Ambiguity in the Definition of Effective Dielectric Permittivity of Layered Heterogeneous Medium

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Abstract—The problem of ambiguity in defining effective dielectric permittivity is studied theoretically in application to a plane layered heterogeneous medium, compounded by two and more alternating homogeneous layers with different dielectric permittivities (water and glass), for the range of wavelengths from 1 to 10 cm. The effective permittivity for such a heterogeneous medium is usually determined by the phenomenological semi-empirical Braggeman's power rule, and the aim of the given investigation is validation of this rule by means of rigorous model of plane wave transmission and reflection. It is shown that the complex values of effective dielectric permittivity for a layered dielectric, determined by measuring its transmission and reflection coefficients, differ noticeably from one to another. It is also shown that in a wide frequency range, the Braggeman's formula gets as a close approximation only for such an effective dielectric permittivity, which is determined by a transmission coefficient.

1. INTRODUCTION

The concept of effective dielectric permittivity is widely used in electrodynamics of heterogeneous materials [1–4]. This is a dielectric permittivity of a certain homogeneous medium, which could have the same influence on electromagnetic field, as the heterogeneous medium, with all other factors being equal. Even in the early stage of investigation of a heterogeneous medium, at measuring its dielectric permittivity, an investigator comes up against this concept, determining in effect permittivity of an equivalent homogeneous material of the same shape. After that, on the bases of additional data about properties of medium components and their mutual arrangement in a volume, one determines sought physical parameters of a medium, for example, relative concentration of various constituents, invoking suitable theoretical models, or experimental calibration data [1–4]. However, the rules determining the effective dielectric permittivity in various physical cases are semi-empirical and not rigorous, which causes certain doubt about their authenticity. Nevertheless, such an approach turned out to be very productive for the study of physical properties of various heterogeneous materials and for the development of control systems in modern technological production of such materials [1, 4]. This technique of simplified phenomenological description of physical properties of heterogeneous structures can be of great importance in the context of a tremendous growth in new avenues of modern science and technology, concerned with active study and use of such physical micro and nano objects, as semiconductor heterostructures, photon crystals, superlattices, metamaterials, etc. [5, 6].

Meanwhile, the very concept of effective dielectric permittivity is not defined uniquely, and its value depends on the manner of its determination. In this work, we discuss this problem by the simple example of layered inhomogeneous medium, when heterogeneous material is represented by multilayered plane dielectric, composed of an aggregate of parallel-plate homogeneous layers of two materials with different

dielectric permittivity. The aim of our theoretical investigation is validation of phenomenological semi-empirical definition of effective permittivity for this example of heterogeneous material by means of rigorous model of plane wave transmission and reflection, based on Maxwell's equations. We consider the simplest and commonly used method of permittivity determination and medium testing, when a medium of the form of a plane layer is placed before a source of electromagnetic waves, forming an incident beam, and desired permittivity value is determined by measuring amplitude coefficient of transmission or reflection for a layer under test.

2. BASIC EQUATIONS OF THE THEORY

From the beginning, let us consider the reflection and refraction of a plane electromagnetic wave by a plane homogeneous dielectric layer with thickness h. We can write the amplitude transmission and reflection coefficients for this layer [7–9] in terms of normal components of parameters of the wave propagation in various media [8, 9]

$$T_{012} = \frac{T_{01}T_{12}}{D_{012}} \exp(ik\alpha_1 h) \quad R_{012} = \frac{R_{01} + R_{12}\exp(2ik\alpha_1 h)}{D_{012}} \tag{1}$$

where $i = \sqrt{-1}$ is the imaginary unit; $k = \omega/c = 2\pi/\lambda$ is the wave number; ω is the circular frequency; c is the light speed in vacuum; λ is the wavelength,

