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Effective Dielectric Permeability of a Medium with Periodic Inclusions

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Abstract. A method for estimating the effective dielectric permittivity tensor is described in the paper. The method is based on variational principle for media with periodic inclusions. It allows one to obtain upper and lower bounds for possible values of the dielectric permittivity of a two-component system. Numerical results for composite structures with dielectric (metal) cubical and spherical inclusions are presented.

Keywords: effective dielectric permittivity tensor, variational principle, periodic inclusionseffective dielectric permittivity tensor, variational principle, periodic inclusions.

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Introduction

Studies on dielectric properties of binary materials have been actively conducted in recent years. The dielectric constant is one of the most important quantities that describes the optical and electrical properties of materials. It is of special interest when composite systems are considered. There is an increasing demand for dielectric materials from a range of industries including telecommunication, medical, auto-mobile, aerospace applications, sensors, actuators, antennas and filters. Effective dielectric permittivity of a binary material is dependent on the dielectric permittivity of inclusions and embedding medium and on the volume fraction and shape of the inclusions. The method of estimation of effective dielectric permittivity based on variational principles is proposed in the paper.

Conception of effective dielectric permittivity was proposed by Maxwell [1]. An up-to-date treatment of effective dielectric permittivity was considered in [2]. Methods based on variational principle were proposed by Kazantsev for problems of electrostatics of dielectrics [3, 4]. Application of these methods to estimating the dielectric permittivity of a medium with periodic inclusions is presented in the paper. Estimations of effective dielectric permittivity with the use of variational principle were also proposed for media with various inclusions [5–7]. Numerical methods are also used to determined dielectric permittivity. Computer simulation data for the

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effective permittivity of a system composed of a periodic lattices of inclusions embedded in a three-dimensional homogeneous matrix was presented in [7]. Results were obtained with the use of the numerical method based on the solution of boundary integral equations. A simulation for dielectric constant of two-phase disordered composites based on a three-dimensional disordered model was presented. Numerical calculations were performed using the finite element method [8].

1. Problem formulation

Let us assume that dielectric permittivity of a medium changes periodically along the axes of the Cartesian coordinate system:

$$\varepsilon\left(x+a,y,z\right)=\varepsilon\left(x,y+b,z\right)=\varepsilon\left(x,y,z+c\right)=\varepsilon\left(x,y,z\right).$$

External homogeneous electric field $\vec{E}_0$ polarizes the medium. Charges induced by the electric field are the sources of electric potential $\varphi\left(\vec{r}\right)$. This potential is a periodic function with the same periods as dielectric permeability. The averaged over the periodic cell the electric displacement field $\vec{\mathbf{D}}$ is related to the external electric field $\vec{E}^{ext}$ by the tensor of effective dielectric permittivity $\hat{\varepsilon}^{ef}$

$$\vec{\mathbf{D}}=\varepsilon_0\hat{\varepsilon}^{ef}\cdot\vec{E}^{ext}.$$

The challenge is to determine $\hat{\varepsilon}^{ef}$ from the known $\varepsilon\left(\vec{r}\right)$.

Let us note that described below method to determine effective dielectric permittivity can be used to determine effective magnetic permeability, electric conductivity and heat conductivity of a medium with periodic inclusions.

2. Variational formulation of the problem

Let us consider the functional of electrostatic energy of the periodic cell

$$W\left(\varphi\right)=\frac{\varepsilon_0}{2}\int\limits_V\varepsilon\left(\vec{r}\right)\left(\vec{E}^{ext}-\nabla\varphi\right)^2dV,\quad V:\left\{0\leqslant x\leqslant a,0\leqslant y\leqslant b,0\leqslant z\leqslant c\right\},\tag{1}$$

where test potential $\varphi(\vec{r})$ is a periodic function for which $W\left(\varphi\right)$ is bounded. The existence of such functions for actual $\varepsilon\left(\vec{r}\right)$ is demonstrated in the given below examples. Let us show [2] that solutions of equation

$$\nabla\cdot\left(\varepsilon\left(\vec{r}\right)\left(\vec{E}^{ext}-\nabla\mathbf{\Phi}\right)\right)=0,\tag{2}$$

provides the minimal value of functional (1) with the assumption that potential $\mathbf{\Phi}$ is continuous and periodic function. Boundedness of energy for the true solution of (2) is obvious as it follows from physical consideration.

