Generalized Clausius-Mossotti relation for semi-infinite artificial periodic structure

M N Anokhin, A A Tishchenko and M N Strikhanov

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoye shosse, 115409, Moscow, Russia

E-mail: MNAnokhin@mephi.ru, Tishchenko@mephi.ru

Abstract. We obtain from the first principles a generalized Clausius-Mossotti relation describing the dielectric permittivity of a semi-infinite artificial periodic structure. The obtained expressions include the spatial dispersion and permit defining resonant conditions for propagating waves.

1. Introduction

Periodicity changes the dielectric properties and, consequently, determines the propagation of electromagnetic waves in periodic structures of various types [1-3]. Periodic structures are widely used in different applications, e.g., in new and perspective class of materials – photonic crystals and metamaterials [4], for producing high-performance filters, in resonators, signal dividers, microwave electronics, etc.

Photonic crystal is a periodic structure which allows controlling light by opening a bandgap within a range of forbidden frequencies. Theoretical calculations of a light propagation in photonic crystals are based on the general theory for periodic structures [5].

In this work we develop the so called local field theory for the case of semi-infinite artificial periodic structure. In our recent paper [6] we considered an infinite structure and now demonstrate that existence of the surface leads to the additional anisotropy and, thus, changes the tensor structure of the dielectric permittivity. The method we use is based on the direct solving Maxwell's equations, and it is known that in case of amorphous medium the natural changing of the dielectric properties near the surface occurs [7, 8].

2. Dielectric properties of semi-infinite artificial periodic structure

We consider the semi-infinite periodic structure occupying half-space $z>0$ composed of N anisotropic particles with the same polarizability $\alpha_{ij}(\omega)$:

$$\alpha_{ij}(\omega)=\alpha_{\perp}(\omega)\left(\delta_{ij}-e_i e_j\right)+\alpha_{\parallel}(\omega)e_i e_j . \tag{1}$$

Let the external field $\mathbf{E}^0$ act on this structure. One can write a solution of the Fourier transform of Maxwell's equations in a medium in the dipole approximation. The microscopic field acting on the a-th particle can be written as [6, 9]:

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$$E_i^{mic}\left(\mathbf{R}_a,\omega\right)=E_i^0\left(\mathbf{R}_a,\omega\right)+ \\ +\frac{1}{2\pi^2}\int d^3lS_{ij}\left(\mathbf{l},\omega\right)\alpha_{jk}\left(\omega\right)\sum_b E_k^{mic}\left(\mathbf{R}_b,\omega\right)\exp\left\{-i\mathbf{l}\left(\mathbf{R}_b-\mathbf{R}_a\right)\right\}, \tag{2}$$

where

$$S_{ij}\left(\mathbf{l},\omega\right)=\frac{k^2\delta_{ij}-l_il_j}{l^2-k^2-i0}, \tag{3}$$

$$k=\omega/c, \tag{4}$$

where index b corresponds to all the other particles of this structure with the exception of a-th particle. Equation (2) can be solved only approximately because of $N>>1$.

The addend in equation (2) is formed by the sum of the fields of the rest particles of matter. The contribution of any particle depends on its position relative to the a-th particle. It determines the dependence of the effective field on the mutual arrangement of the particles, i.e. in fact the structure of matter.

Let $w\left(\mathbf{R}_{ba}\right)$ be the probability density of finding the b-th particle at the distance $\mathbf{R}_{ba}=\mathbf{R}_b-\mathbf{R}_a$ $\left(k=\overline{1,N-1}\right)$ from the a-th one:

$$w\left(\mathbf{R}_{ba}\right)=\frac{1}{N}\sum_{m=1}^{N}\delta\left(\mathbf{R}_{ba}-\mathbf{R}_m\right). \tag{5}$$