$$D_{012} = 1 + R_{01}R_{12}\exp(2ik\alpha_1 h)$$

and the quantities

$$T_{01} = \frac{2\varepsilon_0^\nu \alpha_0}{\alpha_0\varepsilon_1^\nu + \alpha_1\varepsilon_0^\nu}; \quad T_{12} = \frac{2\varepsilon_1^\nu \alpha_1}{\alpha_1\varepsilon_2^\nu + \alpha_2\varepsilon_1^\nu}; \quad R_{01} = \frac{\alpha_0\varepsilon_1^\nu - \alpha_1\varepsilon_0^\nu}{\alpha_0\varepsilon_1^\nu + \alpha_1\varepsilon_0^\nu}; \quad R_{12} = \frac{\alpha_1\varepsilon_2^\nu - \alpha_2\varepsilon_1^\nu}{\alpha_1\varepsilon_2^\nu + \alpha_2\varepsilon_1^\nu} \tag{2}$$

are the amplitude refraction and reflection coefficients of a wave on the plane interfaces "medium 0–medium 1" and "medium 1–medium 2". Here $\nu = 0$ for TE polarization of radiation, whose electric vector is orthogonal to the plane of incidence, and $\nu = 1$ for TM polarization, having magnetic vector to be orthogonal to this plane,

$$\alpha_n = \sqrt{\varepsilon_n - \beta^2}; \quad n = 0, 1, 2 \tag{3}$$

are the parameters of normal wave propagation in each medium; $\beta = \sin\theta$ is the parameter of tangential wave propagation, which is the same in all media (θ is the angle of wave incidence on a layer from vacuum). Below we shall restrict our consideration to the simple case when a homogeneous layer is surrounded on both sides by air (vacuum), i.e., when

$$\varepsilon_0 = \varepsilon_2 = 1; \quad \alpha_0 = \alpha_2 = \sqrt{1 - \beta^2}; \quad R_{12} = -R_{01}$$

Now, let us consider a heterogeneous plate, composed of two layers of homogeneous dielectric materials with the thicknesses h_1 and h_2 (see Fig. 1). The amplitude coefficients of plane wave transmission and reflection by such a layer assume the form [8]

$$T_{0123} = \frac{T_{01}T_{12}T_{23}}{D_{0123}D_{123}} \exp[ik(\alpha_1 h_1 + \alpha_2 h_2)] \quad R_{0123} = \frac{R_{01} + R_{123}\exp(2ik\alpha_1 h_1)}{D_{0123}} \tag{4}$$
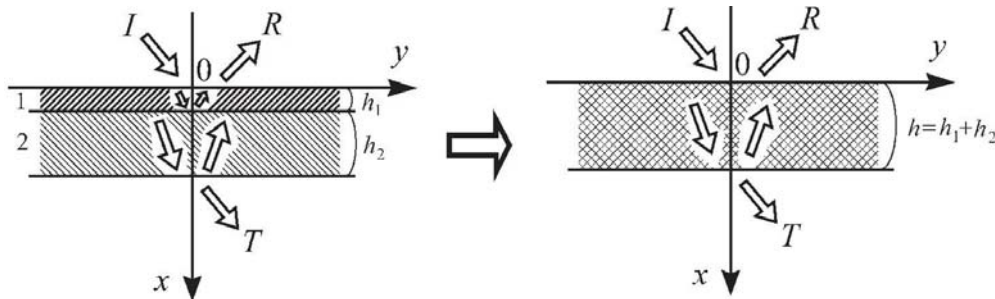

Figure 1. Reflection and refraction in two-layered heterogeneous medium and equivalent homogeneous medium.

where

$$T_{nm} = \frac{2\varepsilon_n^\nu \alpha_n}{\alpha_n \varepsilon_m^\nu + \alpha_m \varepsilon_n^\nu}; \quad R_{nm} = \frac{\alpha_n \varepsilon_m^\nu - \alpha_m \varepsilon_n^\nu}{\alpha_n \varepsilon_m^\nu + \alpha_m \varepsilon_n^\nu}; \quad n = 0,\ 1,\ 2;\ m = n+1. \tag{5}$$

are the amplitude coefficients of refraction and reflection on the plane interface between medium n and medium $m = n + 1$

$$D_{0123} = 1 + R_{01}R_{123}\exp(2ik\alpha_1 h_1); \quad D_{123} = 1 + R_{12}R_{23}\exp(2ik\alpha_2 h_2); \quad R_{123} = \frac{R_{12} + R_{23}\exp(2ik\alpha_2 h_2)}{D_{123}}$$

