Permittivity and permeability of semi-infinite metamaterial

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Abstract. In our work we investigate dielectric and magnetic properties of semi-infinite metamaterial consisting of particles of different possible nature: atoms, molecules, nanoparticles, etc. It is important that these particles would have magnetic properties. Polarization of a near-surface layer is known to differ from its bulk value for non-magnetic materials; for magnetic materials, including metamaterials, the situation should be similar, which is the subject of our research. We obtain analogues of the Clausius-Mossotti relation both for permittivity and permeability taking into account the local field effects in the long-wave approximation for semi-infinite metamaterial. These relations describe the connection between macroscopic characteristics of the semi-infinite metamaterial (permittivity and permeability) and characteristics of constituent particles (dielectric polarizability and magnetic polarizability), which is a bright example of multi-scale approach - method very popular today in physical and computer simulating.

1. Introduction

In recent years engineered materials composed of designed inclusions have drawn significant scientific interest, underscoring the remarkable potential of them to broaden the range of possible wave phenomena not usually observed in nature but being accessible via laboratory experiment [1-3]. These artificially structured composites, known as metamaterials, demonstrate unusual electromagnetic and optical properties, e.g., negative refractive index and subwavelength focusing [4-6]. The properties of metamaterials are derived both from the intrinsic properties of their constituent particles, as well as from the geometrical arrangement of those particles. A striking instance of this fact is a metamaterial constructed from insulating magnetodielectric spherical particles embedded in a background dielectric material [7,8].

Due to their properties metamaterials are in the centre of modern investigations. They find use in various applications. For instance, metamaterial coatings have been employed to enhance the radiation and matching properties of electrically small electric and magnetic dipole antennas [9] and for engineering sensors with specified sensitivity [10]. Metamaterials are very interesting for researches because of their unique electromagnetic properties, which are not realizable in natural materials [11,12]. Most of interesting theoretical problems are connected with the boundary of semi-infinite metamaterial. On the other hand, the local field effects have a strong influence on electromagnetic processes in medium and therefore can be of great interest for different applications in optics, including nonlinear optics and optics of metamaterials [13-15]. In this work we consider a semi-infinite metamaterial starting from the first principles and find its dielectric and magnetic properties on the base of microscopic structure and properties of single particles, which is possible only with help of the local field method.

2. Dielectric and magnetic properties of semi-infinite metamaterial

We consider metamaterial, which occupies the semi-infinite space $z>0$. This material is composed of N anisotropic particles. The particles have both dielectric and magnetic properties:

$$\alpha_{ij}^{e}(\omega)=\alpha_{\perp}^{e}(\omega)\left(\delta_{ij}-e_ie_j\right)+\alpha_{l}^{e}(\omega)e_ie_j, \tag{1}$$

$$\alpha_{ij}^{m}(\omega)=\alpha_{\perp}^{m}(\omega)\left(\delta_{ij}-e_ie_j\right)+\alpha_{l}^{m}(\omega)e_ie_j. \tag{2}$$

The electromagnetic field $(\mathbf{E}_0,\mathbf{B}_0)$ is acting on semi-infinite metamaterial. The Fourier-transform for density of microcurrents in this medium has the form:

$$\begin{aligned}\left\langle j_i^{mic}(\mathbf{r}',\omega)\right\rangle &= -i\omega\alpha_{ij}^{e}(\omega)\left\langle\sum_n E_j^{mic}(\mathbf{R}_n,\omega)\delta(\mathbf{r}'-\mathbf{R}_n)\right\rangle\\ &+c\alpha_{ij}^{m}(\omega)\left\langle\sum_n\left(rot\mathbf{H}^{mic}(\mathbf{R}_n,\omega)\right)_j\delta(\mathbf{r}'-\mathbf{R}_n)\right\rangle,\end{aligned} \tag{3}$$

