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CALCULATION OF THE DIELECTRIC PERMEABILITY OF INHOMOGENEOUS MATERIALS WITH PERIODIC STRUCTURES BY AVERAGING POTENTIAL-FIELD EQUATIONS

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Inhomogeneous materials with periodic structures are considered. Formulas for calculating mean parameters that meet the requirements imposed on them are obtained by averaging the equations of a potential electric field.

It is well known that inhomogeneous materials enjoy very wide application. They increase in number substantially each year, and simultaneously theoretical and experimental studies of their physical properties continue. Ultimately these investigations are reduced to determination of the averaged (effective) parameters of inhomogeneous materials. To solve this problem, one has to calculate physical fields in the components of the inhomogeneous material with subsequent averaging. Exact calculations of these fields involve great difficulties due to the structure, orientation, and shape of the components of the inhomogeneous media. Therefore, the problems of determining the effective parameters of inhomogeneous materials, except for rare cases of the simplest structures, have been solved only approximately [1–9].

The second important problem in the theory of inhomogeneous materials (theory of mixtures) is carrying out experimental investigations, which, however, are associated with great difficulties and expenditures. Therefore, experiments are carried out with one sample of an inhomogeneous material, and the data obtained are extended to the entire material.

Most important here are theoretical results that must satisfy basic requirements: the equivalence between the effective medium and the real inhomogeneous material; acquisition of physically correct results with limiting values of both the coefficient of filling with inclusions and the parameters of the components of theinhomogeneous material; satisfactory agreement between theoretical results and experimental data [4].

We suggest a method that allows one, by averaging the equations of potential fields, to find the effective parameters of inhomogeneous materials. It is based on the definition of Lorenz averaging [10] and also on the theory of averaging of equations of potential fields [11]. The method is applicable to inhomogeneous materials with irregular structures for low volume concentrations $f_2 << 1$ and to inhomogeneous materials with regular structures for $0 \le f_2 \le 1$.

In the present work we consider two-component inhomogeneous dielectrics consisting of a matrix (dispersion) medium and foreign solid particles (inclusions). The results obtained can be extended to other inhomogeneous media that are described by the same divergent-type elliptical equations [11].

It is known that in dielectrics with isotropic physical properties there is a linear relation between the local values of the electric displacement $\vec{D}$ and the electric field intensity $\vec{E}$:

$$\vec{D} = \varepsilon \vec{E} = \varepsilon_0 \vec{E} + \vec{P}, \tag{1}$$

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This relation also holds in macroscopic (averaged) form. We note that in Eq. (1) div $\vec{P} = 0$ (the dielectric is homogeneous) and $\vec{D}$ vanishes simultaneously with $\vec{E}$. But if the dielectric is inhomogeneous, then $\vec{P} \neq 0$ also at $\vec{E} = 0$ and $D \neq 0$. It is assumed in [8] that relation (1) $\vec{D} = \varepsilon\vec{E}$ in macroscopic form is also applicable to inhomogeneous materials. Meanwhile, it has been proved theoretically [11] that Eq. (1) in the averaged form $\langle\vec{D}\rangle = \langle\varepsilon\rangle\,\langle\vec{E}\rangle$ holds only for inhomogeneous materials with periodic structures.

Considering the foregoing, we will try to determine the effective value of $\langle\varepsilon\rangle$ of the inhomogeneous materials under consideration from the nonaveraged equation (1) by averaging $\vec{P}$ and $\vec{E}$. We assume that there is a dispersion medium with the dielectric permeability ε_0; inside a limited region of this medium there is a regular array of foreign solid particles with volumes v_2 and the dielectric permeability ε_2. The applied external electrostatic field of strength $\vec{E}$ is assumed to be uniform. From the local equation (1), which holds within the above-indicated limited region, we determine the magnitude of the dielectric permeability:

$$\langle\varepsilon\rangle = \varepsilon_0 + \langle\vec{P}\rangle / \langle\vec{E}\rangle\,, \tag{2}$$

where the averaging of the quantities from Eq. (2) is carried out according to the Lorenz definition [10]:

$$\langle\Psi\rangle = \frac{1}{v_0}\int\limits_{v_0} \Psi(x, y, z)\,dv \tag{3}$$

in a physically infinitely small volume v_0. We note that the averaged (vector or scalar) parameter $\langle\Psi\rangle$ is independent of the spatial coordinates of the region of averaging and has a period equal to $|v_0|$.