As before, the parameters of normal propagation for a plane wave in various media are determined by Eq. (3). For a heterogeneous layer, we also consider a simpler case when it is surrounded by air on both sides, and

$$\varepsilon_0 = \varepsilon_3 = 1; \quad \alpha_0 = \alpha_3 = \sqrt{1 - \beta^2}.$$

Besides, we shall consider the model of a multilayered dielectric structure, composed of periodically alternating layers of two substances. Usually, the matrix methods are applied to calculation of the fields in layered inhomogeneous materials [7, 9]. But the method of analytical representation of fields in every layer [8] is more suitable and practical for this purpose. Let a plane electromagnetic wave be incident on the structure, containing N plane parallel interfaces. For that, the amplitude transmission and reflection coefficients can be written as follows [8]

$$R_{0123...(N-1)N} = \frac{R_{01} + R_{123...(N-1)N}\exp(2ik\alpha_1 d_1)}{D_{0123...(N-1)N}}; \tag{6a}$$

$$T_{0123...(N-1)N} = T_{01}T_{12}T_{23}...T_{(N-1)N} \frac{\exp[ik(\alpha_1 d_1 + \alpha_2 d_2 + \alpha_3 d_3 + ... + \alpha_{N-1}d_{N-1})]}{D_{0123...(N-1)N}D_{123...(N-1)N}D_{234...(N-1)N}...D_{(N-2)(N-1)N}} \tag{6b}$$

where d_n is the thickness of a plane medium with the number n,

$$\alpha_n = \sqrt{\varepsilon_n - \beta_0^2}$$

ε_n is the dielectric permittivity of the given medium,

$$D_{0123...(N-1)N} = 1 + R_{01}R_{123...(N-1)N}\exp(2ik\alpha_1 d_1) \quad D_{123...(N-1)N} = 1 + R_{12}R_{23...(N-1)N}\exp(2ik\alpha_2 d_2)$$

$$R_{123...(N-1)N} = \frac{R_{12} + R_{23...(N-1)N}\exp(2ik\alpha_2 d_2)}{D_{123...(N-1)N}} \quad D_{234...(N-1)N} = 1 + R_{23}R_{345...(N-1)N}\exp(2ik\alpha_3 d_3)$$

$$R_{234...(N-1)N} = \frac{R_{23} + R_{345...(N-1)N}\exp(2ik\alpha_3 d_3)}{D_{234...(N-1)N}}$$

....

$$D_{(N-2)(N-1)N} = 1 + R_{(N-2)(N-1)}R_{(N-1)N}\exp(2ik\alpha_{N-1}d_{N-1})$$

$$R_{(N-2)(N-1)N} = \frac{R_{(N-2)(N-1)} + R_{(N-1)N}\exp(2ik\alpha_{N-1}d_{N-1})}{D_{(N-2)(N-1)N}}$$

and R_{nm}, T_{nm} are, as before Eq. (5), the amplitude coefficients of reflection and refraction of a plane wave on the interface between media with numbers n and m.

We shall consider a multilayered structure, formed by periodically alternating layers of two different substances, when media $n = 0$ and $n = N$ are air. The layers with numbers $n = 2m-1$ is filled by the 1st substance, and the media with numbers $n = 2m$ is presented by the 2nd substance ($m = 1; 2; 3; ...; M$; $N = 2M + 1$, M is the number of replication of identical layers in dielectric depth). Assume that all layers for the same substance are uniform in thickness: $d_n = h_1/M$ for the 1st substance ($n = 2m - 1$) and $d_n = h_2/M$ for the 2nd substance ($n = 2m$), i.e., our multilayered structure has the thickness of the two-layered dielectric in the previous case.