We do our calculations taking into account the so called local field effects, meaning that the local field is the field acting on the particle of the medium averaged over the positions of other particles [16]. These effects have a strong influence on the optical nonlinear phenomena, in particular, on nonlinear optics of planar metamaterials [17]. We use relation between macroscopic (electric and magnetic) fields and local (electric and magnetic) fields for 3D metamaterials obtained in our work [18]. So, we obtain expressions relating macroscopic and local fields for semi-infinite metamaterials:

$$E_i(\mathbf{p},\omega)=G_{ij}(\mathbf{p},\omega)E_j^{loc}(\mathbf{p},\omega), \tag{4}$$

$$B_i(\mathbf{p},\omega)=F_{ij}(\mathbf{p},\omega)B_j^{loc}(\mathbf{p},\omega), \tag{5}$$

where

$$G_{ij}(\mathbf{p},\omega)=\delta_{ij}+\frac{n}{2\pi^2}\int d^3p\frac{k^2\delta_{ik}-p_ip_k}{p^2-k^2}\int_{z'>0}d^3R'\exp(i\mathbf{p}\mathbf{R}')f(\mathbf{R}')\alpha_{kj}^{e}(\omega), \tag{6}$$

$$F_{ij}(\mathbf{p},\omega)=\delta_{ij}+\frac{n}{2\pi^2}\int d^3p\frac{p^2\delta_{ik}-p_ip_k}{p^2-k^2}\int_{z'>0}d^3R'\exp(i\mathbf{p}\mathbf{R}')f(\mathbf{R}')\alpha_{kj}^{m}(\omega). \tag{7}$$

Let us introduce the notations

$$Q_{ij}(Z)=\frac{n}{2\pi^2}\int d^3p\frac{k^2\delta_{ik}-p_ip_k}{p^2-k^2}\int_{z'>0}d^3R''\exp(i\mathbf{p}\mathbf{R}')f(\mathbf{R}')\alpha_{kj}^{e}(\omega), \tag{8}$$

$$S_{ij}(Z)=\frac{n}{2\pi^2}\int d^3p\frac{p^2\delta_{ik}-p_ip_k}{p^2-k^2}\int_{z'>0}d^3R'\exp(i\mathbf{p}\mathbf{R}')f(\mathbf{R}')\alpha_{kj}^{m}(\omega). \tag{9}$$

For infinite material these tensors become simpler

$$Q_{ij}(Z)=-\frac{1}{3}\delta_{ij},\quad S_{ij}(Z)=\frac{2}{3}\delta_{ij}. \tag{10}$$

Using these values, one can obtain equations (8), (9) in the form

$$Q_{ij}(Z)=-\frac{1}{3}\delta_{ij}-W_{ij}(z),\quad S_{ij}(Z)=\frac{2}{3}\delta_{ij}-V_{ij}(z), \tag{11}$$

where

$$W_{ij}(Z)=\frac{n}{2\pi^2}\int d^3p\frac{k^2\delta_{ik}-p_ip_k}{p^2-k^2}\int_{z'<0}d^3R'\exp(i\mathbf{p}\mathbf{R}')f(\mathbf{R}')\alpha_{kj}^{e}(\omega), \tag{12}$$

$$V_{ij}(Z)=\frac{n}{2\pi^2}\int d^3p\,\frac{p^2\delta_{ik}-p_ip_k}{p^2-k^2}\int_{z'<0}d^3R'\exp(i\mathbf{pR}')f(\mathbf{R}')\alpha^m_{kj}(\omega). \tag{13}$$

Then equations (6),(7) can be rewritten as

$$G_{ij}(\mathbf{p},\omega)=\frac{2}{3}\delta_{ij}-W_{ij}(z),\quad F_{ij}(\mathbf{p},\omega)=\frac{5}{3}\delta_{ij}-V_{ij}(z). \tag{14}$$

In equations (14) $f(\mathbf{R}')$ is the distribution function, which depends on properties of the media and can be found experimentally [19].

