[a, b, i] &= -Bgm[b, i], \\
 \Gamma_{ka} Ag[b, a, k] - Q_a Ae[a, b] &= Blm[b],
 \end{aligned} \tag{21}$$

where

$$\begin{aligned}
 Ac[a, j, b, n] &= \int_Y c_{ijkn} \phi_{,i}^a \phi_{,k}^b dY, & Ag[a, b, n] &= \int_Y g_{ikn} \phi_{,i}^a \phi_{,k}^b dY, \\
 Ae[a, b] &= \int_Y \epsilon_{ik} \phi_{,i}^a \phi_{,k}^b dY, & Bc[a, j, m, n] &= - \int_Y c_{ijmn} \phi_{,i}^a dY, \\
 Bg[a, m, n] &= - \int_Y g_{imn} \phi_{,i}^a dY, & Bga[i, m, a] &= - \int_Y g_{imn} \phi_{,n}^a dY, \\
 Be[a, m] &= - \int_Y \epsilon_{im} \phi_{,i}^a dY, & Blm[a] &= - \int_Y \lambda_i \phi_{,i}^a dY, \\
 Bgm[a, m] &= - \int_Y \gamma_{im} \phi_{,i}^a dY
 \end{aligned} \tag{22}$$

with  $\phi_{,i}^a = \frac{\partial \phi^a}{\partial y_i}$ , and

$$\begin{aligned}
 A[a, j, b, i] &= Ac[a, j, b, i] + AB[d, a, j] Ag[d, b, i], \\
 B[b, i] &= -Bgm[b, i] + AB[d, b, i] Blm[d], \\
 B[j, m, a] &= Bga[j, m, a] - AB[d, a, m] Be[d, j], \\
 B[a, j, m, n] &= Bc[a, j, m, n] - AB[d, a, j] Bg[d, m, n]
 \end{aligned}$$

with

$$AB[d, a, j] = (Ae)^{-1}[c, d] Ag[c, a, j].$$

The solution of the system of equations (21) is given by

$$\begin{aligned}
\chi_{ka}^{(mn)} &= (A)^{-1}[d, i, a, k]B[d, i, m, n], \\
\Theta_a^{(mn)} &= -(Ae)^{-1}[b, a]Bg[b, m, n] + (A)^{-1}[d, i, c, k]B[d, i, m, n]AB[a, c, k], \\
R_a^{(m)} &= (Ae)^{-1}[b, a]Be[b, m] + (A)^{-1}[d, i, c, k]B[m, i, d]AB[a, c, k], \\
\Phi_{ka}^{(m)} &= (A)^{-1}[d, i, a, k]B[m, i, d], \\
\Gamma_{ka} &= (A)^{-1}[d, i, a, k]B[d, i], \\
Q_a &= -(Ae)^{-1}[b, a]Blm[b] + (A)^{-1}[d, i, c, k]B[d, i]AB[a, c, k],
\end{aligned} \tag{23}$$

Symbols  $(Ae)^{-1}$  and  $(A)^{-1}$  denote inverse matrices of  $(Ae)$  and  $(A)$ , defined in this order by

$$(Ae)^{-1}[b, a]Ae[a, c] = \sum_{a=1}^{\bar{a}} (Ae)^{-1}[b, a]Ae[a, c] = \delta_{bc}$$

and

$$(A)^{-1}[b, n, a, m]A[a, m, c, k] = \sum_{a=1}^{\bar{a}} \sum_{m=1}^3 (A)^{-1}[b, n, a, m]A[a, m, c, k] = \delta_{bc}\delta_{kn}.$$

Finally, the homogenized coefficients can be written as follows:

$$\begin{aligned}
c_{ijkl}^h &= \langle c_{ijkl} \rangle + (Ae)^{-1}[b, a]Bg[b, k, l]Bg[a, i, j] \\
&\quad - (A)^{-1}[b, n, a, m]B[b, n, k, l]B[a, m, i, j], \\
g_{kij}^h &= \langle g_{kij} \rangle - (Ae)^{-1}[b, a]Be[b, k]Bg[a, i, j] \\
&\quad - (A)^{-1}[b, n, a, m]B[k, n, b]B[a, m, i, j], \\
\gamma_{ij}^h &= \langle \gamma_{ij} \rangle - (Ae)^{-1}[b, a]Blm[b]Bg[a, i, j] \\
&\quad + (A)^{-1}[b, n, a, m]B[b, n, i, j]B[a, m], \\
\epsilon_{ij}^h &= \langle \epsilon_{ij} \rangle - (Ae)^{-1}[b, a]Be[b, i]Be[a, j] \\
&\quad + (A)^{-1}[b, n, a, m]B[i, n, b]B[j, m, a], \\
\lambda_i^h &= \langle \lambda_i \rangle - (Ae)^{-1}[b, a]Blm[b]Be[a, i] \\
&\quad - (A)^{-1}[b, n, a, m]B[i, n, b]B[a, m], \\
\beta^h &= \langle \beta \rangle - (Ae)^{-1}[b, a]Blm[b]Blm[a] \\
&\quad + (A)^{-1}[b, n, a, m]B[b, n]B[a, m].
\end{aligned} \tag{24}$$

## 5.2. Specific two-dimensional problem: two-phase composite

To illustrate the outlined general procedure we consider a two-phase composite material with piecewise constant coefficients, provided that they do not depend on  $y_3$  (two-dimensional homogenization):

$$c_{\alpha\beta\mu\nu}(y) = \begin{cases} c_{\alpha\beta\mu\nu}^{(1)} & \text{for } y \in Y_1, \\ c_{\alpha\beta\mu\nu}^{(2)} & \text{for } y \in Y_2, \end{cases} \quad \alpha, \beta, \mu, \nu = 1, 2, 3, 4. \quad (25)$$