Let us consider the immediately verified identity

$$W\left(\varphi\right)=W\left(\varphi-\mathbf{\Phi}+\mathbf{\Phi}\right)=W\left(\mathbf{\Phi}\right)+\frac{\varepsilon_0}{2}\int\limits_V\varepsilon\left(\vec{r}\right)\left(\nabla\left(\varphi-\mathbf{\Phi}\right)\right)^2dV-$$
$$-\varepsilon_0\int\limits_V\varepsilon\left(\vec{r}\right)\left(\vec{E}^{ext}-\nabla\mathbf{\Phi}\right)\cdot\nabla\left(\varphi-\mathbf{\Phi}\right)dV.\tag{3}$$

The last integral in (3), providing $\mathbf{\Phi}$ satisfies equation (2), can be transformed into the surface integral

$$\int_V \varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)\cdot\nabla(\varphi-\mathbf{\Phi})\,dV=\int_{\partial V}(\varphi-\mathbf{\Phi})\,\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)\cdot\vec n dS-$$
$$-\int_V(\varphi-\mathbf{\Phi})\,\nabla\cdot\left(\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)\right)dV=\int_{\partial V}(\varphi-\mathbf{\Phi})\,\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)\cdot\vec n dS$$

over the boundary of periodic cell with the use of the Gauss-Ostrogradsky theorem, where $\vec n$ is the unit normal vector to a surface element dS of the boundary ∂V of the periodic cell.

If periodic cell can be chosen so that $\varepsilon(\vec r)$ is continuous on the boundary of the cell then according to (2), $\varepsilon(\vec r)\,\nabla\mathbf{\Phi}$ is also continuous and periodic on ∂V. Then last integral is equal to zero because normal vectors $\vec n$ are oppositely directed on the opposite sides of the periodic cell. Then we transform identity (3) into inequality

$$W(\varphi)-W(\mathbf{\Phi})=\frac{\varepsilon_0}{2}\int_V\varepsilon(\vec r)\,(\nabla(\varphi-\mathbf{\Phi}))^2dV\geqslant 0 \qquad (4)$$

under the natural assumption that dielectric permittivity is positive. Let us note that energy of electric field when $\varphi=\mathbf{\Phi}$ is

$$W(\mathbf{\Phi})=\frac{\varepsilon_0}{2}\left(\vec E^{ext}\cdot\int_V\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)dV-\int_V\nabla\mathbf{\Phi}\cdot\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)dV\right).$$

Second integral in the right hand side is equal to zero (see the similar integral in (3)). Thus

$$W(\mathbf{\Phi})=\frac{1}{2}V\vec E^{ext}\cdot\vec{\mathbf{D}}=\frac{\varepsilon_0}{2}V\vec E^{ext}\cdot\hat\varepsilon^{ef}\cdot\vec E^{ext},$$

where

$$\vec{\mathbf{D}}=\varepsilon_0\varepsilon^{ef}\vec E^{ext}=\frac{1}{V}\int_V\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\mathbf{\Phi}\right)dV,$$

and $\vec{\mathbf{D}}$ can be treated as effective electric displacement field. Because $W(\varphi)$ is a quadratic form with respect to $\vec E^{ext}$ then

$$W(\varphi)=\frac{\varepsilon_0}{2}V\vec E^{ext}\cdot\tilde{\hat\varepsilon}\cdot\vec E^{ext},$$

where $\tilde{\hat\varepsilon}$ is some constant positive definite tensor but it depends on the choice of φ. We call it the approximate tensor of dielectric permittivity.

Moreover, it follows that

$$W(\varphi)=\frac{\varepsilon_0}{2}V\vec E^{ext}\cdot\tilde{\hat\varepsilon}\cdot\vec E^{ext}\geqslant\frac{\varepsilon_0}{2}V\vec E^{ext}\cdot\hat\varepsilon^{ef}\cdot\vec E^{ext}. \qquad (5)$$

It allows one to find an estimate from above $\tilde{\hat\varepsilon}$ for tensor $\hat\varepsilon^{ef}$ with the use of rather arbitrary periodic potentials $\varphi(\vec r)$. Inequality (5) plays a leading part in solving problem on tensor of effective dielectric permittivity of a medium with periodic inclusions.

3. Dual variational principal

Dual variational principle allows one to find an estimate from below for tensor of effective dielectric permittivity of a medium with periodic inclusions. Let us consider the following obvious inequality [2]

$$\frac{1}{2}\int_V\frac{1}{\varepsilon_0\varepsilon(\vec r)}\left(\vec D-\varepsilon_0\varepsilon(\vec r)\left(\vec E^{ext}-\nabla\varphi\right)\right)^2dV\geqslant 0, \qquad (6)$$

where $\vec D$ is an arbitrary vector field. The requirements that should be imposed upon this field are considered below.

