Local field effects in periodic metamaterials

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Abstract. In this article we investigate dielectric and magnetic properties of periodic metamaterials taking into account the so-called local field effect, caused by interaction between single particles the material consists of. We also consider the spatial dispersion effects. As a result, generalized Clausius-Mossotti techniques have been extended to the case of periodic metamaterials; permittivity tensor and permeability tensor were obtained.

1. Introduction

Metamaterials are artificial materials, which attract much attention because of their exotic properties [1]-[3] and promising applications ranging from biosensors to photonic devices [4],[5]. These materials may consist of periodic or random collections of, for example, metallic nanoparticles, metallic split-ring resonators, I-shaped particles and other magnetodielectric objects. The unit elements of metamaterials are usually designed to provide a resonant response to the electric and magnetic fields [6].

In this work we will be focusing on periodic metamaterials taking into consideration the local-field effects.

2. Local field effects in periodic metamaterials

We investigate periodic metamaterial consisting of N anisotropic particles with dielectric polarizability tensor $\alpha_{ij}^{e}(\omega)$ and magnetic polarizability tensor $\alpha_{ij}^{m}(\omega)$:

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

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

The microscopic field in medium is the sum of the primary field $(\mathbf{E}_0,\mathbf{B}_0)$ generated by external charges and secondary fields produced by all particles of the medium. Maxwell's equations for the Fourier transform of the microscopic fields acting at a point $\mathbf{r}$ give [7]:

$$\mathbf{E}^{mic}(\mathbf{r},\omega)=\mathbf{E}^{0}(\mathbf{r},\omega)+\frac{4\pi i}{\omega}\int d^3q e^{i\mathbf{qr}}\frac{k^2\mathbf{j}^{mic}(\mathbf{q},\omega)-\mathbf{q}\left(\mathbf{q},\mathbf{j}^{mic}(\mathbf{q},\omega)\right)}{q^2-k^2}, \tag{3}$$

$$\mathbf{H}^{mic}(\mathbf{r},\omega)=\mathbf{H}^{0}(\mathbf{r},\omega)+\frac{4\pi i}{c}\int d^3q e^{i\mathbf{qr}}\frac{[\mathbf{q},\mathbf{j}^{mic}(\mathbf{q},\omega)]}{q^2-k^2}, \tag{4}$$

where

$$j_i^{mic}(\mathbf{r}',\omega) = -i\omega\alpha_{ij}^{e}(\omega)\sum_{b=1}^{N} E_j^{mic}(\mathbf{R}_b,\omega)\delta(\mathbf{r}'-\mathbf{R}_b) + c\alpha_{ij}^{m}(\omega)\sum_{b}\left(rot\mathbf{H}^{mic}(\mathbf{R}_b,\omega)\right)_j \delta(\mathbf{r}'-\mathbf{R}_b). \quad (5)$$

One can solve this system only approximately because $N \gg 1$. For $\mathbf{r} = \mathbf{R_a}$ one can easily obtain from Eqs.(3),(4) a system of N equations for acting on the a –th particle field with use so-called the local fields. The local field is an effective field can be obtained by averaging over the positions of all particles of the medium except the given one [8]:

$$E_i^{loc}(\mathbf{R}_a,\omega) = E_i^{0}(\mathbf{R}_a,\omega) + \frac{1}{2\omega\pi^2}\int d^3p \frac{k^2\delta_{ij} - p_i p_j}{p^2-k^2}\int d^3R_{ba} e^{-i\mathbf{p}\mathbf{R}_{ba}} Nw(\mathbf{R}_{ba})$$
$$\times\left(\omega\alpha_{jk}^{e}(\omega)E_k^{loc}(\mathbf{R}_a+\mathbf{R}_{ba},\omega) - c\alpha_{jk}^{m}(\omega)\left[\mathbf{p},\mathbf{B}^{loc}(\mathbf{R}_a+\mathbf{R}_{ba},\omega)\right]_k\right), \quad (6)$$