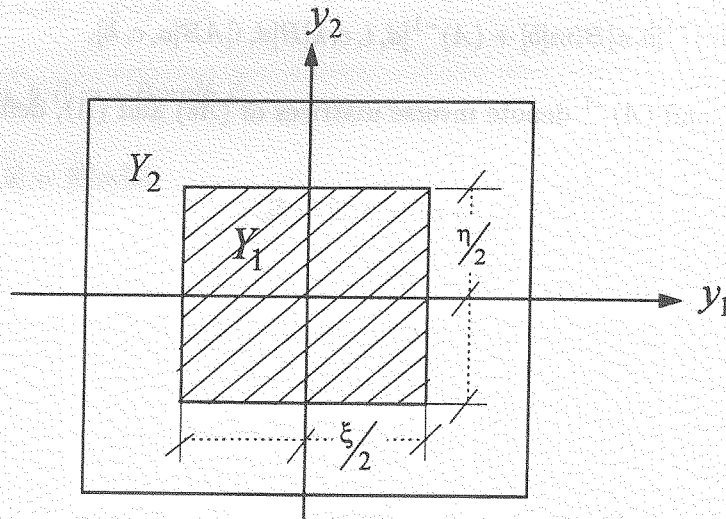


Fig. 2. Basic cell of two-dimensional composite

Fig. 2 describes the basic cell; now  $\phi_3^a = \frac{\partial \phi^a}{\partial y_3} = 0$  while (22) simply takes the form

$$\begin{aligned} Ac[a, k, b, i] &= c_{Lkji}^{(2)} F[a, b, L, J] + [c_{Lkji}] f[a, b, L, J], \\ Ag[a, b, k] &= g_{LkJ}^{(2)} F[a, b, L, J] + [g_{LkJ}] f[a, b, L, J], \\ Ae[a, b] &= \epsilon_{LJ}^{(2)} F[a, b, L, J] + [\epsilon_{LJ}] f[a, b, L, J], \\ Bc[a, i, m, n] &= [c_{Kimn}] f[a, K], & Bg[a, m, n] &= [g_{Kmn}] f[a, K], \\ Bga[k, i, a] &= [g_{kiK}] f[a, K], & Be[a, m] &= [\epsilon_{Km}] f[a, K], \\ Blm[a] &= [\lambda_K] f[a, K], & Bgm[a, i] &= [\gamma_{Ki}] f[a, K]. \end{aligned} \quad (26)$$

Here

$$\begin{aligned} f[a, b, L, J] &= \int_{Y_1} \frac{\partial \phi^a}{\partial y_L} \frac{\partial \phi^a}{\partial J} dY, & F[a, b, L, J] &= \int_Y \frac{\partial \phi^a}{\partial y_L} \frac{\partial \phi^a}{\partial y_J} dY, \\ f[a, K] &= \int_{Y_1} \frac{\partial \phi^a}{\partial y_K} dY & \text{and } K, J, \dots &= 1, 2. \end{aligned}$$



### 5.2.1. Base functions

We take the following base functions

$$\phi^1(y_1, y_2) = \begin{cases} \xi y_1 + \frac{\xi}{2} & \text{for } y_1 \in \left(-\frac{1}{2}, -\frac{\xi}{2}\right), \\ -(1-\xi)y_1 & \text{for } y_1 \in \left(-\frac{\xi}{2}, \frac{\xi}{2}\right), \\ \xi y_1 - \frac{\xi}{2} & \text{for } y_1 \in \left(\frac{\xi}{2}, \frac{1}{2}\right); \end{cases} \quad (27)$$

$$\phi^2(y_1, y_2) = \begin{cases} \eta y_2 + \frac{\eta}{2} & \text{for } y_2 \in \left(-\frac{1}{2}, -\frac{\eta}{2}\right), \\ -(1-\eta)y_2 & \text{for } y_2 \in \left(-\frac{\eta}{2}, \frac{\eta}{2}\right), \\ \eta y_2 - \frac{\eta}{2} & \text{for } y_2 \in \left(\frac{\eta}{2}, \frac{1}{2}\right); \end{cases} \quad (28)$$

$$\phi^3(y_1, y_2) = \cos(\pi y_1) \sin(2\pi y_2), \quad (29)$$

$$\phi^4(y_1, y_2) = \cos(\pi y_2) \sin(2\pi y_1). \quad (30)$$

Next, we calculate

$$\phi_{,1}^1(y_1, y_2) = \begin{cases} -(1-\xi) & \text{for } y_1 \in \left(-\frac{\xi}{2}, \frac{\xi}{2}\right), \\ \xi & \text{for } y_1 \in \left(-\frac{1}{2}, -\frac{\xi}{2}\right) \cup \left(\frac{\xi}{2}, \frac{1}{2}\right); \end{cases}$$

$$\phi_{,2}^1(y_1, y_2) = 0, \quad \phi_{,1}^2(y_1, y_2) = 0,$$

$$\phi_{,2}^2(y_1, y_2) = \begin{cases} -(1-\eta) & \text{for } y_2 \in \left(-\frac{\eta}{2}, \frac{\eta}{2}\right), \\ \eta & \text{for } y_2 \in \left(-\frac{1}{2}, -\frac{\eta}{2}\right) \cup \left(\frac{\eta}{2}, \frac{1}{2}\right); \end{cases}$$

$$\phi_{,1}^3(y_1, y_2) = -\pi \sin(\pi y_1) \sin(2\pi y_2), \quad \phi_{,2}^3(y_1, y_2) = 2\pi \cos(\pi y_1) \cos(2\pi y_2),$$

$$\phi_{,1}^4(y_1, y_2) = 2\pi \cos(2\pi y_1) \cos(\pi y_2), \quad \phi_{,2}^4(y_1, y_2) = -\pi \sin(2\pi y_1) \sin(\pi y_2).$$

## 6. EXAMPLE: COMPOSITE MADE OF QUARTZ AND LITHIUM NIOBATE

In this section we examine a two-phase composite for which the basic cell is two-dimensional, *cf.* Fig. 2. The material of the inclusion  $Y_1$  is quartz, while the matrix  $Y_2 = Y \setminus Y_1$  is made of lithium niobate.

Prior to solving such two-dimensional homogenization problem, we specify the material coefficients characterizing these two components.

## 6.1. Material coefficients

Quartz, cf. [27,32,33]

(i) Density:  $\rho = 2.65 \cdot 10^3 \frac{\text{kg}}{\text{m}^3}$ .

