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Equivalent medium theory of layered sphere particle with anisotropic shells

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ABSTRACT

Researches on the optical properties of small particle have been widely concerned in the atmospheric science, astronomy, astrophysics, biology and medical science. This paper provides an equivalent dielectric theory for the functional graded particle with anisotropic shells, in which inhomogeneous and anisotropic particle was equivalently transformed into a new kind of homogeneous, continuous and isotropic sphere with same size but different permittivity, and then greatly simplify the calculation process of particle's optical property. Meanwhile, the paper also discusses whether the charge on the particle can change the expression of its equivalent permittivity or not. These results proposed in this paper can be used to simulate the electrical, optical properties of layered sphere, it also meet the research requirement in the design of functional graded particles in different subjects.

1. Introduction

Estimation and simulation of the optical properties for small particles became a common research subject in the atmospheric science, astronomy, astrophysics, biology, medical science and the chemistry. Because of its complexities in particle shapes and structures [1,2], several methods to resolve the problem have been suggested, for example, Rayleigh approximation [3], Lorenz–Mie theory [3,4], N-layered Mie theory [5–8], DDA [9,10], T-matrix method [11–16], Separation of Variables Method [2,17], FDTD [18,19], Deby series solution [20–22] etc. Besides, because of its clear physical significance and concision, equivalent medium theory has been obtained much attention, and it has been used to do some numerical simulation works on the optical and electrical properties of intermixed random medium [23,24]. With the help of the equivalent medium theory, Videen et al. discussed the electromagnetic scattering of sphere with an absorptive core [25]. Kolokolova et al. simulated the electromagnetic scattering property of discontinuous particle, and compared it with the experiment results [26]. They found that the equivalent medium theory does not work for calculations of back-scattering characteristics of large particles. Li et al. proposed the equivalent permittivity of a multilayered isotropic sphere, and discussed its application in the calculation of particles' electromagnetic scattering [27]. They found the equivalent permittivity can be used when the Rayleigh hypothesis is meet. Liu et al. compared the similarities and differences of four major theories on the equivalent medium, such as the Bruggeman theory, the Maxwell-Garnett theory, and two different Wiener bounds, and analyzed their scopes of application in

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calculating the electromagnetic scattering properties of inhomogeneous medium particles [28].

However, these models mentioned above are only applicable to the isotropic medium. Meanwhile, functional graded materials make it easy to achieve invisibility at specific frequency ranges, which is attracting more and more attentions from scientific researchers [29,30]. The anisotropic shell can significantly change the electric field distribution inside the particle, so as to realize some interesting features [29]. Numerical simulations of the electromagnetic field both inside and outside of the particle with different structural can give an important guidance to the structural designs, and the equivalent medium theory can significantly simplify related calculations and meet the accurate requirement of engineering design. There are quite a few researches on the optical properties of particles with multilayered structures or some anisotropic shells, but there is still a lack of detailed and systematic research on its equivalent permittivity. Therefore, this paper devoted to the study of equivalent permittivity of these kinds of particles with similar structures. In addition, we also discussed the influences of the surface charge on the particle's equivalent permittivity.

2. Basic theories and models

2.1. Equivalent permittivity of homogeneous particle with some anisotropic shells

Assuming there's a core–shell structured spherical particle with an anisotropic coating, and the core is an isotropic medium, its permittivity is ε_0 and the radius is r_0. The shell is an anisotropic material, its outer radius is r_1, and its permittivity can be expressed with the spherical coordinate as follows,

$$\varepsilon_s = \begin{bmatrix} \varepsilon_r & 0 & 0 \\ 0 & \varepsilon_\theta & 0 \\ 0 & 0 & \varepsilon_\varphi \end{bmatrix} \tag{1}$$

The background medium around the particle is isotropic and its permittivity is ε_h. Considering the electrostatic field component of the incident wave is $\boldsymbol{E}_{in} = E_0\boldsymbol{x}$. With the spherical coordinates (r, θ, φ), the electric potentials both inside of the particle and outside of it can be expressed as [29,30],

$$\phi_c = -E_c r \cos\theta \quad r < r_0 \tag{2a}$$

$$\phi_s = \left(A_1 r^{t_1} + A_2 r^{t_2}\right)\cos\theta \quad r_0 < r < r_1 \tag{2b}$$

$$\phi_h = \left(-r + D/r^2\right)E_0 \cos\theta \quad r > r_1 \tag{2c}$$

Here $t_{1,2} = \left(-1 \pm \sqrt{1 + 8\varepsilon_\theta/\varepsilon_r}\right)/2$, E_0 is the intensity of electrostatic field, and A_1, A_2, E_c, D, are undetermined coefficients, which can be determined through the corresponding boundary conditions,

$$\begin{cases} r = r_0 \quad \phi_c = \phi_s \quad \varepsilon_0 \dfrac{\partial \phi_c}{\partial r} = \varepsilon_r \dfrac{\partial \phi_s}{\partial r} \\ r = r_1 \quad \phi_s = \phi_h \quad \varepsilon_h \dfrac{\partial \phi_h}{\partial r} = \varepsilon_r \dfrac{\partial \phi_s}{\partial r} \end{cases} \tag{3}$$