Let us rewrite this inequality in a more convenient form

$$\frac{1}{2}\int\limits_V \left(\frac{\vec{D}^2}{\varepsilon_0 \varepsilon(\vec{r})} - 2\vec{D}\cdot\vec{E}^{ext}\right) dV + W(\varphi) + \int\limits_V \vec{D}\cdot\nabla\varphi dV \geqslant 0.$$

Taking into account the Gauss-Ostrogradsky theorem, we obtain

$$\int\limits_V \vec{D}\cdot\nabla\varphi dV = \int\limits_{\partial V} \varphi\vec{D}\cdot\vec{n}dS - \int\limits_V \varphi div\vec{D}dV.$$

If test vector field $\vec{D}$ is periodic, continuous on the boundary of the cell and solenoidal field in V then both integrals in the right hand side are equal to zero.

Then inequality (6) can be written in the form

$$W(\varphi) \geqslant -L\left(\vec{D}\right),$$

where

$$L(\vec{D}) = \frac{1}{2}\int\limits_V \left(\frac{\vec{D}^2}{\varepsilon_0\varepsilon(\vec{r})} - 2\vec{D}\cdot\vec{E}^{ext}\right) dV.$$

Similar inequality is valid for the true potential

$$W(\mathbf{\Phi}) \geqslant -L\left(\vec{D}\right). \tag{7}$$

Let us note that we need not use vector potential as it is usually done to formulate dual variational principal [2].

Finding extreme value of $L\left(\vec{D}\right)$ over a class of periodic, solenoidal fields $\vec{D}$ will obviously produce a linear relationship between $\vec{D}$ and $\vec{E}^{ext}$ because $L\left(\vec{D}\right)$ is a quadratic form of $\vec{D}$ and it contains $\vec{D}\vec{E}^{ext}$. Then one can set

$$L\left(\vec{D}\right) = -\frac{\varepsilon_0}{2} V\vec{E}^{ext}\cdot\underset{\sim}{\hat{\varepsilon}}\cdot\vec{E}^{ext}.$$

It follows from (7) that

$$\frac{\varepsilon_0}{2}V\vec{E}^{ext}\cdot\hat{\varepsilon}^{ef}\cdot\vec{E}^{ext} \geqslant -L\left(\vec{D}\right) = \frac{\varepsilon_0}{2}V\vec{E}^{ext}\cdot\underset{\sim}{\hat{\varepsilon}}\cdot\vec{E}^{ext}. \tag{8}$$

This Inequality is similar to inequality (5). Inequality (8) allows one to find an estimate from below for tensor of effective dielectric permittivity of a medium with periodic inclusions with the use of square-integrable solenoidal fields $\vec{D}$.

4. Simple estimates for tensor of effective dielectric permittivity of a medium with periodic inclusions

Let us use the following designation

$$\langle f(\vec{r})\rangle_V = \frac{1}{V}\int\limits_V f(\vec{r})\, dV.$$

Let us obtain simple estimates of effective dielectric permittivity, assuming that $\varphi = 0$ in $W(\varphi)$ and $\vec{D} = \varepsilon_0 \vec{E}^{ext}$ in $L\left(\vec{D}\right)$:

$$\frac{\varepsilon_0}{2} V (\vec{E}^{ext})^2 \langle \varepsilon^{-1} \rangle_V^{-1} \leqslant \frac{\varepsilon_0}{2} V \vec{E}^{ext} \cdot \hat{\varepsilon}^{ef} \cdot \vec{E}^{ext} \leqslant \frac{\varepsilon_0}{2} V (\vec{E}^{ext})^2 \langle \varepsilon \rangle_V . \tag{9}$$

Let us note that anisotropy of material of inclusions is not taken into account in (9). Let us improve the obtained estimates. Let us introduce the coordinate system so that periodic cell is in the first octant with three sides of the cell are on the coordinate planes. To obtain the estimate from below, for example, for $\hat{\varepsilon}^{ef}_{xx}$, let us direct $\vec{E}^{ext}$ and $\vec{D}$ along the x axis and set the test solenoidal field $\vec{D}$ in functional $L\left(\vec{D}\right)$ as follows

$$\vec{D} = (D_x(y,z), 0, 0), \quad \vec{E}^{ext} = (E, 0, 0).$$

Then

$$L\left(\vec{D}\right) = \frac{a}{2\varepsilon_0} \int\limits_{S_{yz}} \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x D_x^2 - 2\varepsilon_0 D_x E \right) dydz,$$

where the averaged over value of inverse dielectric permittivity is

$$\langle \varepsilon^{-1}(\vec{r}) \rangle_x = \frac{1}{a} \int_0^a \varepsilon^{-1}(\vec{r})\, dx.$$