It is well known that electric (magnetic) induction is a vector quantity that equals to the sum of the vector of electric (magnetic) field and the polarization (magnetization) of the medium:

$$D_i(\mathbf{p},\omega)=E_i(\mathbf{p},\omega)+4\pi P_i(\mathbf{p},\omega), \tag{15}$$

$$H_i(\mathbf{p},\omega)=B_i(\mathbf{p},\omega)-4\pi M_i(\mathbf{p},\omega). \tag{16}$$

Considering the fact that polarizability and magnetization can be expressed in terms of both macroscopic and local fields, we can write

$$\left(\varepsilon_{ij}(\mathbf{p},\omega)-\delta_{ij}\right)E_j(\mathbf{p},\omega)=4\pi n\alpha^e_{ij}(\omega)E^{loc}_j(\mathbf{p},\omega), \tag{17}$$

$$\left(\mu^{-1}_{ij}(\mathbf{p},\omega)-\delta_{ij}\right)B_j(\mathbf{p},\omega)=-4\pi n\alpha^m_{ij}(\omega)B^{loc}_j(\mathbf{p},\omega). \tag{18}$$

The equations for permittivity and permeability are obtained by substituting local fields from equations (4), (5) in equations (17), (18) which gives:

$$\varepsilon_{ik}(\mathbf{p},\omega)=\delta_{ik}+4\pi n\alpha^e_{ij}(\omega)G^{-1}_{jk}(\mathbf{p},\omega), \tag{19}$$

$$\mu^{-1}_{ik}(\mathbf{p},\omega)=\delta_{ik}-4\pi n\alpha^m_{ij}(\omega)F^{-1}_{jk}(\mathbf{p},\omega). \tag{20}$$

Finally, using equation(1) we get:

$$\varepsilon_{ik}(\mathbf{p},\omega)=\delta_{ik}+4\pi n\alpha^e_{\perp}(\omega)G^{-1}_{ik}(\mathbf{p},\omega)+4\pi n\left(\alpha^e_l(\omega)-\alpha^e_{\perp}(\omega)\right)e_iG^{-1}_{zk}(\mathbf{p},\omega), \tag{21}$$

$$\mu^{-1}_{ik}(\mathbf{p},\omega)=\delta_{ik}-4\pi n\alpha^m_{\perp}(\omega)F^{-1}_{ik}(\mathbf{p},\omega)-4\pi n\left(\alpha^m_l(\omega)-\alpha^m_{\perp}(\omega)\right)e_iF^{-1}_{zk}(\mathbf{p},\omega). \tag{22}$$

These equations are analogue of the Clausius-Mossotti relations for semi-infinite metamaterial.

Equations (21), (22) describe dielectric and magnetic properties of semi-infinite metamaterial in the near-surface region. In these equations the tensors depend on the radial distribution function $f(\mathbf{R}')$, which can be measured using x-ray diffraction.

As long as we neglect the effects of the polarization of a near-surface layer, it is easy to get the expressions which turn into results obtained in the work [20] for anisotropic non-magnetic media ($\mu=1$).

In the long-wave limit

$$n^{-1/3}<<q^{-1}<<c/\omega \tag{23}$$

for metamaterials consisting of spherically symmetric particles tensors $W_{ij}(Z),V_{ij}(Z)$ have only one preferred direction (Z axis). These tensors are axially symmetric with respect to the Z axis. For this reason components $W_{zz}(Z)$ and $V_{zz}(Z)$ differs from components $W_{xx}(Z)=W_{yy}(Z)$ and $V_{xx}(Z)=V_{yy}(Z)$.

In case of infinite material with magnetic properties from equations (19), (20) we get:

$$\varepsilon(\omega)=\frac{1+(8\pi/3)n\alpha_e(\omega)}{1-(4\pi/3)n\alpha_e(\omega)}, \tag{24}$$

$$\mu(\omega)=\frac{1+(8\pi/3)n\alpha_m(\omega)}{1-(4\pi/3)n\alpha_m(\omega)}. \tag{25}$$

Equations (24), (25) coincide with both results obtained in our previous work [18] and with results from [21] obtained with the help of the other method.