(ii) Heat capacity

$$c_e = 0.188 \frac{\text{cal}}{\text{g}1^0} = 0.7871 \frac{\text{J}}{\text{g}1^0}, \quad C_e = \rho c_e = 2.086 \cdot 10^6 \frac{\text{J}}{\text{m}^3 1^0}, \quad T_0 = 300^0 \text{K},$$

$$\beta = \frac{C_e}{T_0} = 6.953 \cdot 10^3 \frac{\text{J}}{\text{m}^3 (1^0)^2}, \quad \beta^{-1} = 0.1438 \cdot 10^{-3} \frac{\text{m}^2 (1^0)^2}{\text{N}}.$$

The indices used here take the following values, cf. [17]:

$$\begin{array}{cccccc} (ij) \rightarrow & (11) & (22) & (33) & (23) = (32) & (13) = (31) & (12) = (21) \\ K \rightarrow & 1 & 2 & 3 & 4 & 5 & 6 \end{array}$$

(iii) Elastic moduli (units:  $10^{10} \frac{\text{N}}{\text{m}^2}$ )

$$(c_{ijkl}) = (c_{KLM}) = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & \frac{1}{2}(c_{11} - c_{12}) \end{bmatrix}$$

$$\begin{array}{llll} c_{11} = 8.674, & c_{12} = 0.699, & c_{13} = 1.191, & c_{14} = -1.791, \\ c_{33} = 10.72, & c_{44} = 5.794, & c_{66} = 3.988. & \end{array}$$

(iv) Piezoelectric coefficients (units:  $\frac{\text{C}}{\text{m}^2}$ )

$$(g_{ijk}) = (g_{iK}) = \begin{bmatrix} g_{11} & -g_{11} & 0 & g_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -g_{14} & -g_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$g_{11} = 0.171, \quad g_{14} = -0.04.$$

(v) Dielectric coefficients (units:  $10^{-10} \frac{\text{F}}{\text{m}}$ )

$$(\epsilon_{ij}) = \begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{11} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}$$

$$\epsilon_{11} = 0.392, \quad \epsilon_{33} = 0.41.$$

(vi) Heat conductivity (units:  $\frac{\text{cal}}{\text{s}^2 \text{cm}}$ )

$$(k_{ij}) = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{11} & 0 \\ 0 & 0 & k_{33} \end{bmatrix}$$

$$k_{11} = 0.016, \quad k_{33} = 0.030.$$

(vii) Thermal expansion coefficients (units:  $10^{-6} \frac{1}{10}$ )

$$(\alpha_{ij}) = \begin{bmatrix} \alpha_{11} & 0 & 0 \\ 0 & \alpha_{11} & 0 \\ 0 & 0 & \alpha_{33} \end{bmatrix}$$

$$\alpha_{11} = 13.37, \quad \alpha_{33} = 7.97, \quad \gamma_{ij} = c_{ijmn} \alpha_{mn}.$$

**Lithium niobate** (Li Nb O<sub>3</sub>), cf. [32]:

(i) Elastic moduli (units:  $10^{10} \frac{\text{N}}{\text{m}^2}$ )

$$(c_{ijkl}) = (c_{KLM}) = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & \frac{1}{2}(c_{11} - c_{12}) \end{bmatrix}$$

$$c_{11} = 20.3, \quad c_{12} = 5.3, \quad c_{13} = 7.5, \quad c_{14} = 0.9,$$

$$c_{33} = 23.5, \quad c_{44} = 6.0.$$

(ii) Piezoelectric coefficients (units:  $\frac{\text{C}}{\text{m}^2}$ )

$$(g_{ijk}) = (g_{iK}) = \begin{bmatrix} 0 & 0 & 0 & 0 & g_{15} & -g_{22} \\ -g_{22} & g_{22} & 0 & g_{15} & 0 & 0 \\ g_{31} & g_{31} & g_{33} & 0 & 0 & 0 \end{bmatrix}$$

$$g_{15} = 3.7, \quad g_{22} = 2.5, \quad g_{31} = 0.2, \quad g_{33} = 1.3.$$

(iii) Dielectric coefficients (units:  $10^{-10} \frac{\text{F}}{\text{m}}$ )

$$(\epsilon_{ij}) = \begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{11} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}$$

$$\epsilon_{11} = 3.89, \quad \epsilon_{33} = 2.57.$$

## 6.2. Numerical results

We have examined both the one-dimensional and two-dimensional problems. In the first case exact homogenization formulae specified in Section 4 were used.

The superscript "(1)" in the material coefficients corresponds now to the layer made of quartz.

(i) *One-dimensional case*

On the basis of formula (17) we have computed elastic, piezoelectric and dielectric homogenized coefficients. We have considered three laminations determined by three Cartesian axes  $\{y_i\}$ , ( $i = 1, 2, 3$ ): Some of our calculations are depicted in Figs. 3–5. An interesting conclusion can be drawn from the upper and lower parts of Fig. 4. In the case of the lamination determined by  $y_3$ , for a certain range of the volume ratio  $v$  the coefficient  $g_{311}^h$  is negative, though both  $g_{311}^{(1)}$  and  $g_{311}^{(2)}$  are nonnegative. Also, the coefficient  $g_{111}^h$  for the lamination determined by  $y_1$  is larger than  $g_{111}^{(1)}$  and  $g_{111}^{(2)}$  in certain interval of  $v$ , see the lower part of Fig. 4.