Minimizing $L\left(\vec{D}\right)$ with respect to $D_x(y,z)$, we obtain

$$D_x(y,z) = \varepsilon_0 \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x \right)^{-1} E,$$

and

$$L\left(\vec{D}\right) = -\frac{abc}{2} \varepsilon_0 \left\langle \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x \right)^{-1} \right\rangle_{S_{yz}} E^2$$

where

$$\left\langle \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x \right)^{-1} \right\rangle_{S_{yz}} = \frac{1}{bc} \int_0^b \int_0^c \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x \right)^{-1} dydz.$$

Thus we have the estimate from below

$$\hat{\varepsilon}^{ef}_{xx} \geqslant \underset{\sim xx}{\hat{\varepsilon}} = \left\langle \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x \right)^{-1} \right\rangle_{S_{yz}}$$

Estimates for $\hat{\varepsilon}^{ef}_{yy}$ and $\hat{\varepsilon}^{ef}_{zz}$ can be obtained in a similar way. As a result we have

$$\underset{\sim xx}{\hat{\varepsilon}} = \left\langle \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_x \right)^{-1} \right\rangle_{S_{yz}} ; \underset{\sim yy}{\hat{\varepsilon}} = \left\langle \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_y \right)^{-1} \right\rangle_{S_{xz}} ; \underset{\sim zz}{\hat{\varepsilon}} = \left\langle \left(\langle \varepsilon^{-1}(\vec{r}) \rangle_z \right)^{-1} \right\rangle_{S_{yz}} . \tag{10}$$

To obtain the estimate from above, for example, for $\tilde{\hat{\varepsilon}}_{xx}$ let us direct $\vec{E}^{ext}$ along the x axis: $\vec{E}^{ext} = (E, 0, 0)$ and assume that test potential φ depends only on x in functional (1). Then

$$W(\varphi) = \frac{\varepsilon_0 bc}{2} \int_0^a \langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \left(E - \frac{d}{dx}\varphi(x) \right)^2 dx$$

The Euler-Lagrange equation for $\varphi(x)$ is

$$\frac{d}{dx} \left(\langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \left(E - \frac{d}{dx}\varphi(x) \right) \right) = 0.$$

The periodic potential with period a that satisfies this equation has the form

$$\varphi(x) = Ex - E\left\langle \left(\langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \right)^{-1} \right\rangle_x \int_0 \frac{dx}{\langle \varepsilon(\vec{r}) \rangle_{S_{yz}}} + C,$$

where C is some constant.

Then the value of the energy functional is

$$W(\varphi) = \frac{\varepsilon_0 abc}{2} E^2 \left(\left\langle \left(\langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \right)^{-1} \right\rangle_x \right)^{-1},$$

with the estimate

$$\hat{\varepsilon}^{ef}_{xx} \leqslant \tilde{\hat{\varepsilon}}_{xx} = \left(\left\langle \left(\langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \right)^{-1} \right\rangle_x \right)^{-1}$$

Estimates for $\tilde{\hat{\varepsilon}}_{yy}$ and $\tilde{\hat{\varepsilon}}_{zz}$ can be obtained in a similar way. Finally we have

$$\begin{aligned} \tilde{\hat{\varepsilon}}_{xx} &= \left(\left\langle \left(\langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \right)^{-1} \right\rangle_x \right)^{-1}; \\ \tilde{\hat{\varepsilon}}_{yy} &= \left(\left\langle \left(\langle \varepsilon(\vec{r}) \rangle_{S_{xz}} \right)^{-1} \right\rangle_y \right)^{-1}; \\ \tilde{\hat{\varepsilon}}_{zz} &= \left(\left\langle \left(\langle \varepsilon(\vec{r}) \rangle_{S_{xy}} \right)^{-1} \right\rangle_z \right)^{-1}. \end{aligned} \tag{11}$$

Let us note that in the considered case tensors $\underset{\sim}{\hat{\varepsilon}}$ and $\tilde{\hat{\varepsilon}}$ have diagonal form by the construction. Generally, $\vec{E}^{ext} = (E_x, E_y, E_z)$ and one can set $\vec{D} = (D_x(y,z), D_y(x,z), D_z(x,y))$, $\varphi = \varphi_x(x) + \varphi_y(y) + \varphi_z(z)$. Then

