Non local effects in cone-shaped metamaterials

TATJANA GRIC^{1,2,3}, EDIK U. RAFAILOV²

- ¹ Department of Electronic Systems, Vilnius Gediminas Technical University, Vilnius, Lithuania
- ² Aston Institute of Photonic Technologies, Aston University, Birmingham B4 7ET, UK
- ³ Semiconductor Physics Institute, Center for Physical Sciences and Technology, Vilnius, Lithuania *tatjana.gric@vgtu.lt

Abstract: Light-matter interactions in a material may be dramatically influenced by the features of the medium. Moreover, the electromagnetic characteristics of the material in the nearby areas may make a dramatic impact as well. Following the first scenario, the medium is considered to be local, whereas in the other case, it is nonlocal. It has been demonstrated by the current works on light-matter interactions in composites that novel optical phenomena is enabled by nonlocal effects. The former can not be treated in case of local effective medium description.

1. Introduction

The system under consideration is treated as non-local in case of its behavior at a given point depending on its state at another spatially separated area. Quantum states of light and matter are considered as being inherently non-local. The former reflects the fundamental wave-particle duality addressed in the reproduction of an original de Broglie paper in [1]. Quantum entanglement is considered as a very intriguing instance of non-localities in nature [2, 3]. Inherently weak photon-photon interactions enable its successful application in optics with photons [4, 5].

A uniaxial permittivity tensor may stand for to describe the electromagnetic response of these metamaterials from the perspective of the effective medium approximation. It has been demonstrated that accounting for nonlocal corrections in effective medium theory (EMT) is needed aiming to adequately describe new optical phenomena in nanowire structures [6-8]. A granularity has a dramatic impact on the optical properties of the nanowire composite. The former leads to the formation of extra electromagnetic modes. It is worthwhile mentioning, that their features can be accounted for in the effective medium formalism by dealing with spatial dispersion of the effective permittivity. Light propagation studies in different structures with varying material properties, including inhomogeneous materials and optical waveguides open the wide avenues for photonic device design. Usually, either approximate partially analytic methods or entirely numerical approaches have been employed. Particularly in device design a deep insight into light propagation properties is beneficial if an analytic method is available and can be applied. In practice though, one has to resort quite often to numerical approaches as analytical solutions are limited to just a few situations.

Herein, the enhancement of electromagnetic modes in hyperbolic media is considered, making an assumption that wires are made of transparent conducting oxide (TCOs) and silver. We show that such an approach makes a dramatic impact on the field enhancement in metamaterials. Moreover, it is demonstrated that the nonlocal effective permittivity model sufficiently defines the detected optical properties.

2. Theoretical modelling

Fig. 1 displays the transition metamaterial under consideration made of an ordered array of plasmonic cone-shaped rods implanted into a dielectric host material.

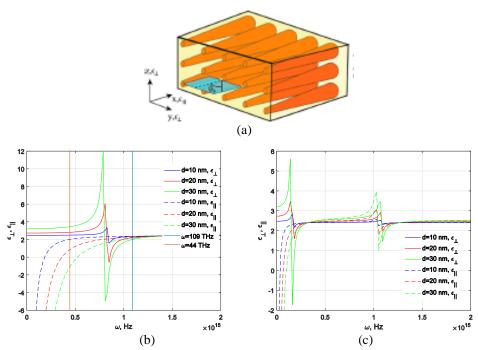


Figure 1. (a) A view of a transition hyperbolic layer consisting of plasmonic cones implanted in the dielectric host material [17]. (b, c) Dependence of the local effective medium parameters of the metamaterials upon frequency: (b) Ag nanorods; (c) TCO nanorods. Herein, d – is the diameter of plasmonic nanorods; d=2R, where R is calculated by Eq. (1).

To have a deeper insight in to the tunability properties of the system, it is worthwhile mentioning that the wavelength λ is much longer than both the radius of the wire R(x) and the distance between the rods a. We have made an assumption that the radius varies from 5 < R(x) < 15 nm as follows

$$R(x) = a\sqrt{\frac{0.12(1 + \tanh(a_1(b_1x + c_1)))}{2\pi}}$$
(1)

with a_1 =0.0018, b_1 =1.5×10⁹ m⁻¹, and c_1 =6000. It is assumed that separation between the rods a = 60 nm. In case of metallic cones, permittivity of plasmonic components of the

$$\varepsilon_m(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\delta\omega}$$

 $\varepsilon_m\left(\omega\right) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\delta\omega} \,.$ The crucial difference between previous works and this work, for investigating optics of hyperbolic composites, is the fact that we consider nanorods with an increasing radius along the transverse position x (Eq. (1)). Moreover, in this case radius increases up to the certain value, after the saturation point is passed, it becomes a constant value. One may obtain the parameters of interest by fitting this permittivity function to a particular frequency range of bulk material [9]. It has been concluded in [10] that a reasonable fit might be provided for silver, if the utilized values are

as follows $\varepsilon_{\infty}=5$, $\omega_p=9.5eV$, $\delta=0.0987eV$. Table 1 presents the parameters of Drude-Lorentz approach for Aluminum-doped Zinc Oxide (AZO) found based on the experimental data [11].

