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Modeling electrical and optical spectral responses of homogeneous nanocomposites

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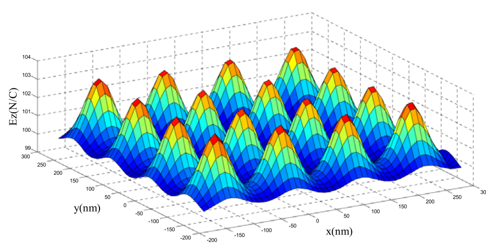
HIGHLIGHTS

- Describing the induced anisotropic electric field as tensor quantities inside a nanocomposite.
- Evaluating the effective electrical conduction and permittivity of a homogeneous nanocomposite.
- Modeling optical dispersion spectrum and UV–visible absorption spectrum of nanocomposites.
- Checking the model in silver nanocolloid.

GRAPHICAL ABSTRACT

Electrical and optical properties of a nano-composite has been studied by the distribution of the electric field on an plane inside it, that is scattered by arrangement of particles.



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ABSTRACT

In this study, electric field diffraction by a nanoparticle is studied using Legender series and extended for many particles in three dimensions. In the presence of an external dc electric field, the electric field induced by all the particles is added together based on the superposition principle and the electric field distribution would be obtained on an unlimited sheet inside the host matrix. Using this field distribution, pure displaced electric charge and passed current would be evaluated and the effective electrical conductivity and permittivity would be obtained. These parameters could predict the optical spectral responses of nano-composites such as the UV–visible absorption spectrum and refractive dispersion spectrum.

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1. Introduction

The most common way to achieve materials with a large linear and nonlinear susceptibility is to use composite materials in which the constituent components possess large intrinsic electrical and optical responses [1]. The formation of composite materials thus constitutes a means for engineering new materials with desired optical properties [2]. In fact, the composite effects arise from strong enhancement or fluctuations of the local fields within the spectral range of collective dipolar resonances like surface plasmon resonances. Surface plasmon resonances on the surface of an individual particle could be illustrated by the solution of Maxwell wave equation which is a Legender series. Legender series could perfectly explain the charge distribution on the particle surface and the electric field distribution outside and inside the particles. Generally, there are three typical theories for calculating the effective permittivity of a nanocomposite, namely: the Maxwell–Garnett theory (Clausius–Mossotti theory), the Bruggeman theory and the Bergman–Milton spectral representation theory. These

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models employ the Legender series in different manners. In Maxwell–Garnett theory [1,3], the effective dielectric constant is given by the ratio of the average displacement to the average electric field inside the composite. Averaging is taken proportional to volume fractions of two components of the composite. The Bruggeman theory [1,4] is based on this fact that the effective dipole factor of the composite should be 0. Its predictions are usually sensible and physically offer a way of quick insight into some problems that are difficult to tackle by other approaches. In Bergman–Milton spectral representation theory [1,5] the electrical potential inside the composite is the solution of Helmholtz equation (colon low of Maxwell equations) that is defined as an integral of free space Green's function over all the space. Similar approximations have been employed to determine dielectric and optical properties of composites. For example, the general sum rule for the effective susceptibilities in a many-body system has been discussed by Lozovski [6,7]. In order to more precision, all these models could been used as boundary conditions to confine the solution area [8,9].

Basically, the electrical and optical responses of a nanocomposite can be tuned by controlling the volume fraction and morphology of constitution.

In this work, we assume an ideal homogenize two-component composite and offer a full mathematical and analytical model based on direct utilization of Legender series (as solution of Helmholtz equation), with the least approximation. First, the effect of a single particle on the applied electrical field would be discussed. Then, the electric field distribution on an inner plane in the medium would be evaluated using superposition principle and this would be the origin of electrical and optical quantities modeling. In other words, this model is an applicable combination of previous models and offers an applicable method.

2. Theory

2.1. Electrical permittivity and conduction tensors of a medium containing a single nanoparticle

Consider a spherical particle with the radius R inside an unlimited dielectric medium. The electrical permittivity of the particle and the medium are ε_1 and ε_2, respectively. The constant electric field in the host medium is $\mathbf{E}=E_{0z}\hat{\mathbf{z}}$. The origin of the coordinates system is considered at the particle center. The electric potential inside and outside the sphere would be a Legender series given by [10]

$$\phi_1(r,\theta)=\phi_0+Ar\cos\theta$$

$$\phi_2(r,\theta)=\phi_0+Br\cos\theta+\frac{C}{r^2}\cos\theta \tag{1}$$

where A, B and C are the Legender constants and would be evaluated under the boundary conditions. Also, r and θ are polar coordinates of a point outside the sphere. The boundary conditions on the sphere's surface (at $r=R$) contain the continuity of the potential and the electric field, which give

$$\phi_1(r,\theta)=\phi_0-E_{0z}\frac{3\varepsilon_2}{2\varepsilon_2+\varepsilon_1}r\cos\theta$$

$$\phi_2(r,\theta)=\phi_0-E_{0z}r\cos\theta+E_{0z}\frac{\varepsilon_1-\varepsilon_2}{2\varepsilon_2+\varepsilon_1}\frac{R^3}{r^2}\cos\theta \tag{2}$$

