Nonlocality in Discrete Metamaterials

M. A. Gorlach[1,2] and P. A. Belov[1]

[1]ITMO University, Russia
[2]Belarusian State University, Belarus

Abstract— We discuss spatial dispersion effects in three-dimensional discrete metamaterials. In the present work, we consider two examples of metamaterials whose behavior can not be described properly by means of the effective medium model and where nonlocality is important. These examples are (i) discrete structure consisting of the uniaxial dipoles operating in the vicinity of the transition from elliptic to the hyperbolic dispersion regime and (ii) structure composed of isotropic particles with electric polarizability where spatial-dispersion-induced birefringence can arise.

1. INTRODUCTION

One of the exciting perspectives provided by the field of metamaterials is a possibility to tailor metamaterial electromagnetic response choosing proper constituent elements of artificial structure as well as the geometry of their arrangement. Engineering composite materials' local material parameters (e.g., permittivity and permeability) is widely discussed in the literature [1, 2]. Besides that, the use of metamaterials provides a novel degree of freedom in material science, namely, a possibility to tailor metamaterial spatially dispersive response. Spatial dispersion or nonlocality of material electromagnetic response means that the polarization of a physically small volume is influenced not only by the field in a given volume but also by the electric field existing in the neighbouring regions of space [3, 4]. Strong spatial dispersion effects are quite uncommon in natural materials [4]. However, there exists a class of metamaterials where nonlocality is important [5]. Therefore, it is of interest to reveal new physical phenomena that arise due to spatial dispersion. In the present work, we address two types of metamaterials operating in such regime that the nonlocal effects are essential: the three-dimensional structure consisting of the uniaxial dipoles in the frequency range corresponding to the transition from elliptic to the hyperbolic dispersion regime (Fig. 1(a)) and the structure composed of isotropic particles (Fig. 1(b)) where spatial-dispersion-induced birefringence can be observed. In our study, we employ the discrete dipole model that provides a self-consistent scheme for the description of the nonlocal effects in discrete metamaterials [6]. Note that we do not employ perturbative expansions of the effective permittivity dyadic with respect to wave vector in this scheme.

2. TOPOLOGICAL TRANSITION IN THE STRUCTURE CONSISTING OF THE UNIAXIAL ELECTRIC SCATTERERS

We consider the structure consisting of the uniaxial electric scatterers located in the sites of a cubic lattice with the period a (Fig. 1(a)). Such scatterers can be realized as short dielectric rods in

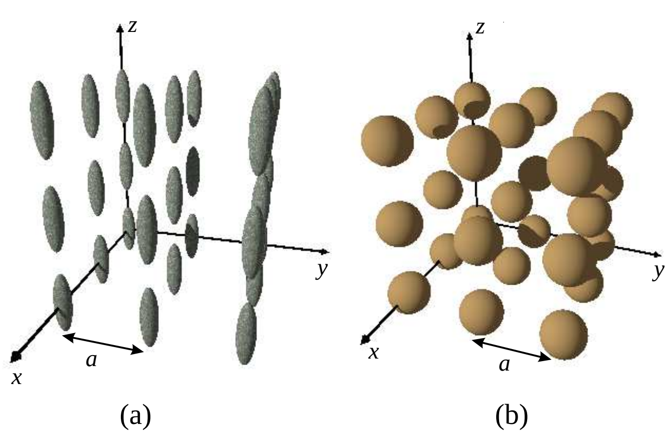


Figure 1: Discrete metamaterials under study. (a) Structure composed of the uniaxial electric scatterers in the sites of a cubic lattice. (b) Structure composed of isotropic particles in the sites of a cubic lattice.

optical metamaterials or short wires with some load, inductive or capacitive, in metamaterials for microwave range. In the further study, we do not concretize the structure of the scatterers, because in this approach their properties are fully described in terms of polarizability tensor $\hat{\alpha} = \alpha_{zz}\vec{e}_z \otimes \vec{e}_z$, where $\vec{e}_z$ is a unit vector directed along the anisotropy axis.