For a heterogeneous plane dielectric (see Fig. 2), the concept of effective dielectric permittivity arises, when one interprets its amplitude transmission or reflection coefficient as a transmission or reflection coefficient of a homogeneous plane layer (1) of the identical thickness $h = h_1 + h_2$. Effective
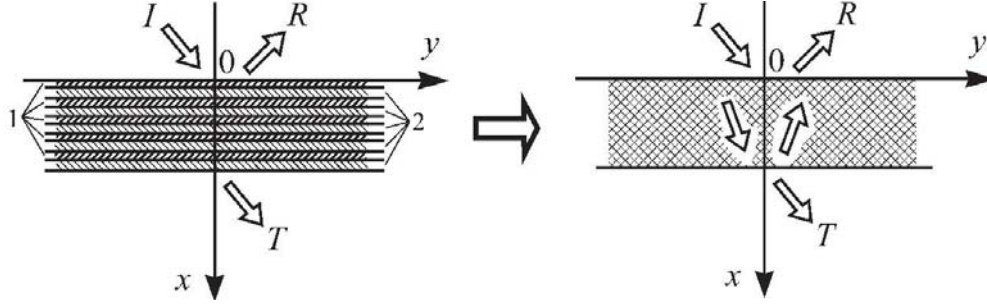
Figure 2. Reflection and refraction in multilayered heterogeneous medium and equivalent homogeneous medium.

permittivity is such that the permittivity of a homogeneous layer $\varepsilon_{eff} = \varepsilon_2$ yields the value of the transmission or reflection coefficient (1), equal to the transmission or reflection coefficient (4) or (6) of a heterogeneous layer. Here, we get transcendent equations for determining the dielectric permittivity of a heterogeneous layer in terms of known value of its transmission or reflection coefficient

$$T_{012}(\varepsilon_T) = T_{0123...(N-1)N}(\varepsilon_1, \varepsilon_2) \quad R_{012}(\varepsilon_R) = R_{0123...(N-1)N}(\varepsilon_1, \varepsilon_2) \tag{7}$$

where the values T_{012}, R_{012} and $T_{0123...(N-1)N}$, $R_{0123...(N-1)N}$ are given by corresponding expressions (1), (6), and different notations ε_T and ε_R for effective permittivity allow for different values, determined by transmission and reflection coefficients, respectively.

3. COMPUTATION RESULTS

As a simple example of calculations of effective dielectric permittivity, let us consider a water layer on a glass plate in the microwave range with the wavelength from 1 to 10 cm. In this range, the frequency dependence for complex dielectric permittivity of both materials is determined by the relaxation polarization mechanism [10, 11]

$$\varepsilon = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - i\omega\tau}$$

where ε_s and ε_∞ are the static (at $\omega \to 0$) and optical (at $\omega \to +\infty$) real values of dielectric permittivity, and τ is the dielectric relaxation time; or

$$\varepsilon = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - i\gamma/\lambda} \tag{8}$$

where $\gamma = 2\pi c\tau$. Setting for water $\varepsilon_\infty = 5.7$, $\varepsilon_s - \varepsilon_\infty = 74.5$, $\gamma = 1.77$ cm [10, 11] and for glass $\varepsilon_\infty = 3.0$, $\varepsilon_s - \varepsilon_\infty = 0.76$, $\gamma = 1.5$ cm, one obtains the relationship between the complex dielectric permittivity of these substances and the wavelength of transmitting radiation, presented graphically in Fig. 3.