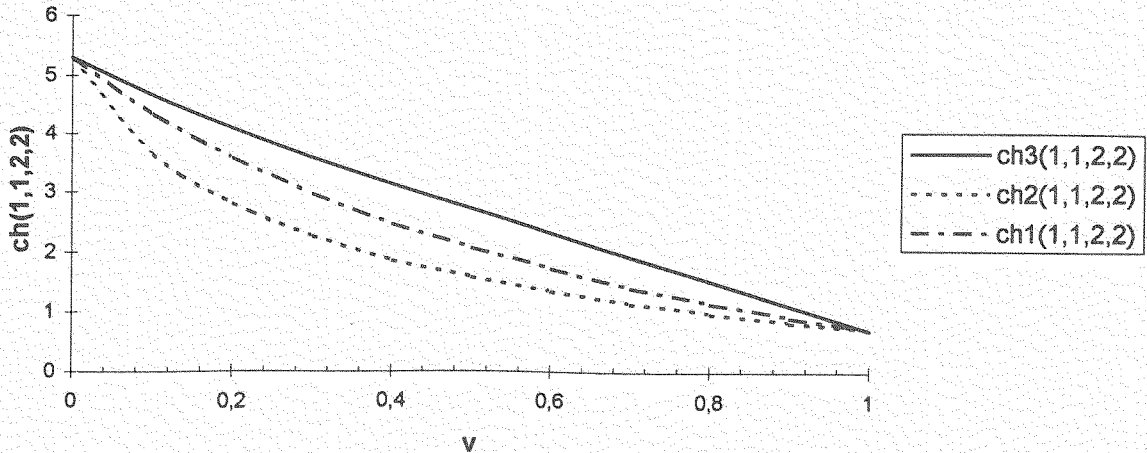
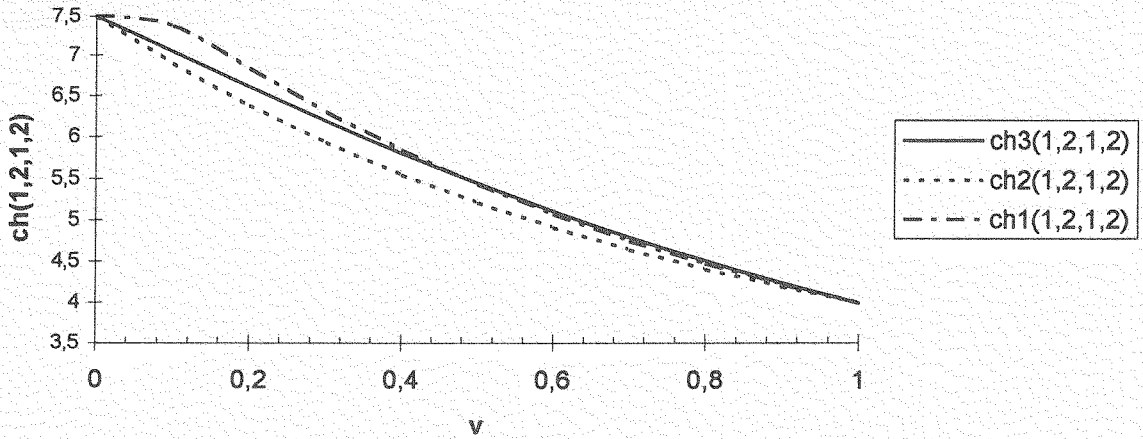
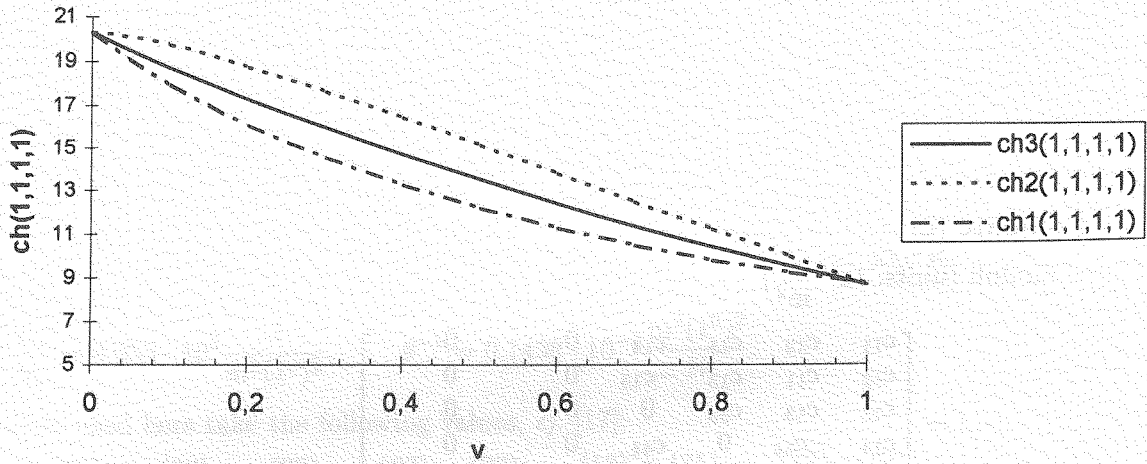


Fig. 3. Selected homogenized elastic coefficients as a function of volume ratio  $v = \xi$ ;  $chk(i, j, m, n) = c_{ijmn}^h$  — lamination in the direction of  $y_k$ ; for instance,  $ch1(i, j, m, n)$  denotes homogenized coefficient  $c_{ijmn}^h$  for lamination in the direction  $y_1$