$$L\left(\vec{D}\right) = \frac{a}{2\varepsilon_0} \int_{S_{yz}} \left(\left\langle \varepsilon^{-1}(\vec{r}) \right\rangle_x D_x^2 - 2\varepsilon_0 D_x E_x \right) dydz + \frac{b}{2\varepsilon_0} \int_{S_{xz}} \left(\left\langle \varepsilon^{-1}(\vec{r}) \right\rangle_y D_y^2 - 2\varepsilon_0 D_y E_y \right) dxdz + \\ + \frac{c}{2\varepsilon_0} \int_{S_{xy}} \left(\left\langle \varepsilon^{-1}(\vec{r}) \right\rangle_z D_z^2 - 2\varepsilon_0 D_z E_z \right) dxdy,$$

$$W(\varphi) = \frac{\varepsilon_0 bc}{2} \int_0^a \langle \varepsilon(\vec{r}) \rangle_{S_{yz}} \left(E_x - \frac{d}{dx}\varphi_x(x) \right)^2 dx + \frac{\varepsilon_0 ac}{2} \int_0^b \langle \varepsilon(\vec{r}) \rangle_{S_{xz}} \left(E_y - \frac{d}{dy}\varphi_y(y) \right)^2 dy + \\ + \frac{\varepsilon_0 ab}{2} \int_0^c \langle \varepsilon(\vec{r}) \rangle_{S_{xy}} \left(E_z - \frac{d}{dz}\varphi_z(z) \right)^2 dz.$$

Minimizing with respect to periodic $\vec{D}$ and φ, we obtain

$$\varepsilon_0 \frac{abc}{2} \left(\underset{\sim xx}{\hat{\varepsilon}} {E_x}^2 + \underset{\sim yy}{\hat{\varepsilon}} {E_y}^2 + \underset{\sim zz}{\hat{\varepsilon}} {E_z}^2 \right) \leqslant \varepsilon_0 \frac{abc}{2} \vec{E}^{ext} \cdot \hat{\varepsilon}^{ef} \cdot \vec{E}^{ext} \leqslant \\ \leqslant \varepsilon_0 \frac{abc}{2} \left(\tilde{\hat{\varepsilon}}_{xx} {E_x}^2 + \tilde{\hat{\varepsilon}}_{yy} {E_y}^2 + \tilde{\hat{\varepsilon}}_{zz} {E_z}^2 \right),$$

where tensors $\underset{\sim}{\hat{\varepsilon}}$ and $\tilde{\hat{\varepsilon}}$ are given in (10) and (11).

One should note that if periodic cell and distribution $\varepsilon(\vec{r})$ have non-trivial rotational symmetry then $\hat{\varepsilon}^{ef}$ has 2 or 3 equal principal values. For example, if periodic cell is a cube and uniform inclusion is in its centre, and the inclusion shape has cubic symmetry then $\hat{\varepsilon}^{ef}$ has diagonal form.

Let us examine the effectiveness of the obtained estimates.

5. Examples of calculation of tensor of effective dielectric permittivity of a medium with periodic inclusions

5.1. Dielectric cube in a dielectric medium

Let us consider a cube of edge $d < a, b, c$ is located in the periodic cell. Cube edges are parallel to the sides of the cell, and the cube centre coincides with the centre of the cell. The dielectric permittivity of the cube differs from the dielectric permittivity of the medium ε by the factor γ.

Using (9), we obtain the following estimate of the effective dielectric permittivity

$$\begin{aligned}\varepsilon_0\varepsilon\frac{abc}{2}(\vec{E}^{ext})^2\left(1-\frac{(\gamma-1)\,d^3}{\gamma abc}\right)^{-1} &< \varepsilon_0\varepsilon\frac{abc}{2}\vec{E}^{ext}\cdot\hat{\varepsilon}^{ef}\cdot\vec{E}^{ext} < \\ &< \varepsilon_0\varepsilon\frac{abc}{2}(\vec{E}^{ext})^2\left(1+\frac{(\gamma-1)\,d^3}{abc}\right).\end{aligned} \tag{12}$$

Using (10), we obtain the following estimates from below of the principal values of tensor of effective dielectric permittivity

$$\begin{aligned}\underset{\sim xx}{\hat{\varepsilon}} &= \left\langle\left(\left\langle\varepsilon^{-1}(\vec{r})\right\rangle_x\right)^{-1}\right\rangle_{S_{yz}} = \varepsilon\left(1-\frac{d^2}{bc}\right)+\frac{\gamma\varepsilon ad^2}{((a-d)\,\gamma+d)\,bc}\\ \underset{\sim yy}{\hat{\varepsilon}} &= \left\langle\left(\left\langle\varepsilon^{-1}(\vec{r})\right\rangle_y\right)^{-1}\right\rangle_{S_{xz}} = \varepsilon\left(1-\frac{d^2}{ac}\right)+\frac{\gamma\varepsilon bd^2}{((b-d)\,\gamma+d)\,ac}\\ \underset{\sim zz}{\hat{\varepsilon}} &= \left\langle\left(\left\langle\varepsilon^{-1}(\vec{r})\right\rangle_z\right)^{-1}\right\rangle_{S_{yz}} = \varepsilon\left(1-\frac{d^2}{ab}\right)+\frac{\gamma\varepsilon cd^2}{((c-d)\,\gamma+d)\,ab}.\end{aligned} \tag{13}$$