Table 1. Drude-Lorentz parameters of transparent conducting oxide obtained from experimental data. It is possible to approximate the materials dielectric function by the equation:

$$\varepsilon_{TCO} = \varepsilon_b - \frac{\omega_p^2}{\omega \left(\omega + i\gamma_p\right)} + \frac{f_1 \omega_1^2}{\left(\omega_1^2 - \omega^2 - i\omega\gamma_1\right)}, \text{ with the values of the parameters outlined in the table}$$
 [11].

	AZO
E _b	3.5402
ω _p [eV]	1.7473
γ _p [eV]	0.04486
f_1	0.5095
ω ₁ [eV]	4.2942
γ1 [eV]	0.1017

One may describe the optical properties of the metamaterials by means of the effective permittivity. The mentioned is valid in case of characteristic sizes of the composite, such as nanowire radius and their period being much smaller than light wavelengths. It is worthwhile mentioning, that the thickness of the structure goes to the infinity. The mentioned formalism can be applied aiming to evaluate transmission, reflection and absorption spectra of the structure. Because of the symmetry, the optical features of a nanowire metamaterial are similar to the properties of an homogeneous uniaxial medium with optical axis parallel to the nanowires (Fig. 1b). From macroscopical perspectives, a diagonal permittivity tensor $\hat{\varepsilon}$ with $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{\perp} \neq \varepsilon_{zz}$ is employed aiming to characterize these optical properties. Following analytical approach, a layer of a metamaterial was treated as homogeneous layer characterized by either local [12] or non-local [13] EMTs.

Following the approach used in [14, 15] permittivity of the wire media is expressed by a diagonal tensor $\hat{\varepsilon} = \{ \varepsilon_{\parallel}, \varepsilon_{\perp}, \varepsilon_{\perp} \}$ with components [16]

$$\varepsilon_{\perp} = \varepsilon_d \frac{(1+f)\varepsilon_m + (1-f)\varepsilon_d}{(1-f)\varepsilon_m + (1+f)\varepsilon_d} \tag{2}$$

$$\varepsilon_{\parallel}(k_x) = f \frac{\varepsilon_m + \varepsilon_d}{\varepsilon_d - (n_{\infty}^l)^2} \frac{c^2}{\omega^2} (k_x^2 - k_x^{l2})$$
(3)

where $f = \frac{\pi R^2}{a^2} = \frac{0.12(1 + \tanh(a_1(b_1x + c_1)))}{2}$ is the filling fraction of plasmonic material, i.

e. either metal or TCO inside a dielectric host, k_x is the component of the wavevector in the direction corresponding to the direction of the nanorods, k_x^l is the wavevector of the longitudinal wave in the nanowire metamaterial, and the performance of a longitudinal wave in a wire medium is described by the parameter $n_\infty^l = \lim_{\varepsilon_m \to -\infty} k_x^l c / \omega$. It has been concluded in [15], that one can calculate dispersion $k_x^l(\omega)$. Aiming to do that, one should solve an eigenvalue-type problem with exact dependence governed by geometrical parameters of the composite as well by permittivity of the wires and the matrix media. It is worthwhile noting, that Eq. 3 can be written as follows [17]

$$\varepsilon_{\parallel}(k_{x}) \Box f \varepsilon_{m} + (1 - f) \varepsilon_{d} + \delta_{x} \frac{k_{x}^{2} c^{2}}{\omega^{2}}$$

$$\tag{4}$$

It is worthwhile noting, that the first two terms represent the local permittivity (given by Maxwell-Garnett effective medium theory [18]) and δ_x is a nonlocality parameter. It is

possible to approximate
$$\delta_x$$
 parameter as follows $\delta_x = f \frac{\varepsilon_m + \varepsilon_d}{\varepsilon_d - \left(n_\infty^l\right)^2}$.