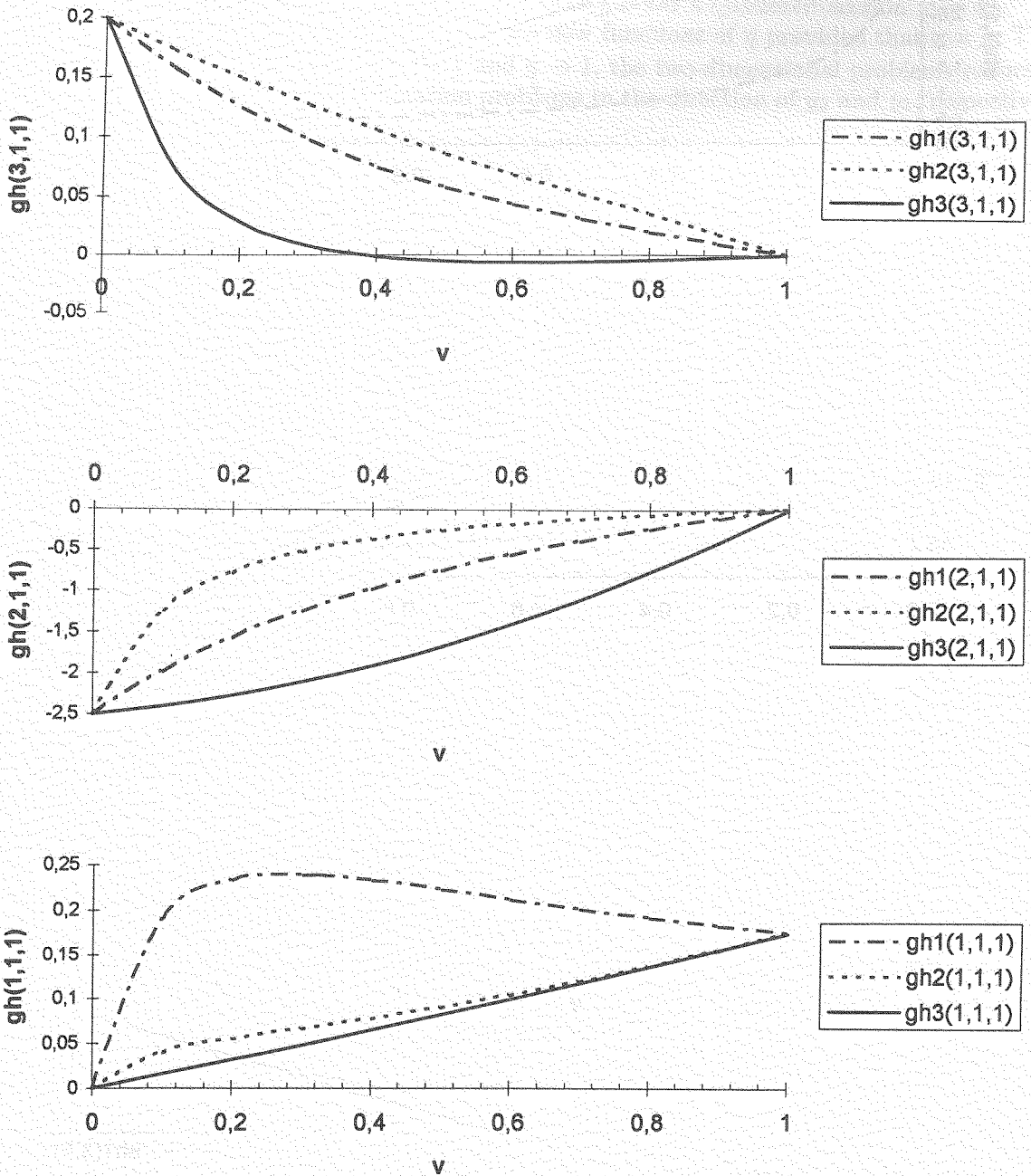


Fig. 4. Selected homogenized piezoelectric coefficients as a function of volume ratio  $v = \xi$ ;  $ghk(m, i, j) = g_{mij}^h$  — lamination in the direction of  $y_k$ ; for instance,  $gh1(m, i, j)$  denotes homogenized coefficient  $g_{mij}^h$  for lamination in the direction  $y_1$

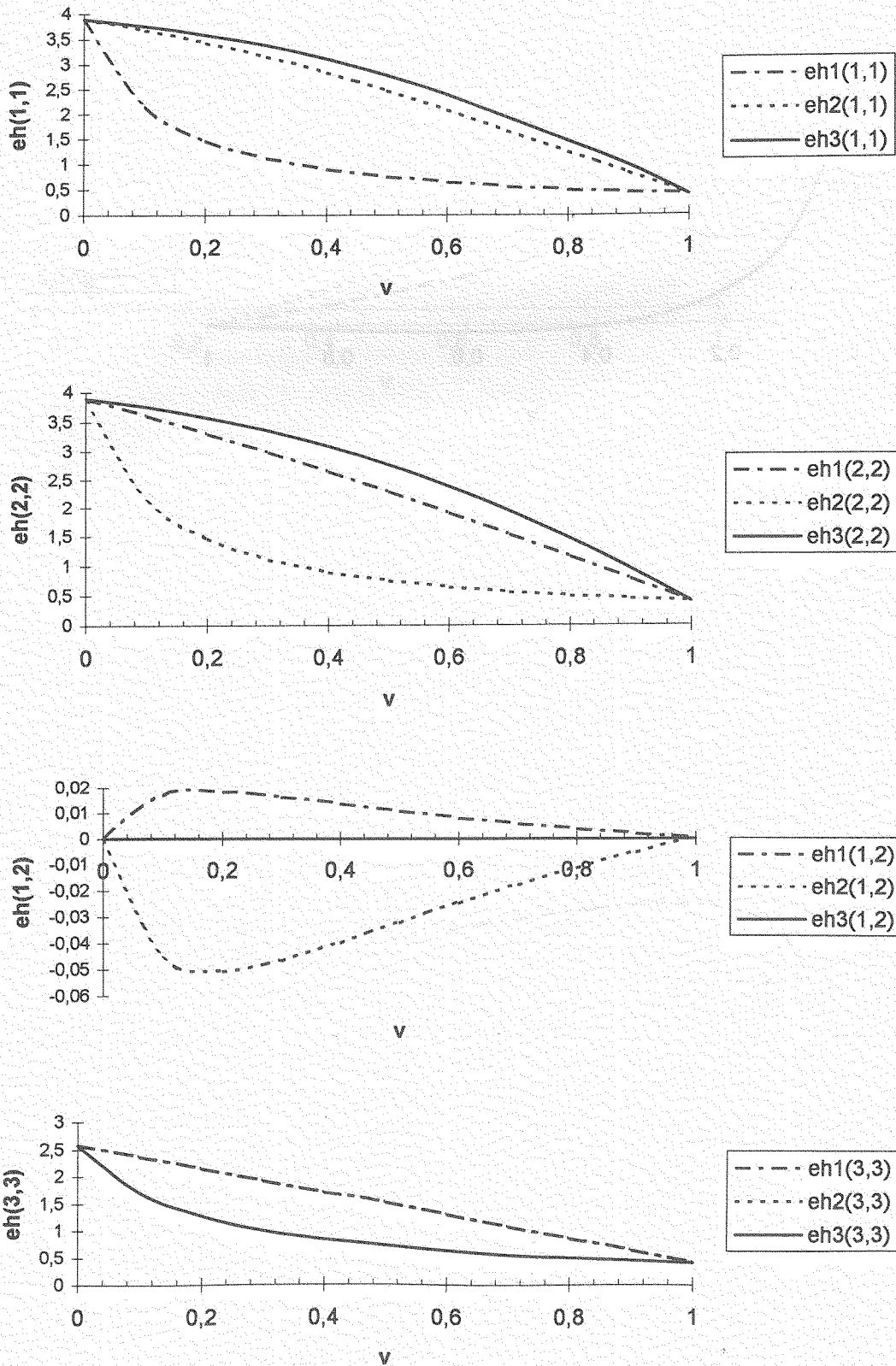


Fig. 5. Selected homogenized dielectric coefficients as a function of volume ratio  $v = \xi$ ;  $ehk(i, j) = \epsilon_{ij}^h$  — lamination in the direction of  $y_k$ ; for instance,  $eh1(i, j)$  denotes homogenized coefficient  $\epsilon_{ij}^h$  for lamination in the direction  $y_1$ .