Let us replace $\mathbf{E}^{mic}$ in the first approximation in equation (2) with its averaged over other particles value called the local field $\mathbf{E}^{loc}$:

$$E_i^{loc}\left(\mathbf{R},\omega\right)=E_i^0\left(\mathbf{R},\omega\right)+\frac{1}{2\pi^2}\sum_{m=1}^{N}S_{ij}\left(-\mathbf{R}_m,\omega\right)\alpha_{jk}\left(\omega\right)E_k^{loc}\left(\mathbf{R}+\mathbf{R}_m,\omega\right), \tag{6}$$

where

$$S_{ij}\left(-\mathbf{R},\omega\right)=\int d^3lS_{ij}\left(\mathbf{l},\omega\right)\exp\left\{-i\mathbf{l}\mathbf{R}\right\}. \tag{7}$$

We take into account that all the particles are located only in the region $z>0$.

One can find the macroscopic field by averaging equation (2) over the coordinates of all the particles:

$$E_i\left(\mathbf{R},\omega\right)=E_i^0\left(\mathbf{R},\omega\right)+ \\ +\frac{1}{2\pi^2}\int d^3lS_{ij}\left(\mathbf{l},\omega\right)\alpha_{jk}\left(\omega\right)\left\langle\sum_b E_k^{loc}\left(\mathbf{R}_b,\omega\right)\exp\left\{-i\mathbf{l}\left(\mathbf{R}_b-\mathbf{R}\right)\right\}\right\rangle, \tag{8}$$

where

$$\left\langle\sum_b E_k^{loc}\left(\mathbf{R}_b,\omega\right)\exp\left\{-i\mathbf{l}\left(\mathbf{R}_b-\mathbf{R}\right)\right\}\right\rangle=\frac{N}{V}\int_{Z''>0}d^3\mathbf{R}''E_k^{loc}\left(\mathbf{R}'',\omega\right)\exp\left\{-i\mathbf{l}\left(\mathbf{R}''-\mathbf{R}\right)\right\}. \tag{9}$$

Then, the macroscopic field can be obtained in form

$$E_i\left(\mathbf{R},\omega\right)=E_i^0\left(\mathbf{R},\omega\right)+\frac{1}{2\pi^2}n\int_{Z'+Z>0}d^3\mathbf{R}'S_{ij}\left(-\mathbf{R}',\omega\right)\alpha_{jk}\left(\omega\right)E_k^{loc}\left(\mathbf{R}'+\mathbf{R},\omega\right). \tag{10}$$

The macroscopic field is expressed through the local field using equations (6) and (10):

$$E_i\left(\mathbf{R},\omega\right)=E_i^{loc}\left(\mathbf{R},\omega\right)+\frac{1}{2\pi^2}n\int_{Z'+Z>0}d^3\mathbf{R}'S_{ij}\left(-\mathbf{R}',\omega\right)\alpha_{jk}\left(\omega\right)E_k^{loc}\left(\mathbf{R}'+\mathbf{R},\omega\right)- \\ -\frac{1}{2\pi^2}\sum_{m=1}^{N}S_{ij}\left(-\mathbf{R}_m,\omega\right)\alpha_{jk}\left(\omega\right)E_k^{loc}\left(\mathbf{R}+\mathbf{R}_m,\omega\right). \tag{11}$$

Equation (11) can be written in variables $\left(\mathbf{q},\omega,z\right)$:

$$E_i(\mathbf{q},\mathrm{z},\omega) = E_i^{loc}(\mathbf{q},\mathrm{z},\omega) + \\ +\frac{1}{2\pi^2} n \int\limits_{Z'+Z>0} d^3\mathbf{R}' \exp\{i\mathbf{q}\mathbf{R}'\} S_{ij}(-\mathbf{R}',\omega)\alpha_{jk}(\omega) E_k^{loc}(\mathbf{q}, z+Z',\omega) - \\ -\frac{1}{2\pi^2}\sum_{m=1}^{N} S_{ij}(-\mathbf{R}_m,\omega)\alpha_{jk}(\omega) E_k^{loc}(\mathbf{q}, z+Z_m,\omega)\exp\{i\mathbf{q}\mathbf{R}_m\}. \tag{12}$$