The fact of considering wires with an increasing radius along the transverse position x (Eq. 1) stands for as the key difference between previous investigations and this study dedicated to the investigation of optics of hyperbolic composites. It means, that the fill fraction f depends on the spatial coordinate x. The material's properties change from elliptical to hyperbolic because of tuning the fill fraction. It is worthwhile noting that the negative permittivity, i. e. $\varepsilon_m < 0$ stands for as the outstanding feature of the plasmonic metals across the visible spectrum. Isofrequency surfaces describing the dispersion of the propagating modes in the Ag and TCO nanowire metamaterial with parameters as in Figure 1 (b), calculated with the local EMT are presented in Figs. 2 and 3. Two particular frequencies were chosen for consideration, i. e. f=200 THz, where $\varepsilon_{\parallel} < 0$ and $\varepsilon_{\perp} > 0$ and f=850 THz, where $\varepsilon_{\parallel} < 0$ and $\varepsilon_{\perp} < 0$.

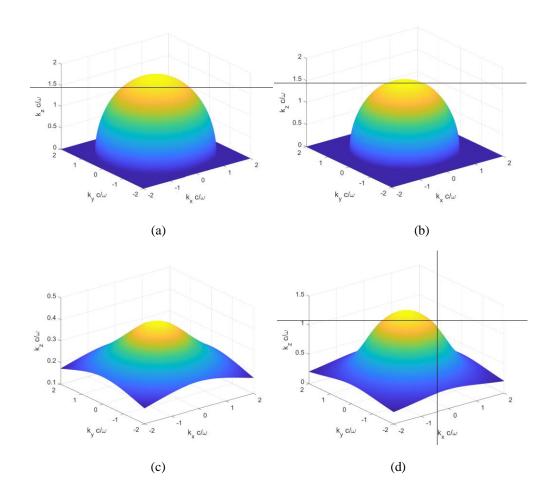


Figure 2. Isofrequency surfaces describing the dispersion of the propagating modes in the Ag nanowire metamaterial with parameters as in Figure 1 (b), calculated with the local EMT: (a, c) d=30nm, (b, d) d=10 nm, (a, b) f=200 THz, (c, d) f=850 THz.

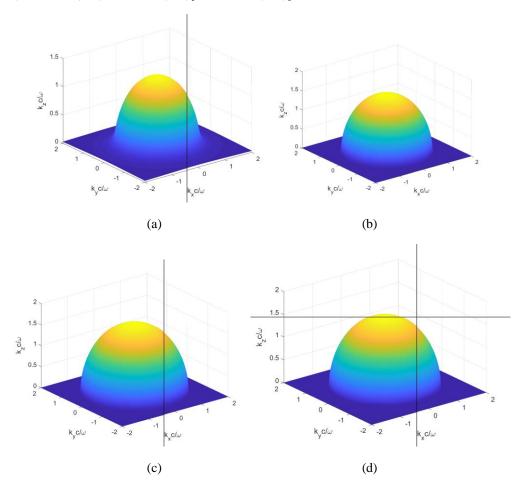


Figure 3. Isofrequency surfaces describing the dispersion of the propagating modes in the TCO nanowire metamaterial with parameters as in Figure 1 (b), calculated with the local EMT: (a, c) d=30nm, (b, d) d=10 nm, (a, b) f=200 THz, (c, d) f=850 THz.

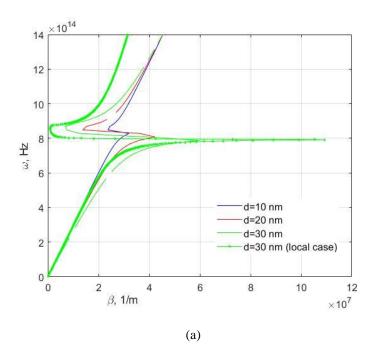
Either an ellipsoid or a hyperboloid is formed by the isofrequency surface defined as the locus of points with coordinates $\{k_x(\omega),k_y(\omega),k_z(\omega)\}$. The former depends on the relationship between the signs of ε_{\perp} and ε_{zz} . It is worthwhile noting that these permittivity components are wavelength-dependent. The geometrical features of this isofrequency surface are treated as the optical topology of a metamaterial [19].

It is demonstrated by the effective permittivity of the metamaterial (with the embedded Ag cones) investigated in this work that metamaterial operates in the elliptic regime for frequencies above 109 THz, exhibits ENZ response at around 109 THz, corresponding to the effective plasma frequency [20] and operates in the hyperbolic regime for frequencies below 44 THz.

$$\frac{k_x^2 + k_y^2}{\varepsilon_{zz}} + \frac{k_z^2}{\varepsilon_{\perp}} = \frac{\omega^2}{c^2}$$
 (5)

Optical topology described by Eq. (5) exhibits typical ellipsoidal isofrequencies for TE modes in both elliptic and hyperbolic regimes.

It is worthwhile mentioning, that the optical topology of metamaterials has a dramatic impact on their quantum optical features. The former leads to a singularity in the local density of optical states in homogeneous hyperbolic media [21]. The rate of spontaneous emission [22], nonradiative energy transfer between molecules [23], and other parameters are drastically affected by the density of optical states.