## (ii) Two-dimensional case

In this case the homogenized coefficients were obtained on the basis of formulae (21). The calculations were performed for two, Eqs. (27) and (28), and for four, Eqs. (27)–(30), base functions. Some of our results are summarized in Figs. 6–9. In Figs. 6 and 8 the homogenized coefficients are functions of the volume fraction  $v = \xi\eta$ , where the inclusion has a quadratic section ( $\xi = \eta$ ).

In Figs. 7 and 9 the homogenized coefficients are now functions of  $\eta$  provided that  $v = \frac{1}{2}$ . Thus the inclusion is a variable rectangle. If  $\eta \rightarrow \frac{1}{2}$  and  $\eta \rightarrow 1$ , the two-dimensional problems reduce to the corresponding one-dimensional lamination problems in the direction of  $y_2$  and  $y_1$ , respectively.

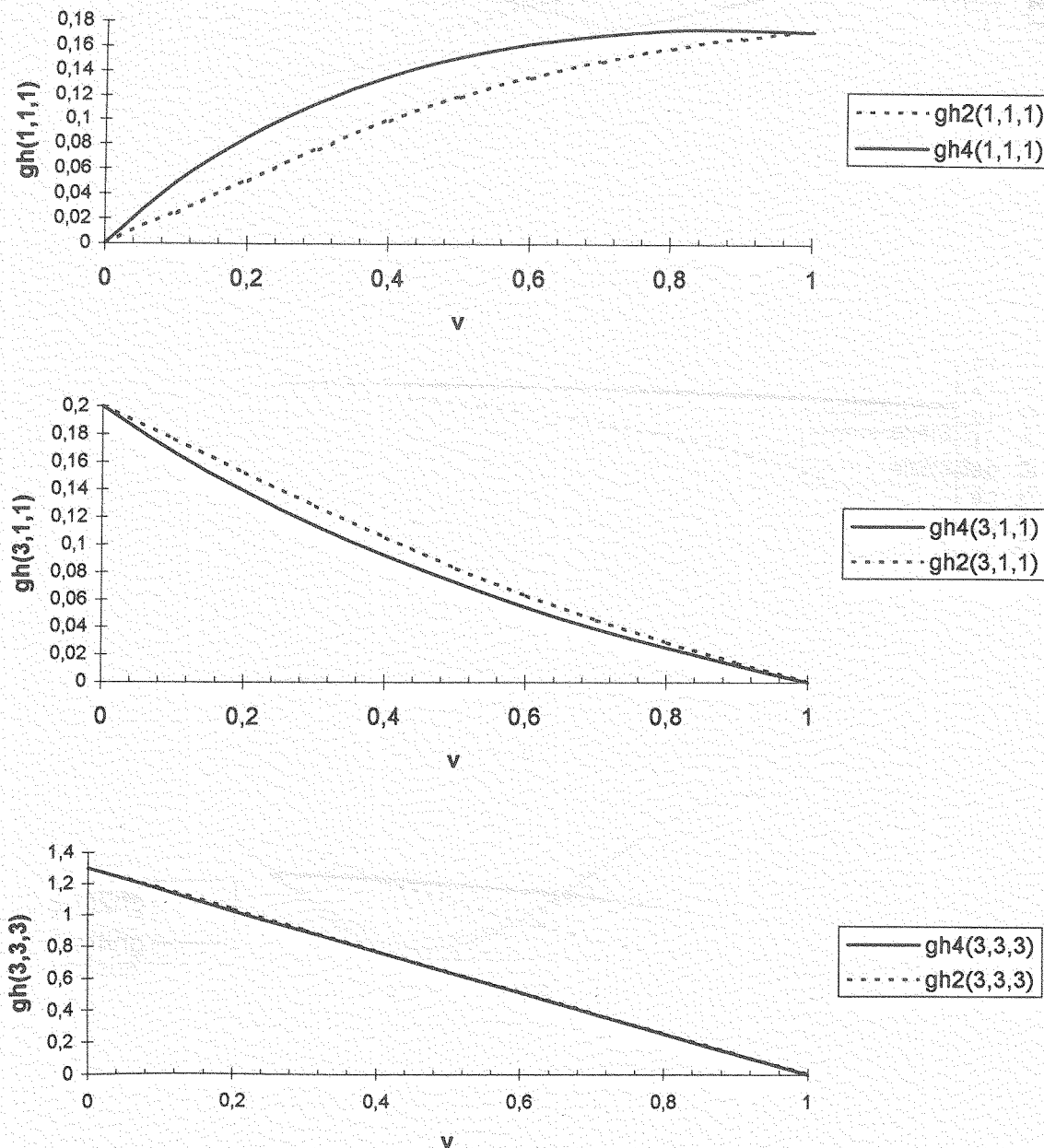


Fig. 6. Selected homogenized piezoelectric coefficients as a function of volume fraction  $v = \xi\eta, \xi = \eta$ ;  $gh2(m, i, j) = g_{mij}^h$  — two base functions;  $gh4(m, i, j) = g_{mij}^h$  — four base functions