It follows from (11) that estimates from above are

$$\begin{aligned}\tilde{\hat{\varepsilon}}_{xx} &= \left(\left\langle\left(\langle\varepsilon(\vec{r})\rangle_{S_{yz}}\right)^{-1}\right\rangle_x\right)^{-1} = \frac{\varepsilon a}{a-d+\frac{bcd}{bc+(\gamma-1)d^2}};\\ \tilde{\hat{\varepsilon}}_{yy} &= \left(\left\langle\left(\langle\varepsilon(\vec{r})\rangle_{S_{xz}}\right)^{-1}\right\rangle_y\right)^{-1} = \frac{\varepsilon b}{b-d+\frac{acd}{ac+(\gamma-1)d^2}};\\ \tilde{\hat{\varepsilon}}_{zz} &= \left(\left\langle\left(\langle\varepsilon(\vec{r})\rangle_{S_{xy}}\right)^{-1}\right\rangle_z\right)^{-1} = \frac{\varepsilon c}{c-d+\frac{bad}{ba+(\gamma-1)d^2}}.\end{aligned} \tag{14}$$

In particular, if then it follows from (12) that

$$\frac{18}{17} < \frac{\vec{E}^{ext}}{|\vec{E}^{ext}|}\cdot\frac{\hat{\varepsilon}^{ef}}{\varepsilon}\cdot\frac{\vec{E}^{ext}}{|\vec{E}^{ext}|} < \frac{7}{6}.$$

Using (13) and (14), we obtain more accurate estimates

$$\left(\frac{15}{14}{E_x}^2+\frac{13}{12}{E_y}^2+\frac{13}{12}{E_z}^2\right) < \vec{E}^{ext}\cdot\hat{\varepsilon}^{ef}\cdot\vec{E}^{ext} < \left(\frac{9}{8}{E_x}^2+\frac{8}{7}{E_y}^2+\frac{8}{7}{E_z}^2\right).$$

Relative error of estimates Δ is defined as the ratio between the difference of upper and lower bounds and the sum of upper and lower bounds. In this example, for two cases when $\vec{E}^{ext}$ is parallel or perpendicular to the x axis we have

$$\Delta = \frac{3}{246} \approx 0,012;\quad \vec{E}^{ext}||x,\ \Delta = \frac{5}{374} \approx 0,013;\quad \vec{E}^{ext}\perp x.$$

Relative error of estimate (12) is

$$\Delta = \frac{11}{454} \approx 0,024.$$

The relative error of estimates (10) and (11) is almost two times less then the relative error of estimate (9). This is because estimates (10) and (11) take better into account the no uniformity of distribution of dielectric permittivity in comparison with estimate (9).

5.2. Dielectric ball in a dielectric medium

Let us now consider a ball of radius R, $(2R \leqslant a,b,c)$ located in the periodic cell. Using (9), we obtain the following estimate of the effective dielectric permittivity

$$\left(1 - \frac{4\pi\,(\gamma-1)\,R^3}{\gamma abc}\right)^{-1} < \frac{\vec{E}^{ext}}{|\vec{E}^{ext}|} \cdot \frac{\hat{\varepsilon}^{ef}}{\varepsilon} \cdot \frac{\vec{E}^{ext}}{|\vec{E}^{ext}|} < \left(1 + \frac{4\pi\,(\gamma-1)\,R^3}{abc}\right). \tag{15}$$

Using (10) and (11), after some cumbersome mathematical treatment we obtain the following estimates

$$\frac{\tilde{\hat{\varepsilon}}_{\alpha\alpha}}{\varepsilon} = \left(1 - \frac{2R}{l_\alpha}\left(1 - \frac{h_\alpha^2}{\sqrt{1+h_\alpha^2}} \ln\left(\frac{\sqrt{1+h_\alpha^2}+1}{|h_\alpha|}\right)\right)\right)^{-1}, \tag{16}$$

where index α takes the values $\alpha = x, y.z$, $l_x = a$, $l_y = b$, $l_z = c$, $h_\alpha^2 = \frac{abc}{\pi(\gamma-1)R^2 l_\alpha}$.