So, using the Clausius-Mossotti relation, one can transform our results to the following form:

$$\varepsilon_{xx}(z,\omega)=\varepsilon_{yy}(z,\omega)=\frac{\varepsilon(\omega)+\left(\varepsilon(\omega)-1\right)W_{xx}(z)}{1+\left(\varepsilon(\omega)-1\right)W_{xx}(z)}, \tag{26}$$

$$\varepsilon_{zz}(z,\omega)=\frac{\varepsilon(\omega)+\left(\varepsilon(\omega)-1\right)W_{zz}(z)}{1+\left(\varepsilon(\omega)-1\right)W_{zz}(z)}, \tag{27}$$

$$\mu_{zz}(z,\omega)=\frac{\mu(\omega)+\left(\mu(\omega)-1\right)V_{zz}(z)}{1+\left(\mu(\omega)-1\right)V_{zz}(z)}, \tag{28}$$

$$\mu_{xx}(z,\omega)=\mu_{yy}(z,\omega)=\frac{\mu(\omega)+\left(\mu(\omega)-1\right)V_{xx}(z)}{1+\left(\mu(\omega)-1\right)V_{xx}(z)}, \tag{29}$$

where

$$W_{xx}(z)=\frac{n\alpha^{e}(\omega)}{2\pi^{2}}\int d^{3}p\,\frac{k^{2}-p_{x}^{2}}{p^{2}-k^{2}}\int\limits_{z'<0} d^{3}R'\exp(i\mathbf{pR}')\,f(\mathbf{R}'), \tag{30}$$

$$W_{zz}(z)=\frac{n\alpha^{e}(\omega)}{2\pi^{2}}\int d^{3}p\,\frac{k^{2}-p_{z}^{2}}{p^{2}-k^{2}}\int\limits_{z'<0} d^{3}R'\exp(i\mathbf{pR}')\,f(\mathbf{R}'), \tag{31}$$

$$V_{xx}(Z)=\frac{n\alpha^{m}(\omega)}{2\pi^{2}}\int d^{3}p\,\frac{p^{2}-p_{x}^{2}}{p^{2}-k^{2}}\int\limits_{z'<0} d^{3}R'\exp(i\mathbf{pR}')\,f(\mathbf{R}'), \tag{32}$$

$$V_{zz}(Z)=\frac{n\alpha^{m}(\omega)}{2\pi^{2}}\int d^{3}p\,\frac{p^{2}-p_{z}^{2}}{p^{2}-k^{2}}\int\limits_{z'<0} d^{3}R'\exp(i\mathbf{pR}')\,f(\mathbf{R}'). \tag{33}$$

Equations (26)-(29) describe dielectric properties of near-surface layer macroscopically, using permittivity tensor depending on the coordinate Z. The result for the permittivity coincides with those from the work [22].

3. Discussion

In this paper dielectric and magnetic properties of semi-infinite metamaterials were investigated with taking into account the local field effects. We have obtained equations for permittivity tensor (21) and permeability tensor (22) in the near-surface region. These tensors allow analyzing dielectric and magnetic properties of semi-infinite metamaterials and considering qualitatively new phenomena in metamaterials. Thus, using these equations for permittivity and permeability one can construct semi-infinite metamaterials based on the properties of their constituent particles of different shapes and nature. For example, in our recent work [23] we obtained an analogue of the Clausius-Mossotti relations for 3D metamaterials based on colloidal quantum dots.

We have obtained the permittivity and permeability tensors (26)-(29) in long-wave limit in case of spherically symmetric particles as well.

The results obtained are important for understanding the influence of polarization and magnetization of the near-surface layer of metamaterial on the properties of electromagnetic surface waves, reflection and refraction and other optical phenomena. Also, the expressions for permittivity and permeability can serve as the theoretical foundation for engineering and designing general metamaterial-based devices.

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