We could write the electric field in the medium as

$$\mathbf{E_2}(r,\theta)=-\vec{\nabla}\phi_2=-\left(\hat{\mathbf{r}}\frac{\partial\phi_2}{\partial r}+\hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial\phi_2}{\partial\theta}\right)$$
$$=(E_{0z}\cos\theta\hat{\mathbf{r}}-E_{0z}\sin\theta\hat{\boldsymbol{\theta}})+\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}\frac{E_{0z}R^3}{r^3}[2\cos\theta\hat{\mathbf{r}}+\sin\theta\hat{\boldsymbol{\theta}}] \tag{3}$$

Polar coordinates unit vectors could be expressed in terms of the fixed direction Cartesian unit vectors as

$$\hat{\mathbf{r}}=\hat{\mathbf{z}}\cos\theta+\hat{\mathbf{y}}\sin\theta$$

$$\hat{\boldsymbol{\theta}}=-\hat{\mathbf{z}}\sin\theta+\hat{\mathbf{y}}\cos\theta \tag{4}$$

In terms of the Cartesian unit vectors, one could write

$$\mathbf{E_2}(r,\theta)=E_{0z}\hat{\mathbf{z}}+\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}\frac{E_{0z}R^3}{r^3}[3\sin\theta\cos\theta\hat{\mathbf{y}}+(2\cos^2\theta-\sin^2\theta)\hat{\mathbf{z}}] \tag{5}$$

This solution is valid on the yz-plane. In three dimensions system, because of independency of the electric field to the azimuth angle, one could rotate the system around the z-axis. Under these conditions the vector $\hat{\mathbf{y}}$ could be substituted with $\hat{\boldsymbol{\rho}}$. Therefore, the solution could be expanded in three dimensions cylindrical coordinates using a unit vector $\hat{\boldsymbol{\rho}}$:

$$\mathbf{E_2}(r,\theta)=E_{0z}\hat{\mathbf{z}}+\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}\frac{E_{0z}R^3}{r^3}[3\sin\theta\cos\theta\hat{\boldsymbol{\rho}}+(2\cos^2\theta-\sin^2\theta)\hat{\mathbf{z}}] \tag{6}$$

where

$$\hat{\boldsymbol{\rho}}=\hat{\mathbf{x}}\cos\phi+\hat{\mathbf{y}}\sin\phi \tag{7}$$

and φ is the azimuth angle in cylindrical coordinates (the angle between $\hat{\boldsymbol{\rho}}$ and $+\hat{\mathbf{x}}$ direction).

Transforming the electric field in terms of the Cartesian unit vectors gives

$$\mathbf{E_2}(r,\theta)=\left[E_{0z}+\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}\frac{E_{0z}R^3}{r^3}(2\cos^2\theta-\sin^2\theta)\right]\hat{\mathbf{z}}$$
$$+\left[\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}\frac{E_{0z}R^3}{r^3}\times 3\sin\theta\cos\theta\cos\phi\right]\hat{\mathbf{x}}$$
$$+\left[\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}\frac{E_{0z}R^3}{r^3}\times 3\sin\theta\cos\theta\sin\phi\right]\hat{\mathbf{y}}. \tag{8}$$

Furthermore, using

$$x=r\sin\theta\cos\phi,\quad y=r\sin\theta\sin\phi,\quad z=r\cos\theta$$

one could obtain

$$\cos\phi=\frac{x}{\sqrt{x^2+y^2}},\quad \cos\theta=\frac{z}{r},\quad r=\sqrt{x^2+y^2+z^2}.$$

These give

$$\mathbf{E_2}(x,y,z)=\left[3\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}R^3\frac{xz}{r^5}\right]E_{0z}\hat{\mathbf{x}}$$
$$+\left[3\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}R^3\frac{zy}{r^5}\right]E_{0z}\hat{\mathbf{y}}$$
$$+\left[1+\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+2\varepsilon_2}R^3\frac{(2z^2-x^2-y^2)}{r^5}\right]E_{0z}\hat{\mathbf{z}}. \tag{9}$$

The displacement vector in the host medium would be

$$\mathbf{D}_2(x,y,z)=\varepsilon_2\mathbf{E}_2(x,y,z)\equiv\boldsymbol{\varepsilon}^{eff}(x,y,z)\mathbf{E}_0 \tag{10}$$

where $\boldsymbol{\varepsilon}^{eff}$ is the effective permittivity of the nano-composite and is a second-rank order tensor. We have

$$\begin{bmatrix}D_{2x}\\D_{2y}\\D_{2z}\end{bmatrix}=\begin{bmatrix}\varepsilon^{eff}_{xx}&\varepsilon^{eff}_{xy}&\varepsilon^{eff}_{xz}\\\varepsilon^{eff}_{yx}&\varepsilon^{eff}_{yy}&\varepsilon^{eff}_{yz}\\\varepsilon^{eff}_{zx}&\varepsilon^{eff}_{zy}&\varepsilon^{eff}_{zz}\end{bmatrix}\begin{bmatrix}E_{0x}\\E_{0y}\\E_{0z}\end{bmatrix} \tag{11}$$

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