Within the frame of discrete dipole model the effective nonlocal permittivity tensor of the composite is given by

$$\varepsilon_{zz}\left(\omega, \bar{k}\right) = 1 + \frac{4\pi}{a^3}\left[\alpha_{zz}^{-1} - C_{\bar{k}}^{zz}\left(\omega, \bar{k}\right)\right]^{-1}, \tag{1}$$

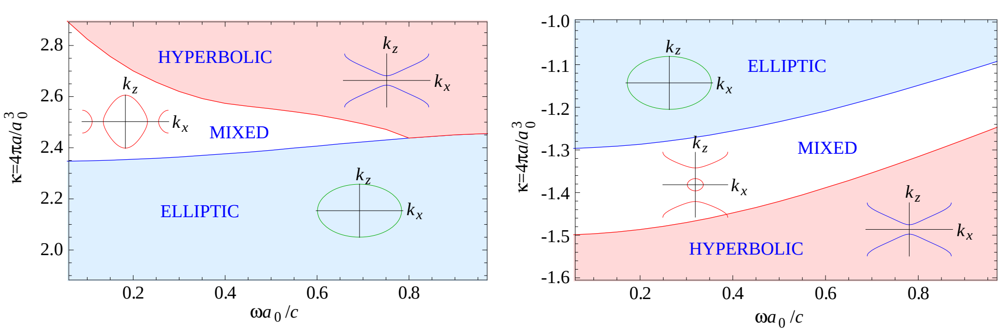
where $C_{\bar{k}}^{zz}(\omega, \bar{k}) = G_{\bar{k}}^{zz}(\omega, \bar{k}) + 4\pi/a^3(q^2 - k_z^2)/(q^2 - k^2)$, $G_{\bar{k}}^{zz} \equiv \sum\limits_{(m,n,l)\neq(0,0,0)} G^{zz}(\omega; \bar{r}_{mnl})e^{-i\bar{k}\cdot\bar{r}_{mnl}}$, and $G^{zz}(\omega; \bar{r})$ is a matrix element of the dyadic Green's function that determines the electric field created by the point dipole. $\alpha_{zz}^{-1} = \alpha_{0zz}^{-1} - 2i\omega^3/(3c^3)$, the latter imaginary term takes into account the radiation loss contribution, and α_{0zz} is a bare polarizability of the scatterer. In the limit $ka \ll 1$, $\omega a/c \ll 1$, one can derive Clausius-Mossotti formula that does not contain spatial dispersion corrections:

$$\varepsilon_{zz}^{\mathrm{loc}}(\omega) = \frac{1 + 2\varkappa/3}{1 - \varkappa/3}, \tag{2}$$

where $\varkappa = 4\pi\alpha_{0zz}/(3\,a^3)$. From Eqs. (1), (2), it follows that spatial dispersion corrections to local permittivity Eq. (2) are the most essential when the numerator or the denominator of the fraction Eq. (2) tends to zero. But this situation corresponds to the topological transition in metamaterial when ε_{zz} changes its sign and the topology of isofrequency contours changes from a closed quasi-ellipsoid to an open quasi-hyperboloid, i.e., the dispersion regime changes from elliptic to the hyperbolic one. Using the expression for the effective permittivity Eq. (1) we derive the dispersion equation

$$\alpha_{zz}^{-1}(\omega) - G_{\bar{k}zz}\left(\omega, \bar{k}\right) = 0. \tag{3}$$

Solving Eq. (3) numerically one can plot the system of isofrequency contours for different frequencies. The analysis of isofrequency contours system suggests that the transition from elliptic dispersion regime (that corresponds to the quasi-elliptic closed isofrequency contours) to the hyperbolic one (corresponding to the quasi-hyperbolic opened isofrequency contours) is not instantaneous. Namely, there exists a transition dispersion regime that combines elliptic and hyperbolic isofrequency contours. Further, we refer this regime as mixed dispersion regime. The conditions of observation of the mixed dispersion regime are shown in the "frequency-polarizability" diagram Fig. 2; the typical isofrequency contours are also sketched in Fig. 2. The detailed investigation of the mixed dispersion regime properties is provided in our recent work [7]. It is interesting that the complicated structure of isofrequency contours in the mixed dispersion regime gives rise to the threerefringence of the wave incident from air at the boundary of the discrete structure with a special orientation of the anisotropy axis. Note also, that the discrete dipole model allows one to describe low- and high-ε mixed regime within a single framework (i.e., by the single formula for the effective permittivity) whereas in the perturbative description of spatial dispersion effects one



(a) (b)

Figure 2: Different dispersion regimes in the discrete dipole structure composed of the uniaxial electric scatterers shown on "frequency-polarizability" diagram. The isofrequency contours typical for the given regime are sketched. (a) The vicinity of high-ε mixed regime. (b) The vicinity of low-ε mixed regime.

deals with the expansions of $\varepsilon_{zz}(\omega, \bar{k})$ or $\varepsilon_{zz}^{-1}(\omega, \bar{k})$ with respect to wave vector in low- and high-ε mixed regimes, respectively.