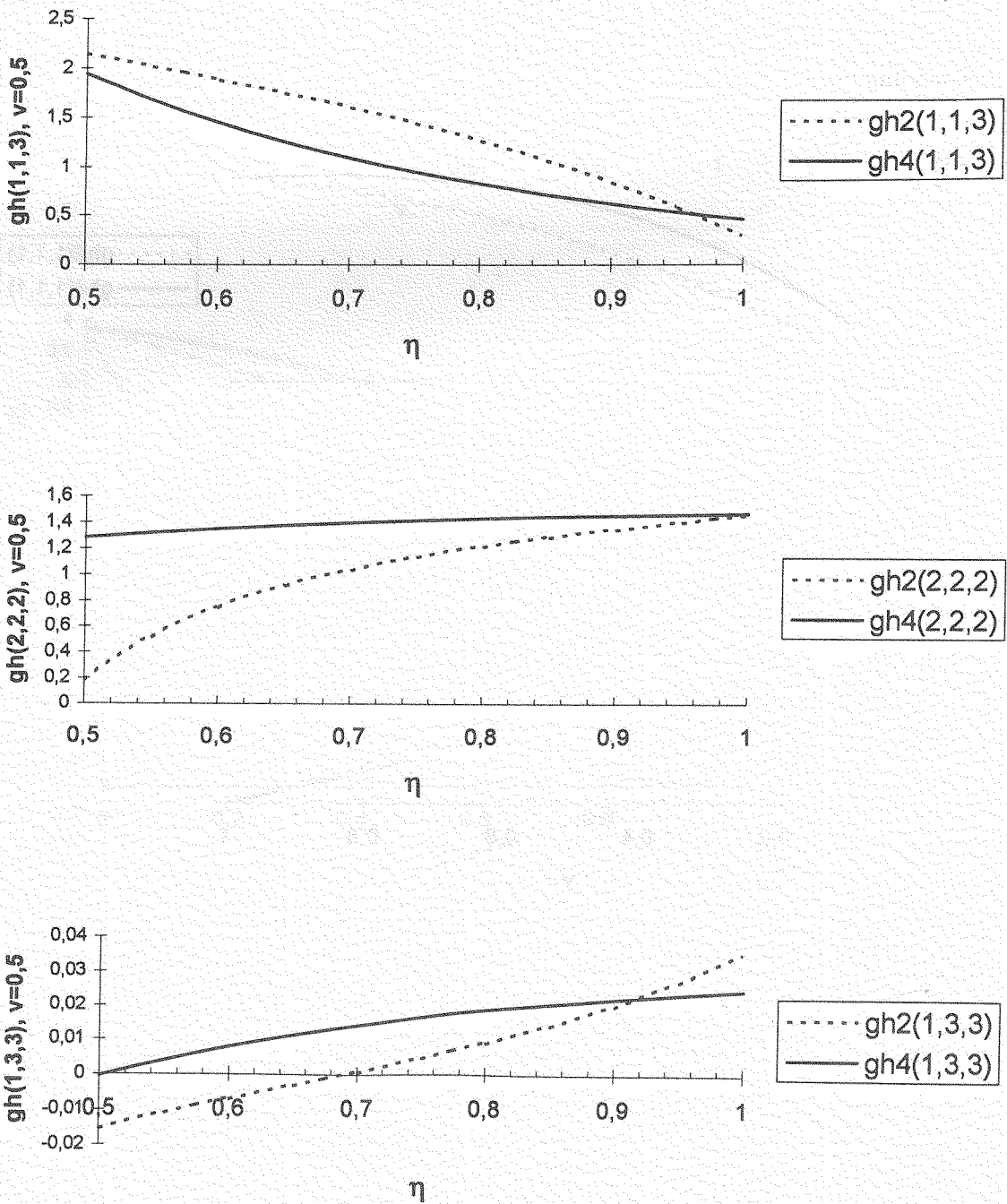


Fig. 7. Selected homogenized piezoelectric coefficients as a function of  $\eta$  for  $\nu = 1/2$ ;  $gh2(m, i, j) = g_{mij}^h$  — two base functions;  $gh4(m, i, j) = g_{mij}^h$  — four base functions