A relation between the Fourier transforms of the local and macroscopic fields [10]:

$$t_{ik}(\mathbf{q},\mathrm{z},\omega) E_k^{loc}(\mathbf{q},\mathrm{z},\omega) = E_i(\mathbf{q},\mathrm{z},\omega), \tag{13}$$

where

$$t_{ik}(\mathbf{q},\mathrm{z},\omega) = \delta_{ik} + \frac{1}{2\pi^2} n \int\limits_{Z'+Z>0} d^3\mathbf{R}' \exp\{i\mathbf{q}\mathbf{R}'\} S_{ij}(-\mathbf{R}',\omega)\alpha_{jk}(\omega) - \\ -\frac{1}{2\pi^2}\sum_{m=1}^{N}\exp\{i\mathbf{q}\mathbf{R}_m\} S_{ij}(-\mathbf{R}_m,\omega)\alpha_{jk}(\omega). \tag{14}$$

Let us make some auxiliary manipulations:

$$S_{ij}(-\mathbf{R},\omega) = \int d^3 l S_{ij}(\mathbf{l},\omega)\exp\{-i\mathbf{l}\mathbf{R}\} = a(R)\delta_{ij} + b(R)\frac{R_i R_j}{R^2}. \tag{15}$$

Thus, tensor $t_{ik}(\mathbf{q},\mathrm{z},\omega)$ has the form:

$$t_{ik}(\mathbf{q},\mathrm{z},\omega) = \delta_{ik} + \frac{1}{2\pi^2} n \int\limits_{Z'+Z>0} d^3\mathbf{R}' \exp\{i\mathbf{q}\mathbf{R}'\}\left\{a(R')\delta_{ij} + b(R')\frac{R_i' R_j'}{R'^2}\right\}\alpha_{jk}(\omega) - \\ -\frac{1}{2\pi^2}\sum_{m=1}^{N}\exp\{i\mathbf{q}\mathbf{R}_m\}\left\{a(R_m)\delta_{ij} + b(R_m)\frac{R_i^m R_j^m}{R_m^2}\right\}\alpha_{jk}(\omega), \tag{16}$$

where

$$a(R) = -2\frac{\pi^2 k}{R^2}\sin(kR) - 2\frac{\pi^2}{R^3}\cos(kR); \\ b(R) = 4\frac{\pi^2 k^2}{R}\cos(kR) + 6\frac{\pi^2 k}{R^2}\sin(kR) + 6\frac{\pi^2}{R^3}\cos(kR). \tag{17}$$

As a result, we find expression for the dielectric permittivity:

$$\varepsilon_{ik}(\mathbf{q},\mathrm{z}.\omega) = \delta_{ik} + 4\pi n\alpha_{ij}(\omega) t_{jk}^{-1}(\mathbf{q},\mathrm{z},\omega), \tag{18}$$

where $z > 0$.

Let us neglect the anisotropy of individual particles, i.e.:

$$\alpha(\omega) \equiv \alpha_{\perp}(\omega) \equiv \alpha_{\parallel}(\omega). \tag{19}$$

We can find a tensor $t_{ik}^{-1}(\mathbf{q},\mathrm{z},\omega)$ by presenting tensor $t_{ik}(\mathbf{q},\mathrm{z},\omega)$ in the form:

$$t_{ik}(\mathbf{q},\mathrm{z},\omega) = c_1(\mathbf{q},\mathrm{z},\omega)\delta_{ik} + c_2(\mathbf{q},\mathrm{z},\omega)\frac{q_i q_k}{q^2} + \\ + c_3(\mathbf{q},\mathrm{z},\omega) e_i e_k + c_4(\mathbf{q},\mathrm{z},\omega) e_i q_k + c_5(\mathbf{q},\mathrm{z},\omega) q_i e_k. \tag{20}$$