Let the water layer of the thickness $h_1 = 0.6$ cm is placed on the glass plate of the thickness $h_2 = 0.5$ cm. These layers constitute a two-layered dielectric structure, whose transmission and reflection coefficients can be calculated by the formulae (4). Fig. 4 depicts the modulus of the values of these coefficients dependent on the wavelength of incident radiation. Besides, this figure presents the results of analogous computations of Eq. (6) for multilayered periodical structure with the same total thickness and 20 homogeneous layers, formed by these substances, water and glass. In the phenomenological model of heterogeneous materials, the effective dielectric permittivity of such structures is usually determined by the simplified semi-empirical Braggeman's power formula [2, 3], when this permittivity is equated to the sum of permittivities of separate components with the coefficients, equal to their volume concentrations in a medium

$$\varepsilon_B = \varepsilon_1 h_1/h + \varepsilon_2 h_2/h \tag{9}$$

where h_1 and h_2 are the combined thickness of all layers of one or the other mixture component, and $h = h_1 + h_2$ is the total thickness of the heterogeneous medium. The transmission and reflection coefficients of the homogeneous layer with the permittivity in Eq. (9) are also presented in Fig. 4.
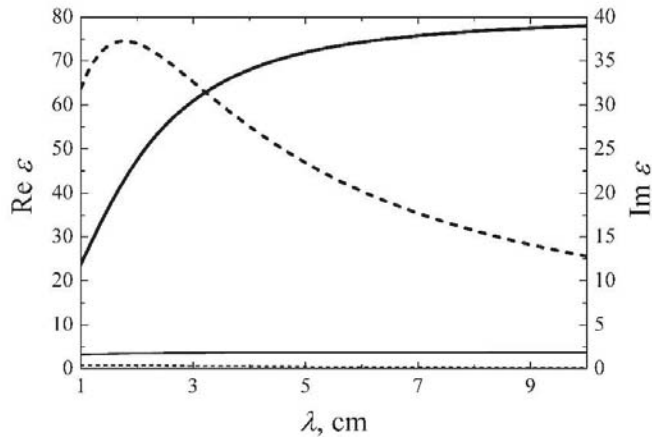
Figure 3. Real (solid lines) and imaginary (dashed curves) parts of the complex dielectric permittivity as functions of transmitting radiation wavelength for water (thick lines) and for glass (thin lines).
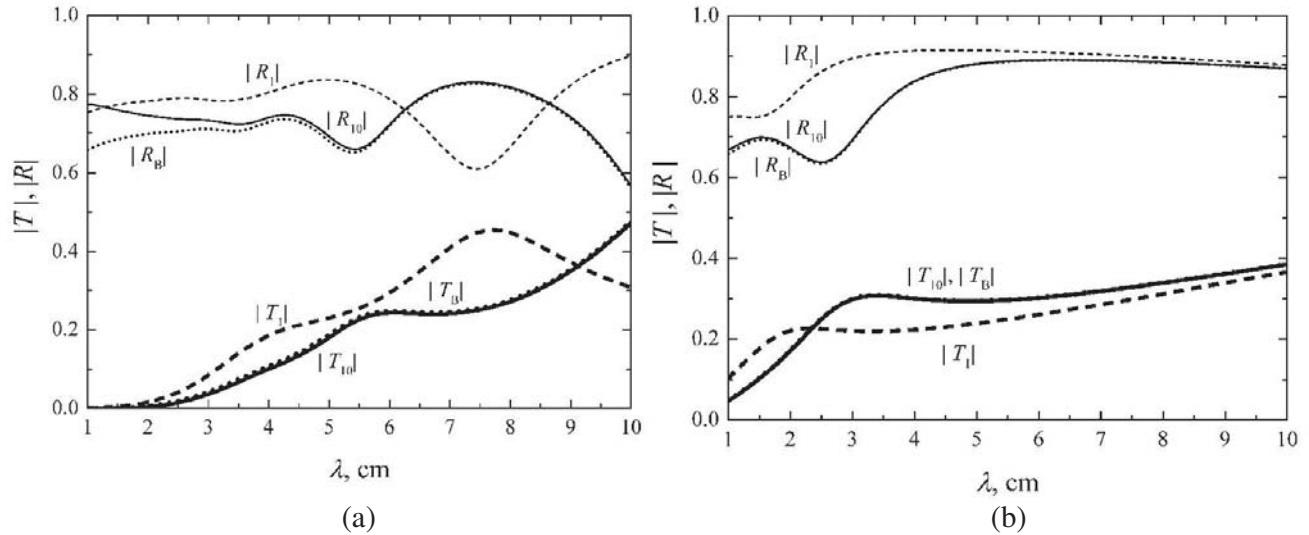