Using (10), we obtain the following estimate

$$\frac{\underset{\sim}{\hat{\varepsilon}}_{\alpha\alpha}}{\varepsilon} = \left(1 - \frac{\pi R^2}{S_\alpha}\left(1 + 2p_\alpha - 2{p_\alpha}^2 \ln\left(\frac{p_\alpha}{p_\alpha - 1}\right)\right)\right), \tag{17}$$

where $S_\alpha = \dfrac{abc}{l_\alpha}$, $p_\alpha = \dfrac{\gamma l_\alpha}{2\,(\gamma-1)\,R}$.

In particular, if $\gamma = 3$, $a = b = c = 3R$ then tensor of effective dielectric permittivity is a scalar tensor, that is, all principal values of the tensor are equal: $\hat{\varepsilon}^{ef}_{xx} = \hat{\varepsilon}^{ef}_{yy} = \hat{\varepsilon}^{ef}_{zz} = \varepsilon^{ef}$. Using inequalities (15), we obtain the following estimates

$$1,11 < \frac{\varepsilon^{ef}}{\varepsilon} < 1,31. \tag{18}$$

Considering now inequalities (16) and (17), we find

$$1,16 < \frac{\varepsilon^{ef}}{\varepsilon} < 1,25. \tag{19}$$

The relative error of estimate (19) is equal to 0,04. It is two times less then the relative error of estimate (18).

It is obvious that relative error of estimates (16) and (17) increases with increasing γ. For example, if $\gamma \to \infty$, $a = b = c = 3R$ then we obtain the following estimates

$$1,13 < \frac{\varepsilon^{ef}}{\varepsilon} < 3,00. \tag{20}$$

The relative error of estimate (20) is increased to 45%. Let us show how to improve this estimate.

Let us now compare the obtained estimates with the results of numerical calculations. For comparison we take results for $\gamma = 30$ [8]. Fig. 1 shows numerical results [8] and estimates (16), (17). From this figure we notice that numerical results are between estimates from below and estimates from above.

Fig.1 also shows that it is necessary to improve the estimate from above (16). Let us show how to achieve this for the case $\gamma \to \infty$.

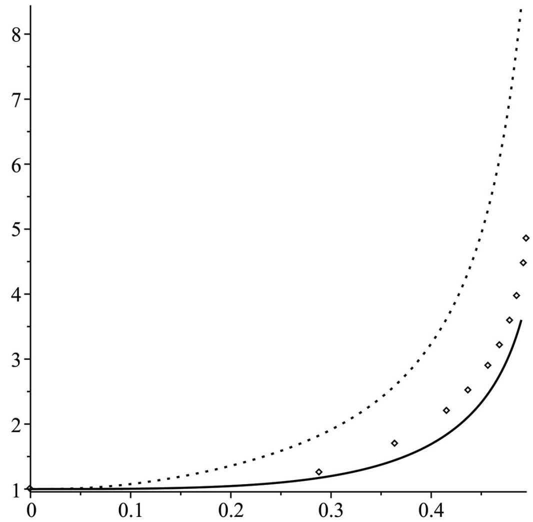

Fig. 1. Effective dielectric permittivity versus radius of the ball for $\gamma = 30$; upper line corresponds to estimate from above (16); line in the middle corresponds to numerical results [8]; lower line corresponds to estimate from below (17).

5.3. Cubic lattice of uniform in size conductive balls in a dielectric medium (improved estimate)

Let us improve estimate from above (16) for the case of cubic lattice of conductive spherical inclusions. Let us consider a cube of edge a and dielectric permittivity ε with a conductive ball of radius $R < a/2$. The centre of the cube is at the origin of coordinate system, and cube edges are parallel to the coordinate axes.

External homogeneous electric field $\vec{E}^{ext}$ is directed along the x-axis: $\vec{E}^{ext} = (E, 0, 0)$. This electric field induces electric charges on the boundary of the conductive ball. Electric field of these charges compensates the external field on the boundary of the ball, and in the case of isolated ball it coincides outside of the ball with the electric field of dipole located at the origin. It is clear from the symmetry of the problem that one needs to consider the domain $x > 0$. Let us divide this domain by the plane $x = R$ into two parts. For $0 < x < R$ the trial potential outside the ball is

$$\varphi_{x<R} = \frac{ExR^3}{(x^2+y^2+z^2)^{\frac{3}{2}}} + Ax\left(1 - \frac{R^3}{(x^2+y^2+z^2)^{\frac{3}{2}}}\right), \tag{21}$$

where A is some arbitrary constant. The value of this constant is determined from the condition of minimum of energy functional. On the boundary of the ball second term in (21) is equal to zero, and first term in (21) compensates potential of the external field .