$$B_i^{loc}(\mathbf{R}_a,\omega) = B_i^{0}(\mathbf{R}_a,\omega) + \frac{1}{2c\pi^2}\int d^3p \frac{1}{p^2-k^2}\int d^3R_{ba} e^{-i\mathbf{p}\mathbf{R}_{ba}} Nw(\mathbf{R}_{ba})$$
$$\times\left(\omega\alpha_{ij}^{e}(\omega)\left[\mathbf{p},\mathbf{E}^{loc}(\mathbf{R}_a+\mathbf{R}_{ba},\omega)\right]_j - c\alpha_{ij}^{m}(\omega)\left[\mathbf{p},\left[\mathbf{p},\mathbf{B}^{loc}(\mathbf{R}_a+\mathbf{R}_{ba},\omega)\right]\right]_j\right). \quad (7)$$

On the other hand, dependence of the local field on the structure of the medium is provided by the function of distribution $w(\mathbf{R}_{an})$. For periodic material one can write:

$$w(\mathbf{R}_{an}) = \frac{1}{N}\sum_{m=1}^{N}\delta(\mathbf{R}_{an}-\mathbf{R}_m). \quad (8)$$

At the same time, averaging equations Eqs. (3),(4) over the positions of all the particles one gets equations for usual average macroscopic fields. Combining these expressions, we obtain equations connecting the Fourier transforms of the local and macroscopic fields:

$$G_{ij}(\mathbf{q},\omega)E_j^{loc}(\mathbf{q},\omega) = E_i(\mathbf{q},\omega), \quad (9)$$

$$F_{ij}(\mathbf{q},\omega)B_j^{loc}(\mathbf{q},\omega) = B_i(\mathbf{q},\omega), \quad (10)$$

where

$$G_{ik}(\mathbf{q},\omega) = \delta_{ik} - \frac{1}{2\pi^2}\sum_{m=1}^{N} S_{ij}(-\mathbf{R}_m,\omega)e^{i\mathbf{q}\mathbf{R}_m}\alpha_{jk}^{e}(\omega) + 4\pi n S_{ij}(\mathbf{q},\omega)\alpha_{jk}^{e}(\omega), \quad (11)$$

$$F_{ik}(\mathbf{q},\omega) = \delta_{ik} - \frac{1}{2\pi^2}\sum_{m=1}^{N} F_{ij}(-\mathbf{R}_m,\omega)e^{i\mathbf{q}\mathbf{R}_m}\alpha_{jk}^{m} + 4\pi n F_{ij}(\mathbf{q},\omega)\alpha_{jk}^{m}(\omega), \quad (12)$$

$$S_{ij}(-\mathbf{R}_m,\omega) = \int d^3p \frac{k^2\delta_{ij} - p_i p_j}{p^2-k^2} e^{-i\mathbf{p}\mathbf{R}_m}, \quad (13)$$

$$F_{ij}(-\mathbf{R}_m,\omega) = \int d^3p \frac{p^2\delta_{ij} - p_i p_j}{p^2-k^2} e^{-i\mathbf{p}\mathbf{R}_m}. \quad (14)$$

We do our calculations in a long-wave limit. According to this limit, if

$$d << L << c/\omega, \quad (15)$$

the effective field acting on a molecule is formed by adding the fields of many molecules lying in some volume of the crystal [9]. In (15) d is the lattice constant, L is the linear dimension of the region responsible for the formation of the local field.

Neglecting the anisotropy of individual particles

$$\alpha_l(\omega) \equiv \alpha_\perp(\omega) \equiv \alpha(\omega) \quad (16)$$

we can rewrite Eqs. (13),(14) in the following form:

$$\int d^3p \frac{k^2\delta_{ij} - p_i p_j}{p^2-k^2} e^{-i\mathbf{p}\mathbf{R}_m} = a(R_m)\delta_{ij} + b(R_m)\frac{R_i^m R_j^m}{R^2}, \quad (17)$$

$$\int d^3p \frac{p^2\delta_{ij} - p_i p_j}{p^2 - k^2} e^{-i\mathbf{p}\mathbf{R}_m} = c(R_m)\delta_{ij} + d(R_m)\frac{R_i^m R_j^m}{R^2}. \tag{18}$$

