ON THE EFFECTIVE DIELECTRIC PERMITTIVITY OF NANOCOMPOSITE STRUCTURES

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Effective medium methods [1] are widely used to describe the optical properties of nanocomposite structures [2-6]. A nanodispersed structure can be considered as a new homogeneous medium with an effective permittivity ε_{ef} , which has the same optical properties as the given nanodispersed structure. Since the size of nanoparticles and the distance between them is less than the wavelength of light in the medium, it is sufficient to restrict ourselves to the electrostatic approximation to calculate the effective permittivity ε_{ef} of such a medium.

This article considers a multicomponent nanodispersed structure consisting of randomly oriented ellipsoidal nanoparticles in a matrix with a permittivity ε_m.

If the particles have the same ellipsoidal shape and are oriented in the one direction, and the external field E is directed along the direction of one of the main axes of the ellipsoids $i = a, b, c,$ then the particles will have the same polarization [2], and the particle polarization coefficient is determined by the formula:

$$\alpha_i = \frac{1}{4\pi}\frac{\varepsilon - \varepsilon_m}{\varepsilon_m + f_i(\varepsilon - \varepsilon_m)}. \tag{1}$$

Where, f_i is the shape factor of the ellipsoid in the direction of one of its principal axes. The formula for calculating the effective permittivity of the medium is written as follows

$$\frac{\varepsilon_{ef} - \varepsilon_m}{\varepsilon_m + f_i\left(\varepsilon_{ef} - \varepsilon_m\right)} = \sum q_i \cdot \frac{\varepsilon_i - \varepsilon_m}{\varepsilon_m + f_i(\varepsilon_i - \varepsilon_m)} \tag{2}$$

Formula (2) is a generalized formula for the Maxwell-Garnett effective medium model for a multicomponent nanodispersed medium with anisotropic (ellipsoidal) particles. f_i depends on the ratio of the principal axes of the ellipsoid and is calculated by the integral [4]

$$f_i = \frac{abc}{2}\int_0^\infty \frac{ds}{(s+i^2)\left((s+a^2)(s+b^2)(s+c^2)\right)^{1/2}} \tag{3}$$

The depolarization factors f_a, f_b and f_c satisfy the condition: $f_a + f_b + f_c = 1$. Also, if $a < b < c$, then $f_a > f_b > f_c$.

In the case of a spheroid, $b = c \neq a$ and therefore $f_b = f_c \neq f_a$.

If the nanocomposite medium is an ensemble of nanoparticles with dielectric permittivity ε, in the matrix of permittivity ε_m, then in formula (2) $\varepsilon_i = \varepsilon$, $q_i = q$, therefore, with simple transformations, we obtain the following formula for calculating the effective permittivity:

$$\varepsilon_{ef} = \varepsilon_m\left(1 + \frac{q(\varepsilon - \varepsilon_m)}{\varepsilon_m + f_i(1-q)(\varepsilon - \varepsilon_m)}\right) \tag{4}$$

In the case of randomly oriented ellipsoidal particles, we use the average value of the ellipsoidal polarization in the direction of the principal axes.

$$\bar{\alpha} = \frac{1}{3}\sum \alpha_i = \frac{1}{12\pi}\sum \frac{\varepsilon - \varepsilon_m}{\varepsilon_m + f_i(\varepsilon - \varepsilon_m)} \tag{5}$$

It can be shown that the determination of the average value of the polarization of an ellipsoid is reduced to the introduction of the effective form factor f_{ef}. In this case, the value of f_{ef} must be placed in the interval [0;1] and the relation must be satisfied:

$$\bar{\alpha_i} = \frac{1}{4\pi}\frac{\varepsilon - \varepsilon_m}{\varepsilon_m + f_{ef}(\varepsilon - \varepsilon_m)} = \frac{1}{12\pi}\sum \frac{\varepsilon - \varepsilon_m}{\varepsilon_m + f_i(\varepsilon - \varepsilon_m)} \tag{6}$$

In the case of a spheroidal shape of the particles, from eq. (6) is determined:

$$f_{ef} = \frac{1}{\xi - 1} \cdot \left(\frac{3 \cdot (1 + (\xi - 1) f_a)(1 + (\xi - 1) f_b)}{3 + (\xi - 1)(2 f_a + f_b)} - 1 \right) \tag{7}$$

The effective form factor is determined by the relative permittivity of the particle and the medium around the particle $\xi = \boldsymbol{\varepsilon}/\boldsymbol{\varepsilon_m}$ and depends on the ratio of the principal axes of the spheroid $\boldsymbol{\vartheta} = \frac{\boldsymbol{a}}{\boldsymbol{b}}$.

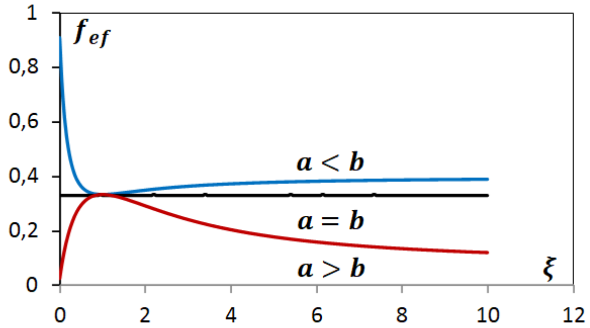

Fig.1. Dependencies of the f_{ef} on the ξ with different ϑ

Fig.1 shows the dependences of the f_{ef} on the ξ with different ϑ: $a > b$, $a = b$ and $a < b$. It can be seen that the value of the effective depolarization factor is always in the range 0-1. This makes it possible to prove that an ensemble of anisotropic nanoparticles can be replaced by an ensemble of nanoparticles with a depolarization coefficient f_{ef} uniformly oriented with respect to the external electric field.

Taking into account the effective depolarization factor, formula (4) is written in the following form:

$$\varepsilon_{ef} = \varepsilon_m \left(1 + \frac{q(\varepsilon - \varepsilon_m)}{\varepsilon_m + f_{ef}(1 - q)(\varepsilon - \varepsilon_m)} \right) \tag{8}$$

From formula (8) for given values of the parameters q, ε and ε_m, when f_{ef} =0, we obtain

$$\varepsilon_{ef} = q\varepsilon + (1 - q)\varepsilon_m, \tag{9}$$

and when $f_{ef} = 1$ we get

$$\frac{1}{\varepsilon_{ef}} = \frac{q}{\varepsilon} + \frac{1 - q}{\varepsilon_m} \tag{10}$$

For any configuration of nanocomposite structures, formulas (9) and (10) determine the minimum and maximum values of the effective dielectric permittivity.

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