To determine $\langle\vec{P}\rangle$ and $\langle\vec{E}\rangle$, we assume that the number of inclusions within the region of averaging v_0 is n_0. The region occupied by the dispersion medium with the dielectric permeability $\varepsilon_1 = \varepsilon_0$ (vacuum) is $v_1 = v_0 - n_0 v_2$. There is no material medium inside v_1; therefore here $\vec{P} = 0$. Then, for the averaged polarization vector determined from (3) we have

$$\langle\vec{P}\rangle = \frac{1}{v_0}\int\limits_{v_0 - v_1} \vec{P}\,dv\,. \tag{4}$$

Considering the density of dipole moments inside the inclusions to be constant and denoting it by $\vec{P}_2$, from (4) for $\langle\vec{P}\rangle$ we obtain

$$\langle\vec{P}\rangle = \frac{1}{v_0}\sum_{i=1}^{n_0}\int\limits_{v_2} \vec{P}_2\,dv = f_2\,\vec{P}_2\,, \tag{5}$$

where $f_2 = n_0 v_2 / v_0$, i is the number of the inclusion. We note that relation (5) is valid for an inhomogeneous material with an irregular structure for low concentrations $f_2 << 1$ and also for concentrated inhomogeneous materials with a periodic structure when the foreign particles are polarized identically and uniformly under the action of a uniform field $\vec{E}_0$. In such cases, the equivalent dipole moment of a particle $\vec{p}_2$ and the polarization vector $\vec{P}_2$ are interrelated by $\vec{p}_2 = \vec{P}_2 v_2$. Within these inclusions, the following relationship holds:

$$\vec{D}_2 = \varepsilon_2\vec{E}_2 = \varepsilon_0\vec{E}_2 + \vec{P}_2\,. \tag{6}$$

For $\vec{P}_2$ Eq. (6) yields

$$\vec{P}_2 = (\varepsilon_2 - \varepsilon_0)\,\vec{E}_2\,. \tag{7}$$

Now, we will determine $\langle\vec{E}\rangle$. Since we consider linear systems, at any point of a limited space the local intensity $\vec{E}$ will be equal to

$$\vec{E} = \vec{E}_0 + \vec{E}_p \, . \tag{8}$$

With a uniform external field applied, averaging of Eq. (8) yields for $\langle\vec{E}\rangle$

$$\langle\vec{E}\rangle = \langle\vec{E}_0\rangle + \langle\vec{E}_p\rangle \, , \tag{9}$$

where $\langle\vec{E}_0\rangle = \vec{E}_0$.

To determine the mean value of the polarization field intensity, we will consider the same limited region with foreign inclusions inside it and free charges and the sources of the fields $\vec{D}_0$ and $\vec{E}_0$ outside. Within the region,

$$\operatorname{div}\vec{D} = 0 \, , \quad \operatorname{div}\vec{E}_0 = 0 \, , \tag{10}$$

since coupled charges are also sources of the intensity of the electrostatic field $\vec{E}$.

In determining $\vec{E}_p$, we exclude the vector of the displacement $\vec{D}$ from Eq. (1) in order to relate the remaining vectors to their sources. For this, we represent Eq. (1), with account for Eq. (8), in the form

$$\operatorname{div}\left(\vec{E}_p + \frac{1}{\varepsilon_0}\vec{P}\right) = \frac{1}{\varepsilon_0}\operatorname{div}\vec{D} - \operatorname{div}\vec{E}_0 \, . \tag{11}$$

Since the dielectric is inhomogeneous, $\operatorname{div}\vec{P} \neq 0$. Then Eq. (11), with account for Eq. (10), will take the form

$$\operatorname{div}\left(\vec{E}_p + \frac{1}{\varepsilon_0}\vec{P}\right) = 0 \, . \tag{12}$$

This condition will be satisfied if

$$\vec{E}_p = -\frac{1}{\varepsilon_0}\vec{P}, \tag{13}$$

whence

$$\langle\vec{E}_p\rangle = -\frac{1}{\varepsilon_0}\langle\vec{P}\rangle = -\frac{1}{\varepsilon_0} f_2\vec{P}_2 \, . \tag{14}$$

Relation (13) is also valid inside the inclusions, where

$$\vec{E}_2 - \vec{E}_0 = \vec{E}_{p2} = -\frac{1}{\varepsilon_0}\vec{P}_2 \, . \tag{15}$$