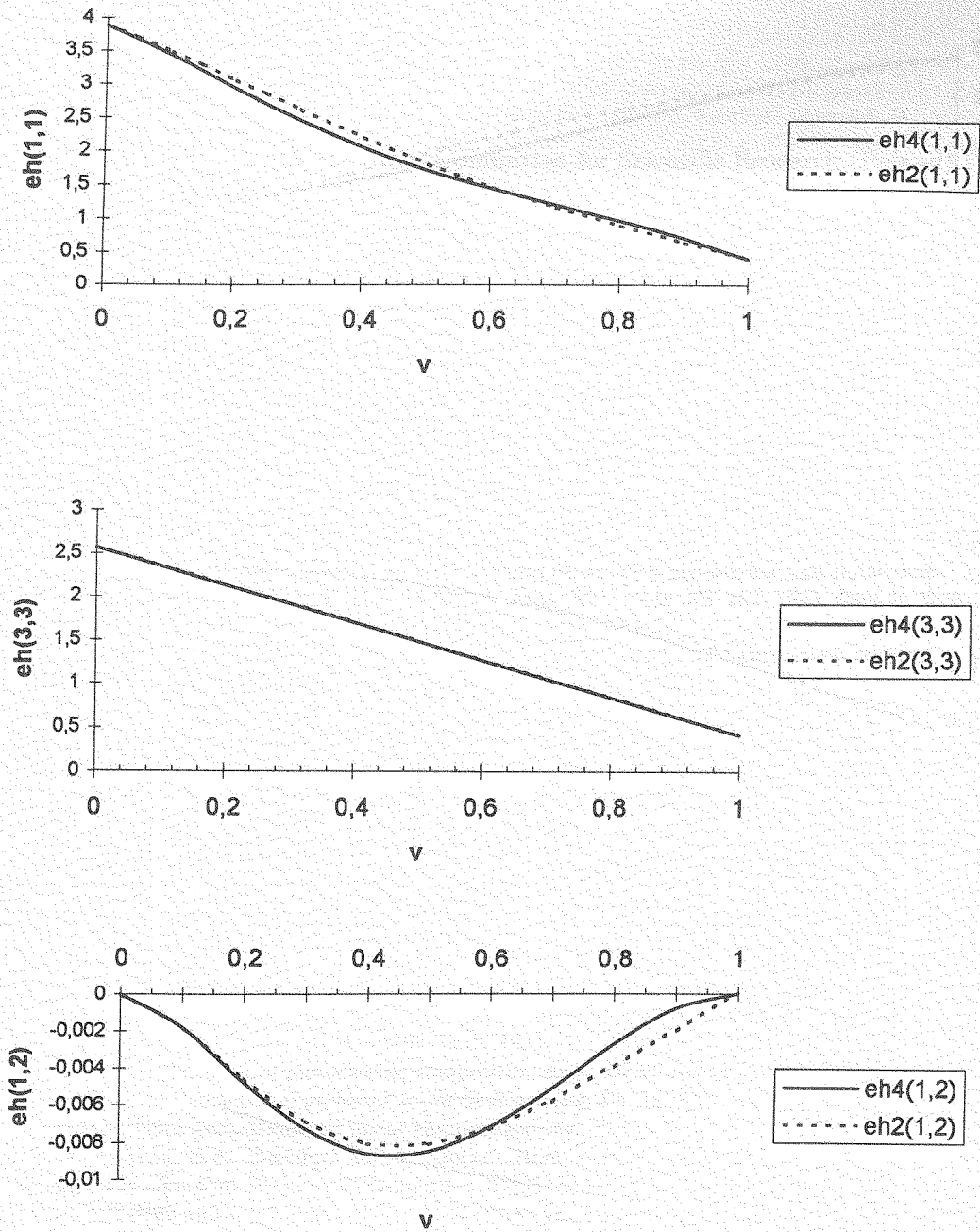


Fig. 8. Selected homogenized dielectric coefficients as a function of  $v = \xi\eta, \xi = \eta$ ;  $eh2(i, j) = \epsilon_{ij}^h$  — two base functions;  $eh4(m, i, j) = \epsilon_{ij}^h$  — four base functions

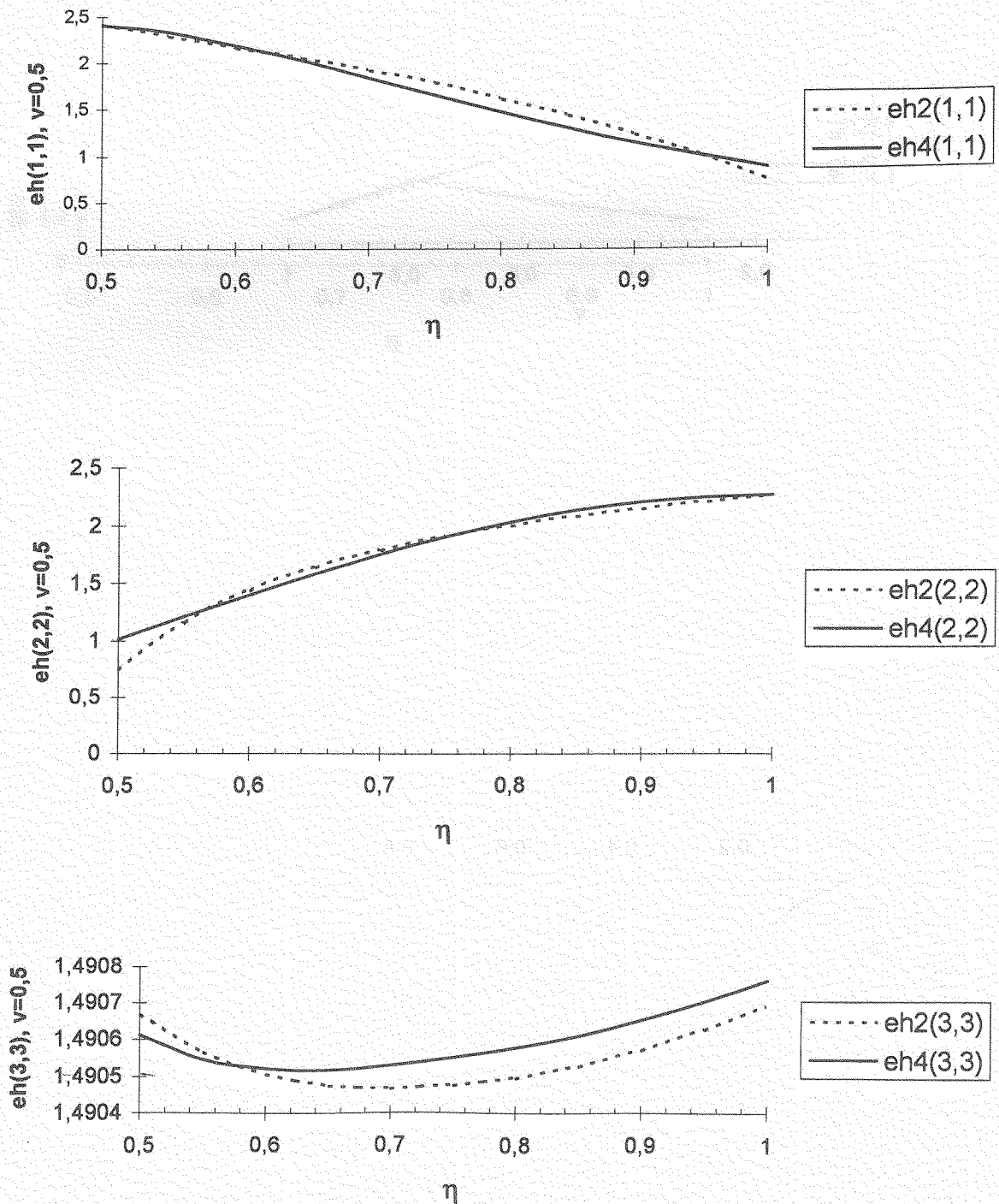


Fig. 9. Selected homogenized dielectric coefficients as a function of  $\eta$  for  $v = 1/2$ ;  $eh2(i, j) = \epsilon_{ij}^h$  — two base functions;  $eh4(m, i, j) = \epsilon_{ij}^h$  — four base functions

The exact one-dimensional results ( $\nu = \frac{1}{2}$ ) for lamination in the corresponding direction were compared with approximate two-dimensional results obtained for  $\eta = 0.551 \cong \frac{1}{2}$  and  $\eta = 0.999 \cong 1$ , for dielectric and piezo-electric coefficients. Good agreement (within 1% of error) of the results was observed for all components.

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