Figure 4. Modulus of the amplitude transmission $|T_M|$ (thick curves) and reflection $|R_M|$ (thin lines) coefficients of a multilayered dielectric with the thickness (a) 0.9 cm and (b) 0.225 cm, having the number of layers $2M$ ($M = 1$ and $M = 10$), in dependence of testing radiation wavelength at its normal incidence ($\theta = 0°$). The data for transmission $|T_B|$ and reflection $|R_B|$ coefficients, computed for a homogeneous layer with the permittivity ε_B by the Braggeman's formula (9) are displayed for comparison.

In this figure, the values of transmission and reflection coefficients are shown by thick and thin lines, respectively, being depicted by dashed curves for two-layered dielectric, by solid ones for multilayered material, and by dotted lines for a homogeneous layer with the Braggeman's permittivity in Eq. (9). In the following figures, the identical curves display the values, determined in terms of the given coefficients by Equation (7).

Figures 5 and 6 depict the results, obtained by solving Equation (7) for effective complex dielectric permittivity of a multilayered material (with the number of layers 20) dependent on radiation wavelength, and of the angle of incidence, when the total dielectric thickness comprises $h = h_1 + h_2 = 0.4 \, \text{cm} + 0.5 \, \text{cm} = 0.9 \, \text{cm}$. Computations have been performed for the cases, when the number of layers is 2 and 20 (a further increase in their number has little effect on the final result). In right-hand sides of the given equations, we have used the values of transmission and reflection coefficients of Eq. (4)