From the condition

$$t_{ik}(\mathbf{q},\mathrm{z},\omega) = t_{ki}(\mathbf{q},\mathrm{z},\omega), \tag{21}$$

one can see that

$$c_4(\mathbf{q},\mathrm{z},\omega) = c_5(\mathbf{q},\mathrm{z},\omega). \tag{22}$$

Therefore, equation (20) goes to

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$$t_{ik}\left(\mathbf{q},\mathrm{z},\omega\right)=c_1\left(\mathbf{q},\mathrm{z},\omega\right)\delta_{ik}+c_2\left(\mathbf{q},\mathrm{z},\omega\right)\frac{q_iq_k}{q^2}+ \\ +c_3\left(\mathbf{q},\mathrm{z},\omega\right)e_ie_k+c_4\left(\mathbf{q},\mathrm{z},\omega\right)\left(e_iq_k+q_ie_k\right). \tag{23}$$

Comparing equations (16) and (23) we find the coefficient $c_1\left(\mathbf{q},\mathrm{z},\omega\right)$:

$$c_1\left(\mathbf{q},\mathrm{z},\omega\right)=1+a_1\left(\mathbf{q},\mathrm{z},\omega\right)-a_2\left(\mathbf{q},\mathrm{z},\omega\right), \tag{24}$$

where

$$a_1\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}n\alpha\left(\omega\right)\int\limits_{Z'+Z>0}d^3\mathbf{R}'\exp\left\{i\mathbf{qR}'\right\}a\left(R'\right); \\ a_2\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}\alpha\left(\omega\right)\sum_{m=1}^{N}\exp\left\{i\mathbf{qR}_m\right\}a\left(R_m\right). \tag{25}$$

The other coefficients can be obtained by multiplying equation (23) by δ_{ki}, e_ke_i, e_kq_i:

$$c_2\left(\mathbf{q},\mathrm{z},\omega\right)=b_1\left(\mathbf{q},\mathrm{z},\omega\right)-b_2\left(\mathbf{q},\mathrm{z},\omega\right); \\ c_3\left(\mathbf{q},\mathrm{z},\omega\right)=b_3\left(\mathbf{q},\mathrm{z},\omega\right)-b_4\left(\mathbf{q},\mathrm{z},\omega\right); \\ c_4\left(\mathbf{q},\mathrm{z},\omega\right)=b_5\left(\mathbf{q},\mathrm{z},\omega\right)-b_6\left(\mathbf{q},\mathrm{z},\omega\right), \tag{26}$$

where

$$b_1\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}n\alpha\left(\omega\right)\int\limits_{Z'+Z>0}d^3\mathbf{R}'\exp\left\{i\mathbf{qR}'\right\}b\left(R'\right)\left[1-\frac{Z'^2}{R'^2}\right]; \\ b_2\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}\alpha\left(\omega\right)\sum_{m=1}^{N}\exp\left\{i\mathbf{qR}_m\right\}b\left(R_m\right)\left[1-\frac{Z'^2_m}{R^2_m}\right]; \\ b_3\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}n\alpha\left(\omega\right)\int\limits_{Z'+Z>0}d^3\mathbf{R}'\exp\left\{i\mathbf{qR}'\right\}b\left(R'\right)\frac{Z'^2}{R'^2}; \\ b_4\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}\alpha\left(\omega\right)\sum_{m=1}^{N}\exp\left\{i\mathbf{qR}_m\right\}b\left(R_m\right)\frac{Z'^2_m}{R^2_m}; \\ b_5\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}n\alpha\left(\omega\right)\int\limits_{Z'+Z>0}d^3\mathbf{R}'\exp\left\{i\mathbf{qR}'\right\}b\left(R'\right)\frac{\left(\mathbf{qR}\right)Z'_k}{q^2R'^2}; \\ b_6\left(\mathbf{q},\mathrm{z},\omega\right)=\frac{1}{2\pi^2}\alpha\left(\omega\right)\sum_{m=1}^{N}\exp\left\{i\mathbf{qR}_m\right\}b\left(R_m\right)\frac{\left(\mathbf{qR}\right)Z_m}{q^2R^2_m}. \tag{27}$$