Taking into account that trial potential is a periodic, continuous and piecewise smooth function, we assume for that

$$\begin{aligned}\varphi_{x>R} = \frac{ERR^3}{(x^2+y^2+R^2)^{\frac{3}{2}}}\frac{\frac{1}{2}a - x}{\frac{1}{2}a - R} + AR\left(1 - \frac{R^3}{(x^2+y^2+R^2)^{\frac{3}{2}}}\right)\frac{\frac{1}{2}a - x}{\frac{1}{2}a - R} + \\ + B(y^2+z^2)\sin\left(\pi\frac{\frac{1}{2}a - x}{\frac{1}{2}a - R}\right).\end{aligned} \tag{22}$$

where B is some arbitrary constant. Potential (22) is a continuous extension of potential (21) in $R < x < a/2$, and it is equal to zero at $x = \frac{a}{2}$.

Let us minimize functional (1) with respect to parameters A and B. Then we obtain expression for the upper bound of effective dielectric permittivity. To obtain parameters A and B that minimize the value of functional $W(\varphi)$ the mathematical software MAPLE was used. The obtained expression for $W(\varphi)$ is rather cumbersome, and it is omitted here.

Fig. 2 shows the relationship between estimates of the relative effective dielectric permittivity and parameter $\frac{R}{a}$ for $0 < \frac{R}{a} < 0.45$.

Fig. 3 presents the relationship between the upper bound of relative error for best estimates of effective dielectric permittivity and parameter $\frac{R}{a}$.

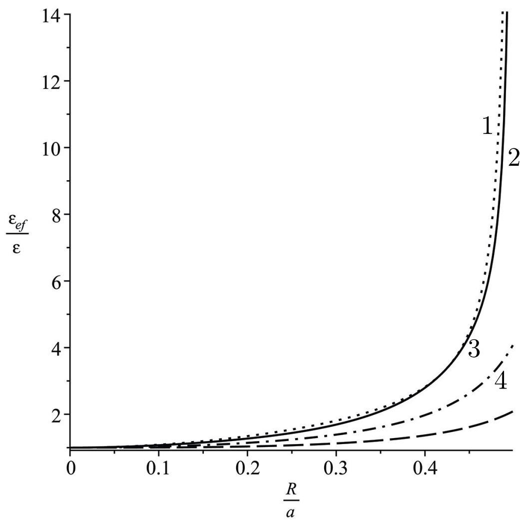

Fig. 2. Relative effective dielectric permittivity versus parameter R/a: 1) estimate from above based on potentials (21), (22); 2) estimate from above based on potentials (21), (22) for $A = 0$, $B = 0$; 3) estimate from below from (15) for $\gamma \to \infty$; 4) estimate from below (17).

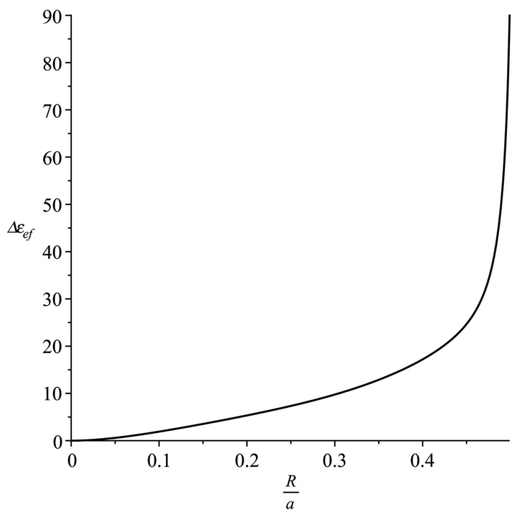

Fig. 3. Upper bound of relative error in percentage for estimates of effective dielectric permittivity (16, 17) based on potentials (21), (22) versus parameter $\frac{R}{a}$.

Conclusions

A medium with periodic inclusions is considered. A method for estimating the effective dielectric permittivity tensor of the medium is proposed. The method is based on variational principle. One should note that proposed method can be used not only for a medium with periodic inclusions but also in the case when dielectric permittivity tensor of a medium varies periodically in space.

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Эффективная диэлектрическая проницаемость среды с периодическими включениями

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Аннотация. В статье описывается метод оценки тензора эффективной диэлектрической проницаемости, основанный на вариационных принципах для сред с периодическими включениями, который позволяет получить двусторонние границы области возможных значений диэлектрической проницаемости двухкомпонентной системы. В качестве примеров показаны расчёты для композитных структур с кубическими и шаровыми включениями из диэлектрика и металла.

Ключевые слова: тензор эффективной диэлектрической проницаемости, вариационный метод оценки, среда с периодическими включениями