3. SPATIAL-DISPERSION-INDUCED BIREFRINGENCE IN THE STRUCTURE COMPOSED OF ISOTROPIC PARTICLES

In the similar manner we analyse spatial dispersion effects in the structure consisting of isotropic particles (for example, plasmonic spheres) located in the sites of a cubic lattice with the period a (Fig. 1(b)). Homogenization of the structure within the frame of the discrete dipole model yields [8]:

$$\hat{\varepsilon}\left(\omega, \bar{k}\right) = 1 + \frac{4\pi}{a^3}\left[\hat{I}\alpha^{-1}(\omega) - \hat{C}_{\bar{k}}\left(\omega, \bar{k}\right)\right]^{-1}, \tag{4}$$

where α is a polarizability of isotropic particle. Note, that the tensor $\hat{C}_{\bar{k}}(\omega, \bar{k})$ representing the lattice interaction constant is not proportional to the identity matrix in the general case. Therefore, Eq. (4) suggests that the effective permittivity tensor of the structure consisting of isotropic particles is not proportional to the identity matrix and, consequently, the structure exhibits anisotropy at least in a certain spectral range. The intrinsic reason for this anisotropy is spatial dispersion, because the direction of the wave vector with respect to the lattice axes provides a selected direction in space. One can also envision the frequency range where spatial-dispersion-induced birefringence can be notable. Indeed, as the anisotropy of the structure is determined by anisotropic tensor $\hat{C}_{\bar{k}}$, the anisotropy would be the strongest if the isotropic term $\hat{I}\alpha^{-1}$ vanishes. This situation corresponds to the resonance of the individual particle. The described phenomenon of spatial-dispersion-induced birefringence was discussed in the theoretical works [3, 9] employing the perturbative expansions of the effective permittivity tensor and some symmetry considerations. The effect was also observed experimentally for such natural materials as Cu_2O [10], CaF_2 and BaF_2 [11], but expectedly was sufficiently weak. For that reason, the study of spatial-dispersion-induced birefringence in the field of metamaterials with strong nonlocal response is promising.

To provide a quantitative demonstration of the effect, we plot the dispersion diagram Fig. 3 for metamaterial consisting of spherical isotropic particles with the radius $R = a/2.1$, permittivity of material $\varepsilon_p = 1 - 3\frac{\omega_0^2}{\omega^2}$, where the resonance frequency of a single particle is $\omega_0 a/c = 0.132$. The inverse particle polarizability is set to $\alpha^{-1} = \frac{\varepsilon_p+2}{\varepsilon_p-1}R^3 - \frac{2iq^3}{3}$ with the latter term describing the radiation loss contribution. The dispersion diagram Fig. 3 shows that the degeneracy of the two transverse eigenmodes inherent to anisotropic media is removed for the direction of propagation ΓK. One can also see that the anisotropy of the structure is the most essential in the frequency interval in the vicinity of a single particle resonance as it was discussed above. The phenomenon of spatial-dispersion-induced birefringence in metamaterials can be detected experimentally by measuring the reflection coefficients for two polarizations of the wave incident from air at the boundary of the