Having substituted the value of $\vec{P}_2$ from (15) into (14), for the averaged quantity $\langle\vec{E}_p\rangle$ we obtain

$$\langle\vec{E}_p\rangle = f_2\vec{E}_{p2} = f_2\,(\vec{E}_2 - \vec{E}_0) \, . \tag{16}$$

For the averaged intensity $\langle\vec{E}\rangle$ of (9), with account for Eq. (16), we then obtain

$$\langle\vec{E}\rangle = \vec{E}_0 + f_2\,(\vec{E}_2 - \vec{E}_0) \, . \tag{17}$$

Determining $\langle \vec{P} \rangle$ of (5) and $\langle \vec{E} \rangle$ of (17), from Eq. (2) with account for Eq. (7), for the averaged value of the dielectric permeability of the inhomogeneous materials considered we finally obtain the relation

$$\langle \varepsilon \rangle = \varepsilon_0 + \frac{f_2 (\varepsilon_2 - \varepsilon_0) A}{1 + f_2 (A - 1)}, \tag{18}$$

in which $A = |\vec{E}_2| / |\vec{E}_0|$.

The proposed definition of (18) derived from the potential-field equation meets the above requirements. Thus, the real inhomogeneous medium defined by Eq. (1) and the averaged medium defined by Eq. (2) are equivalent by virtue of condition (5). And since Eq. (2) is the result of averaging Eq. (1), relation (18) is free of internal inconsistency, and it gives physically correct results not only for $f_0 = 0$ and $f_2 = 1$ but also for $\nu = \varepsilon_2/\varepsilon_0 = 0$ and $\nu = \infty$. The degree of accuracy of equations derived from Eq. (18) for $\langle \varepsilon \rangle$ will be discussed below when inhomogeneous media with inclusions of specific forms are considered.

We give, as an example, the derivation of a formula for calculating the dielectric permeability of an inhomogeneous material with ellipsoidal (spherical, cylindrical) inclusions. We assume that these inclusions are oriented identically along the x axis, which is also the direction of the external field $\vec{E}_0 = \vec{E}_{0x}$. When the particles are arranged regularly, they are polarized uniformly. It is known that a uniformly polarized particle can be represented as equivalent to a dipole. For a particle of ellipsoidal shape the field $\vec{E}_{ax}$ acting on the dipole, which differs from the mean one $\langle \vec{E}_{0x} \rangle$ [10], is equal to

$$\vec{E}_{ax} = \vec{E}_{0x} + \frac{N_x \vec{P}_x}{\varepsilon_0}. \tag{19}$$

The mean value of $\vec{E}_{ax}$ of (19) is

$$\langle \vec{E}_{ax} \rangle = \langle \vec{E}_{0x} \rangle + \frac{N_x f_2 \vec{P}_{2x}}{\varepsilon_0}. \tag{20}$$

Then, for the electric-field intensity inside an inclusion we obtain

$$\vec{E}_{2x} = \langle \vec{E}_{ax} \rangle + \vec{E}_{p2x} = \vec{E}_{0x} + \frac{N_x f_2 \vec{P}_{2x}}{\varepsilon_0} - \frac{N_x \vec{P}_{2x}}{\varepsilon_0}. \tag{21}$$

Taking into account relation (7), from Eq. (21) we have for $\vec{E}_{2x}$

$$\vec{E}_{2x} = \frac{\varepsilon_0 \vec{E}_{0x}}{\varepsilon_0 + (\varepsilon_2 - \varepsilon_0)(1 - f_2) N_x}. \tag{22}$$

Substituting (22) into (18), for $\langle \varepsilon_x \rangle$ of the inhomogeneous material considered we obtain a new formula:

$$\langle \varepsilon_x \rangle = \varepsilon_0 \frac{\varepsilon_0 + (\varepsilon_2 - \varepsilon_0)(f_2 + (1 - f_2)^2 N_x)}{\varepsilon_0 + (\varepsilon_2 - \varepsilon_0)(1 - f_2)^2 N_x}. \tag{23}$$

Analysis of this formula shows that it gives physically correct results at the limiting values of the coefficient of filling. Indeed, $\langle \varepsilon_x \rangle = \varepsilon_0$ when $f_2 = 0$, whereas $\langle \varepsilon_x \rangle = \varepsilon_2$ when $f_2 = 1$. Formula (23) also gives correct results at the limiting values of the parameters of the inhomogeneous-material components. Thus, for $\nu = \varepsilon_2/\varepsilon_0 = \infty$ Eq. (23) yields

TABLE 1. Dielectric Permeability Calculated from Formula (26) and Compared with Existing Formulas