It is well known that the probability of unlimited approaching of molecules is negligibly small [10]. For this reason, convolutions of Eqs. (17),(18) with δ_{kj} and $\frac{R_j^m R_i^m}{R^2}$ allow us to obtain coefficients $a(R_m), b(R_m), c(R_m), d(R_m)$:

$$a(R_m) = -2\frac{\pi^2 k}{R_m^2}\sin(kR_m) - 2\frac{\pi^2}{R_m^3}\cos(kR_m), \tag{19}$$

$$b(R_m) = 6\frac{\pi^2 k}{R_m^2}\sin(kR_m) + 6\frac{\pi^2}{R_m^3}\cos(kR_m) + 4\frac{\pi^2 k^2}{R_m}\cos(kR_m), \tag{20}$$

$$c(R_m) = -2\frac{\pi^2 k}{\mathrm{R}_m^2}\sin(k\,\mathrm{R}^m) - 2\frac{\pi^2}{\mathrm{R}_m^3}\cos(k\,\mathrm{R}^m) + 2\frac{\pi^2 k^2}{\mathrm{R}_m}\cos(\mathrm{kR}^m), \tag{21}$$

$$d(R_m) = 6\frac{\pi^2}{\mathrm{R}_m^3}\cos(k\,\mathrm{R}^m) + 6\frac{\pi^2 k}{\mathrm{R}_m^2}\sin(k\,\mathrm{R}^m) - 2\frac{\pi^2 k^2}{\mathrm{R}_m}\cos(k\,\mathrm{R}^m). \tag{22}$$

So, we get tensors $G_{ik}(\mathbf{q},\omega), F_{ik}(\mathbf{q},\omega)$ in the form

$$G_{ik}(\mathbf{q},\omega) = \delta_{ik} - \frac{1}{2\pi^2}\sum_{m=1}^{N}\left(a(\mathbf{R}_m)\delta_{ik} + b(\mathbf{R}_m)\frac{R_i^m R_k^m}{R_m^2}\right)e^{i\mathbf{q}\mathbf{R}_m}\alpha^e(\omega) + 4\pi n\frac{k^2\delta_{ij} - p_i p_j}{p^2 - k^2}\alpha^e(\omega), \tag{23}$$

$$F_{ik}(\mathbf{q},\omega) = \delta_{ik} - \frac{1}{2\pi^2}\sum_{m=1}^{N}\left(c(\mathbf{R}_m)\delta_{ik} + d(\mathbf{R}_m)\frac{R_i^m R_k^m}{R_m^2}\right)e^{i\mathbf{q}\mathbf{R}_m}\alpha^m(\omega) + 4\pi n\frac{p^2\delta_{ij} - p_i p_j}{p^2 - k^2}\alpha^m(\omega). \tag{24}$$

Considering that polarization and magnetization of the medium can be expressed in terms of both the macroscopic fields and the local fields, one can obtain equations for permittivity and permeability of periodic metamaterials:

$$\varepsilon_{ij}(\mathbf{q},\omega) = \delta_{ij} + 4\pi n\alpha^e(\omega)G_{ij}^{-1}(\mathbf{q},\omega), \tag{25}$$

$$\mu_{ij}(\mathbf{q},\omega) = \delta_{ij} + 4\pi n\alpha^m(\omega)F_{ij}^{-1}(\mathbf{q},\omega). \tag{26}$$

Eqs. (25),(26) are analogues of the well-known Clausius-Mossotti relation, but for periodic metamaterial. In case of non-magnetic media our results coincide with those from work [11].

3. Discussion

In this paper dielectric and magnetic properties of periodic metamaterials were investigated taking into account the local field effects. We have obtained permittivity tensor (25) and permeability tensor (26). Our results describe relation between macroscopic properties of periodic metamaterial and microscopic properties of the particles it consists of. This fact is important, because it allows the potential features of metamaterials to be incorporated into a design and analysis of new devices, such as transmission devices, electromagnetic absorbers, *etc* [12],[13].

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