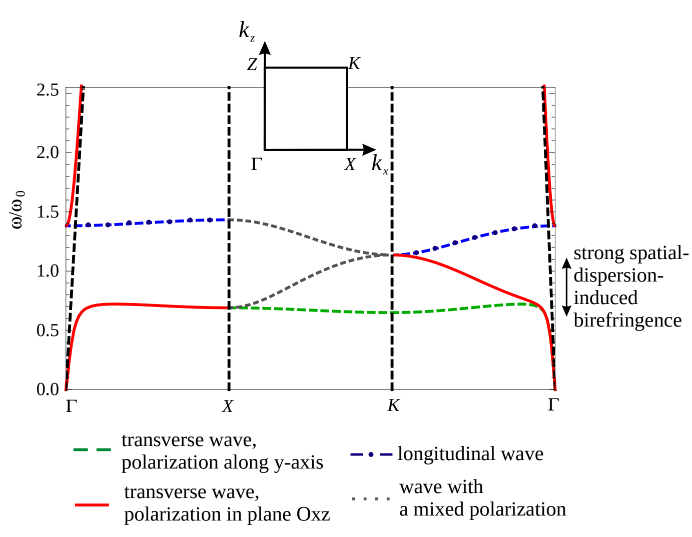


Figure 3: The dispersion diagram for the structure composed of isotropic particles with electric polarizability. Propagation in the plane $k_y = 0$ is studied.

discrete structure with the wave vector aligned along ΓK direction of the cubic crystal. Further details regarding the observation of spatial-dispersion-induced birefringence in metamaterials and the corresponding calculations are expounded in our work [12].

4. CONCLUSION

Metamaterials with the pronounced nonlocal effects constitute an important class of materials. The possibility to tailor their spatially dispersive response provides a novel degree of freedom in material science and challenges metamaterial engineers. In the present work, we apply the discrete dipole model to describe nonlocal effects in discrete three-dimensional metamaterials. We demonstrate the existence of the mixed dispersion regime accompanying topological transition in discrete metamaterials composed of the uniaxial electric scatterers. We also consider the phenomenon of spatial-dispersion-induced birefringence in metamaterials based on three-dimensional cubic arrays of isotropic particles.

ACKNOWLEDGMENT

The present work was supported by the Government of the Russian Federation (Grant No. 074-U01), grant of the President of the Russian Federation No. MD-6805.2013.2, Russian Foundation for Basic Research (grant No. 15-02-08957 A), "Dynasty" foundation, the Ministry of Education and Science of the Russian Federation (projects 14.584.21.0009 10, GOSZADANIE 2014/190, Zadanie No. 3.561.2014/K) and the Ministry of Education of the Republic of Belarus (grant No. 625/02).

REFERENCES

1. Capolino, F., *Theory and Phenomena of Metamaterials*, CRC Press, New York, 2009.
2. Milton, G. W., *The Theory of Composites*, Cambridge University Press, Cambridge, 2002.
3. Agranovich, V. M. and V. L. Ginzburg, *Spatial Dispersion in Crystal Optics and the Theory of Excitons*, Wiley-Interscience, New York, 1966.
4. Landau, L. D. and E. M. Lifshitz, *Electrodynamics of Continuous Media*, Pergamon Press, New York, 1984.
5. Belov, P. A. and R. Marques, "Strong spatial dispersion in wire media in the very large wavelength limit," *Phys. Rev. B*, Vol. 67, 113103, 2003.
6. Belov, P. A. and C. R. Simovski, "Homogenization of electromagnetic crystals formed by uniaxial resonant scatterers," *Phys. Rev. E*, Vol. 72, 036615, 2005.
7. Gorlach, M. A. and P. A. Belov, "Effect of spatial dispersion on the topological transition in metamaterials," *Phys. Rev. B*, Vol. 90, 115136, 2014.
8. Silveirinha, M. G., "Generalized Lorentz-Lorenz formulas for microstructured materials," *Phys. Rev. B*, Vol. 76, 245117, 2007.
9. Ginzburg, V. L., "Ob elektromagnitnyh volnah v izotropnyh sredah pri ychete yavleniya prostranstvennoi dispersii dielectricheskoi pronicaemosti," *Journal of Experimental and Theoretical Physics*, Vol. 34, No. 6, 1593–1604, 1958 (in Russian).
10. Gross, E. F. and A. A. Kaplianskiy, "Opticheskaya anizotropiya cubicheskih cristallov, vyzvannaya yavleniyem prostranstvennoi dispersii," *Reports of the USSR Academy of Sciences*, Vol. 132, No. 1, 98–101, 1960 (in Russian).
11. Burnett, J. N., Z. H. Levine, and E. L. Shirley, "Intrinsic birefringence in calcium fluoride and barium fluoride," *Phys. Rev. B*, Vol. 64, 241102, 2001.
12. Chebykin, A. V., M. A. Gorlach, and P. A. Belov, "Spatial-dispersion-induced birefringence in metamaterials with cubic symmetry," in Preparation.