Volume concentration f_2	Experimental data on $\langle\varepsilon\rangle$	Formulas					
		1	2	3	4	5	6
0.05	2.3170	2.3165	2.3168	2.3149	2.3154	2.3177	2.3170
		–5	–2	–21	–16	+7	0
0.10	2.4110	2.4074	2.4085	2.4116	2.4026	2.4124	2.4120
		–36	–25	–6	–84	+14	+10
0.15	2.5110	2.5006	2.5032	2.5077	2.4901	2.5124	2.5106
		–92	–78	–33	–209	+14	+6
0.20	2.6110	2.5968	2.6009	2.6072	2.5750	2.6183	2.6138
		–142	–101	–38	–360	+73	+28
0.25	2.7140	2.6954	2.7017	2.7099	2.6618	2.7306	2.7213
		–186	–123	–41	–762	+166	+73
0.30	2.8240	2.7968	2.8055	2.8181	2.7522	2.8496	2.8330
		–272	–185	–59	–718	+258	+90
0.35	2.9490	2.9012	2.9124	2.9255	2.8396	2.9766	–
							2.9480
		–478	–366	–235	–1094	+276	–10

Note. Comparison of formulas: 1) Maxwell–Lorenz; 2) Bruggeman–Hanai; 3) Odelevskii–Kondorskii; 4) Landau–Lifshits; 5) Aramyan's formula [9]; 6) formula (26) with experimental data obtained by Reynolds.

$$\langle\varepsilon_x\rangle = \varepsilon_0 \frac{f_2 + (1 - f_2)^2 N_x}{(1 - f_2)^2 N_x}\,. \tag{24}$$

And if in Eq. (24) the concentration is varied from $f_2 = 0$ to $f_2 = 1$, the dielectric permeability varies from $\langle\varepsilon_x\rangle = \varepsilon_0$ to $\langle\varepsilon_x\rangle = \infty$.

The present authors are unaware of experimental data for an inhomogeneous material with ellipsoidal inclusions. Therefore, a comparison with experiment will be made for an inhomogeneous material with spherical inclusions. For this purpose, assuming in Eq. (23) that $N_x = 1/3$, we obtain a formula for the dielectric permeability of an inhomogeneous dielectric whose inclusions are spherical:

$$\langle\varepsilon\rangle = \varepsilon_0 \frac{\varepsilon_2 + 2\varepsilon_0 + f_2(\varepsilon_2 - \varepsilon_0)(1 + f_2)}{\varepsilon_2 + 2\varepsilon_0 - f_2(\varepsilon_2 - \varepsilon_0)(2 - f_2)}\,. \tag{25}$$

In the general case, where the dispersion medium is not a vacuum $\langle\varepsilon_0\rangle$, but a medium with the relative dielectric permeability ε_1, formula (25) takes the form

$$\langle\varepsilon\rangle = \varepsilon_1 \frac{\varepsilon_2 + 2\varepsilon_1 + f_2(\varepsilon_2 - \varepsilon_1)(1 + f_2)}{\varepsilon_2 + 2\varepsilon_1 - f_2(\varepsilon_2 - \varepsilon_1)(2 - f_2)}\,. \tag{26}$$

Table 1 contains results of calculation by formula (26) for $\varepsilon_1 = 2.228$ and $\varepsilon_2 = 4.594$ for $0 \le f_2 \le 0.35$. Experimental data obtained by Reynolds are taken from [1]. The table presents the deviations of the theoretical data (multiplied by 10^4), where the plus sign denotes values higher than the experimental data and the minus sign denotes ones lower.

It follows from the data given in the table that formula (26) is more accurate, especially at relatively high concentrations, than the existing Maxwell–Lorenz [3], Odelevskii–Kondorskii [4], Bruggeman–Hanai, Aramyan [9], and Landau–Lifshits formulas [8].*)

Thus, a method is suggested that allows one, by averaging equations of potential fields, to derive equations for calculating mean parameters of inhomogeneous materials. The method meets the requirements imposed on the theory of inhomogeneous media of regular structure.

NOTATION

ε, dielectric permeability of the homogeneous medium; ε_0, electric constant; $\vec{P}$, electric polarization vector; f_2, relative volume concentration of the inclusions; $\vec{D}_2$, electric displacement inside an nclusion; $\vec{E}_2$, intensity of the field inside an inclusion; $\vec{E}_p$, polarization field intensity; N_x, coefficient of depolarization of an ellipsoid along the x axis.

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