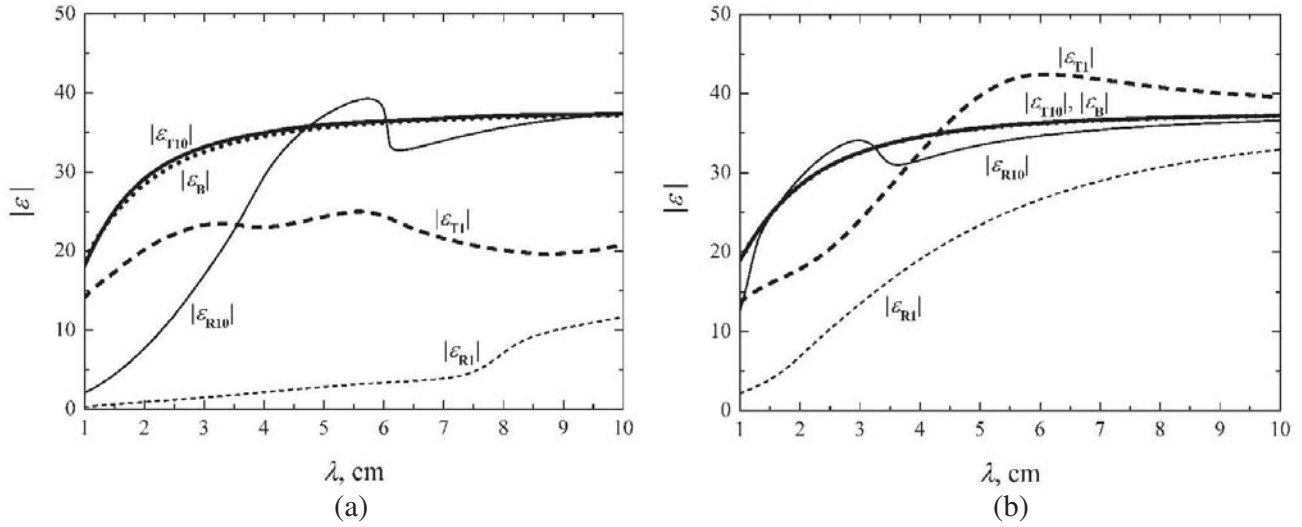
Figure 5. Modulus of the complex effective dielectric permittivities ε_{TM} and ε_{RM}, determined from equations for amplitude transmission (thick curves) and reflection (thin lines) coefficients of a multilayered dielectric with the thickness (a) 0.9 cm and (b) 0.225 cm, having the number of layers $2M$ ($M = 1$ and $M = 10$), in dependence of testing radiation wavelength at its normal incidence ($\theta = 0°$).
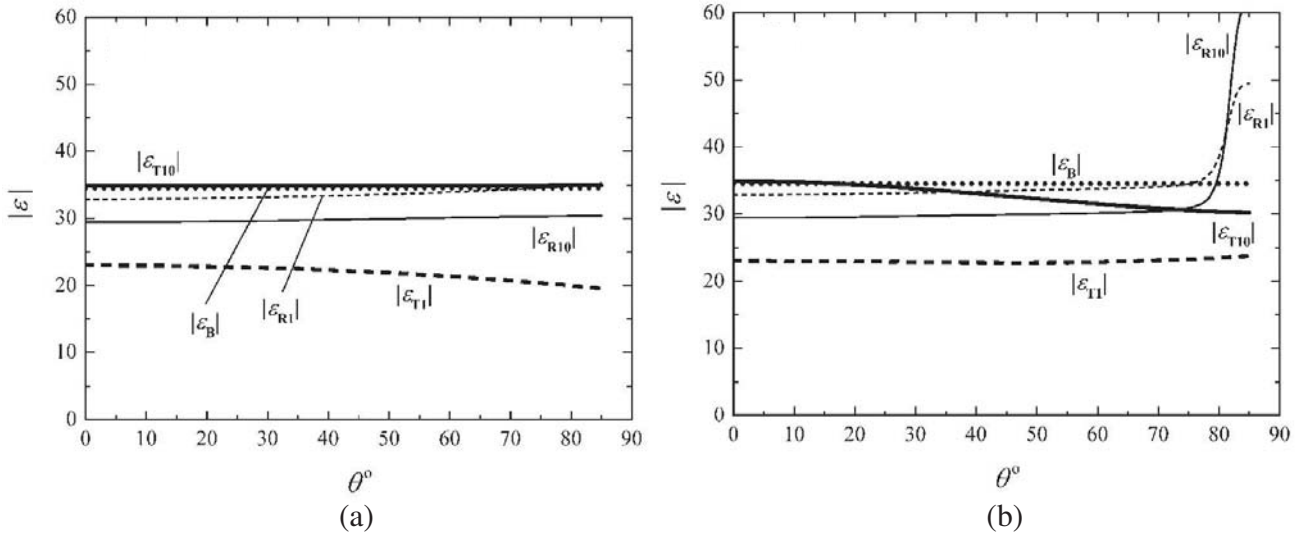

Figure 6. Modulus of the complex effective dielectric permittivities ε_{TM} (thick curves) and ε_{RM} (thin lines), determined from equations for amplitude transmission and reflection coefficients of a multilayered dielectric with the thickness 0.9 cm, having the number of layers $2M$ ($M = 1$ and $M = 10$), in dependence of the angle of incidence θ of testing radiation with the wavelength $\lambda = 4$ cm in the cases of (a) TE and (b) TM polarization.

or Eq. (6) of a multilayered dielectric at various values of the wavelength or of the angle of incidence. Besides, for comparison, the values of effective permittivity ε_B, calculated by formula (9), are shown in Figs. 5 and 6 by dotted lines. The real and imaginary parts of all these values demonstrate similar behavior, that is why we present only magnitudes of the given complex values.