Through Eqs. (2), (3) we can obtain

$$E_c = \frac{3\varepsilon_r \varepsilon_h (t_2 - t_1) E_0}{(\varepsilon_r t_2 - \varepsilon_0) a_1 - (\varepsilon_r t_1 - \varepsilon_0) a_2} \tag{4}$$

$$A_1 = -\frac{(\varepsilon_r t_2 - \varepsilon_0) E_c}{\varepsilon_r (t_2 - t_1) r_0^{t_1 - 1}} \quad A_2 = \frac{(\varepsilon_r t_1 - \varepsilon_0) E_c}{\varepsilon_r (t_2 - t_1) r_0^{t_2 - 1}} \quad D = \frac{\tilde{\varepsilon} - \varepsilon_h}{\tilde{\varepsilon} + 2\varepsilon_h} r_0^3$$

Here

$$a_{1,2} = (\varepsilon_r t_{1,2} + 2\varepsilon_h)\lambda^{t_{1,2} - 1}, \lambda = r_1/r_0, a_{1,2} = (\varepsilon_r t_{1,2} + 2\varepsilon_h)\lambda^{t_{1,2} - 1}$$

and

$$\tilde{\varepsilon} = \frac{(\varepsilon_r t_2 - \varepsilon_0) t_1 \lambda^{t_1 - t_2} - (\varepsilon_r t_1 - \varepsilon_0) t_2}{(\varepsilon_r t_2 - \varepsilon_0)\lambda^{t_1 - t_2} - (\varepsilon_r t_1 - \varepsilon_0)} \varepsilon_r \tag{5}$$

Compared (2c) with the expression of outer potential for a homogeneous sphere in a uniform electric field, $\tilde{\varepsilon}$ can be considered as the equivalent permittivity of spherical particle with an anisotropic coating. As shown in the above equation, the coefficient before E_0 in E_c is a constant, which related to the core–shell radius ratio and the permittivity of the particle, which means that the core–shell geometric parameters and the electrical properties of shell all can change the electric field in the particle.

Based on the new parameter expression $\tilde{\varepsilon}$, the equivalent dielectric constant of the coated sphere with an anisotropic shell, and the method proposed by Li et al. [27], we can expand this result to other conditions, and then obtain the equivalent parameter of any particle with some types of special structures. Those results are discussed as follows.

1) *N-layered core–shell particle with an anisotropic shell and $N-1$ isotropic shells*
For this kind of special particle, supposed the radius for the core and shells are $r_0, r_1, r_2, r_3, \cdots r_N$, the permittivity is $\varepsilon_0, \varepsilon_1, \varepsilon_2, \varepsilon_3, \cdots \varepsilon_N$, respectively. Here the dielectric constant ε_1 for the first shell have a similar expression with the Eq. (1). In order to obtain the equivalent permittivity of this multi-layered particle, we can set the core and the first shell as a new core, whose dielectric constant can be obtained through the Eq. (5). With a similar operation with reference [27] we can obtain its permittivity,

$$\tilde{\varepsilon}_n = \frac{(\beta_{n-1} + 2g_n) + 2\delta_n(\beta_{n-1} - g_n)}{(\beta_{n-1} + 2g_n) - \delta_n(\beta_{n-1} - g_n)} \varepsilon_n \overset{\text{signed as}}{\rightarrow} \beta_n \varepsilon_n \tag{6}$$

here

$$\delta_n = r_{n-1}^3 / r_n^3, g_n = \varepsilon_n / \tilde{\varepsilon}_{n-1}, \beta_1 = 1, \tilde{\varepsilon}_1 = \tilde{\varepsilon},$$
$$\beta_n = \frac{(\beta_{n-1} + 2g_n) + 2\delta_n(\beta_{n-1} - g_n)}{(\beta_{n-1} + 2g_n) - \delta_n(\beta_{n-1} - g_n)}, n = 2, 3, \ldots\ldots N.$$

The parameter E_c in the electric potential of the core-zone can be expressed as,

$$E_c = \frac{3\varepsilon_r \varepsilon_h (t_2 - t_1) A E_0}{(\varepsilon_r t_2 - \varepsilon_c) a_1 - (\varepsilon_r t_1 - \varepsilon_c) a_2} \tag{7}$$

$$A = \prod_{i=2}^{N} \frac{9\varepsilon_h \varepsilon_i}{(\varepsilon_i + 2\varepsilon_h)(\widetilde{\varepsilon_{i-1}} + 2\varepsilon_i) + 2\delta_i(\varepsilon_i - \varepsilon_h)(\widetilde{\varepsilon_{i-1}} - \varepsilon_i)} \tag{8}$$