Tensor $t^{-1}_{ik}\left(\mathbf{q},\mathrm{z},\omega\right)$ has the same structure as $t_{ik}\left(\mathbf{q},\mathrm{z},\omega\right)$ in equation (23):

$$t^{-1}_{ik}\left(\mathbf{q},\mathrm{z},\omega\right)=d_1\left(\mathbf{q},\mathrm{z},\omega\right)\delta_{ik}+d_2\left(\mathbf{q},\mathrm{z},\omega\right)\frac{q_iq_k}{q^2}+ \\ +d_3\left(\mathbf{q},\mathrm{z},\omega\right)e_ie_k+d_4\left(\mathbf{q},\mathrm{z},\omega\right)\left(e_iq_k+q_ie_k\right). \tag{28}$$

For finding the coefficients $d_{1,2,3,4}\left(\mathbf{q},\mathrm{z},\omega\right)$ in equation (28) it is necessary to carry out some additional calculations:

$$t^{-1}_{ki}\left(\mathbf{q},\mathrm{z},\omega\right)t_{ij}\left(\mathbf{q},\mathrm{z},\omega\right)=\delta_{kj}. \tag{29}$$

To make the calculations easier, let us put

$$c_\alpha\left(\mathbf{q},\mathrm{z},\omega\right)\equiv c_\alpha; \\ d_\alpha\left(\mathbf{q},\mathrm{z},\omega\right)\equiv d_\alpha, \tag{30}$$

where $\alpha=1,2,3,4$.

The tensor coefficients in equation (29) are grouped:

$$\delta_{kj} = d_1 c_1 \delta_{kj} + \left[d_1 c_2 + d_2 c_1 + d_2 c_2 + d_4 c_4 q^2 \right] \frac{q_k q_j}{q^2} + \left[d_1 c_3 + d_3 c_1 + d_3 c_3 + d_4 c_4 q^2 \right] e_k e_j + \\ + \left[d_1 c_4 + d_3 c_4 + d_4 c_1 + d_4 c_2 \right] e_k q_j + \left[d_1 c_4 + d_2 c_4 + d_4 c_1 + d_4 c_3 \right] q_k e_j , \quad (31)$$

after which one can write the system of equations for unknown coefficients:

$$\begin{cases} d_1 c_1 = 1; \\ d_1 c_2 + d_2 c_1 + d_2 c_2 + d_4 c_4 q^2 = 0; \\ d_1 c_3 + d_3 c_1 + d_3 c_3 + d_4 c_4 q^2 = 0; \\ d_3 c_4 + d_4 c_2 - d_2 c_4 - d_4 c_3 = 0. \end{cases} \quad (32)$$

It is easy to solve this system:

$$\begin{aligned} d_1 &= \frac{1}{c_1}; \\ d_2 &= -\frac{c_1 c_2 + c_2 c_3 - q^2 c_4^2}{c_1 \left(c_1^2 + c_1 c_2 + c_1 c_3 + c_2 c_3 - q^2 c_4^2 \right)}; \\ d_3 &= -\frac{c_1 c_3 + c_2 c_3 - q^2 c_4^2}{c_1 \left(c_1^2 + c_1 c_2 + c_1 c_3 + c_2 c_3 - q^2 c_4^2 \right)}; \\ d_4 &= -\frac{c_4}{c_1^2 + c_1 c_2 + c_1 c_3 + c_2 c_3 - q^2 c_4^2}. \end{aligned} \quad (33)$$

According to equations (18) and (28) the coefficients obtained determine the dielectric permittivity.

3. Discussion

The results obtained here describe the dielectric properties of semi-infinite artificial periodic structure, which consists of particles. These particles can be of different nature: atoms, molecules, nanoparticles, quantum dots, etc. equations (16) - (18) and (28), (33) describe this structure in the transparency band of the optical frequency range in the dipole approximation. The expression for the dielectric permittivity is obtained taking into account the spatial dispersion.

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