   Figures 5 and 6 show that the effective permittivities ε_T and ε_R, calculated by transmission and reflection coefficients, differ one from the other and do not equal to values, computed by Bruggeman in Eq. (9). The fact that effective permittivities vary under wavelength change is not unexpected owing to

dielectric dispersion of various components (see Fig. 3). However, the occurrence of effective permittivity dependence on polarization of testing field (TE or TM), on the type of initial coefficient (transmission or reflection), and also on the angle of incidence, for heterogeneous material is not obvious, because for homogeneous dielectric all these dependences are absent. It says that the physical sense of effective dielectric permittivity of heterogeneous material is not fully identical to that of the permittivity of a homogeneous layer.

From the graphs in Figs. 5 and 6 for two-layered and multilayered dielectrics, one can see that increase of the number of layers gives rise to that the properties of these dielectric become closer to the properties of a homogeneous layer with effective value of dielectric permittivity. For multilayered structures with number of layers more than 20, the model of such a homogeneous layer produces quite satisfactory results. However, it is typical only for the effective permittivity, determined by transmission coefficient and only for TE polarization, but for TM polarization, at the values of angle of incidence more than 20°, one observes noticeable discrepancies from the Braggeman's values. The matter is that formula (9) is applicable to the cases, when the electric field is parallel to the boundaries of layers of a multilayered structure, as it occurs for TE polarization, but in the cases of field orthogonal to the layers, the mixing formula (9) must be written with the index of a power -1 for all dielectric permittivities [2, 3]. That is why for TM polarization, whose electric vector lies in the plane of incidence, its normal component increases with increase of the angle of incidence, and formula (9) becomes inapplicable. Besides, noticeable disagreements from Braggeman's values arise for effective permittivities, determined by reflection coefficients, for both polarizations. Calculations show that the presence of great number of periodical layers by itself is not an essential feature. The relation between the wavelength of transmitting radiation and total thickness of a homogeneous layer is of importance to a far greater extent. The greater the wavelength is in comparison with the given thickness, the more accurate description one obtains using the Braggeman's formula as for transmission, as for reflection from a layer. This formula provides sufficiently complete description of dielectric properties of a plane layered heterogeneous medium only in the limiting case of negligibly small thickness of a medium in comparison with the wavelength of transmitting radiation. It is clear, because the Braggeman's formula (9) was established for electrostatic fields.

It should be noted that Equation (7) have more than one solution for effective dielectric permittivities at specified values of medium and radiation parameters. For Figs. 5 and 6, we have selected the solutions, which are most close to the Braggeman's values of Eq. (9) of permittivity.

4. CONCLUSION

In the given work, we have computed the transmission and reflection coefficients of layered heterogeneous media at various frequencies of monochromatic electromagnetic radiation and at various angles of incidence, determining effective dielectric permittivities of an equivalent homogeneous dielectric layer from the equations with these coefficients. It appears that the complex effective permittivities of layered media depend on transmitting radiation wavelength, on the angle of wave incidence on the layer, and on its polarization. If the wavelength is much more than the medium thickness, and it contains many layers of various substances (no less than 10), then the effective permittivity no longer depends on the properties of transmitting radiation and becomes practically equal to the dielectric permittivity, determined by the classical Braggeman's mixing formula for heterogeneous medium containing parallel layers. However, with decreasing the wavelength, one observes increasing distinctions between effective permittivities, determined for different coefficients (of transmission and reflection), different polarizations, and various angles of incidence. At any values of wavelength and of angle of incidence, the Braggeman's formula gives a close approximation only for TE polarization with the electric vector, orthogonal to the plane of incidence on a multilayer heterogeneous substance, when the effective permittivity is determined by transmission coefficient, but for TM polarization it is true only at small values of the angle of incidence. At the same time, the effective permittivities, determined by reflection coefficient of a layered medium, can be noticeably different from the Braggeman's value.

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