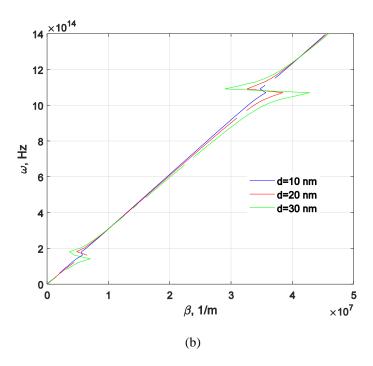


Figure 4. The dispersion of main mode for different cases: (a) – Ag nanowires; (b) – TCO nanowires.

Comparing Figs. 2 and 3, one might conclude that while in the TCO case the differences are minimal, the behavior in the Ag case is drastically different.

One may engineer the dispersion of modes in metamaterials by scaling the unit cell. Figure 4 displays the foreseen changes in the dispersion of the modes. The former modifications are caused by the geometry scaling. One may modify material losses by either the choice of plasmonic metal or by fabrication (for example, annealing). The mentioned features serve as a fertile ground for engineering the optical properties of a metamaterial. One may conclude from Fig. 4 that usage of TCO nanowires serves as a perfect mechanism aiming to increase frequency range of the surface waves existence. It is worthwhile mentioning, that two different types of the modes are present in case of the TCO nanowires. Both modes have finite-frequency solutions with the longitudinal propagation constant β approaching infinity, which leads to the characteristic curve, that extends to infinitely large wavevectors. It is worthwhile mentioning, that we have presented comparisons of the results obtained by applying non-local and local cases in Fig. 4 (a).

Conclusions

Herein, we consider propagation of the electromagnetic wave through a hyperbolic transition layer. It is worthwhile mentioning, that local and nonlocal effective medium approximation are considered. It has been concluded that nonlocality must be considered aiming to properly deal with the field enhancement. It can be concluded that nonlocal effects make a dramatic impact on the field behavior inside a transition hyperbolic layer. Dealing with a system allowing to accurately predict the field distribution through these materials will provide a fertile background for the design and practical applications of this new fascinating metamaterial platform.

Acknowledgement

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska Curie grant agreement No 713694 and from Engineering and Physical Sciences Research Council (EPSRC) (Grant No. EP/R024898/1).

Disclosures. The authors declare no conflicts of interest.

References

- L. de Broglie, "A tentative theory of light quanta," Philos. Mag. Lett. 86, 411-423 (2006).
- A. Einstein, B. Podolsky, N. Rosen, "Can quantum-mechanical description of physical reality be considered complete?," Phys. Rev. 47, 777 -780 (1935).
- J. S. Bell, "On the problem of hidden variables in quantum mechanics," Rev. Mod. Phys. 38, 447-452 (1966).
- S. J. Freedman, J. F. Clauser, "Experimental test of local hidden-variable theories," Phys. Rev. Lett. 28, 938 -941 (1972).
- A. Aspect, P. Grangier, G. Roger, "Experimental realization of einstein-podolsky-rosenbohm gedankenexperiment: a new violation of Bell's inequalities," Phys. Rev. Lett. 49, 91-94 (1982).
- J. Elser, V. A. Podolskiy, I. Salakhutdinov, I. Avrutsky, "Nonlocal effects in effective-medium response of nanolayered metamaterials," Appl. Phys. Lett. 90, 191109 (2007).
- M. G. Silveirinha, "Nonlocal homogenization model for a periodic array of ϵ -negative rods," Phys. Rev. E 73, 046612 (2006).
- G. W. Hanson, E. Forati, M. G. Silveirinha, "Modeling of spatially-dispersive wire media: transport representation, comparison with natural materials, and additional boundary conditions," IEEE Trans. Antennas Propag. 60, 4219-4232 (2012).
- P. B. Johnson, R. W. Christy, "Optical constants of the noble metals," Phys. Rev. B 6, 4370 (1972).
- 10. C. Oubre, P. Nordlander, "Finite-difference time-domain studies of the optical properties of nanoshell dimers," J. Phys. Chem. B 109(20), 10042-10051 (2005).
- 11. G. V. Naik, V. M. Shalaev, A. Boltasseva, "Alternative plasmonic materials: beyond gold and silver," Adv. Mater. 25, 3264-3294 (2013).
- 12. R. Wangberg, J. Elser, E. E. Narimanov, V. A. Podolskiy, "Nonmagnetic nanocomposites for optical and infrared negative-refractive-index media," J. Opt. Soc. Am. B 23, 498-505 (2006).
- S. V. Zhukovsky, A. Andryieuski, O. Takayama, E. Shkondin, R. Malureanu, F. Jensen, and A. V. Lavrinenko, "Experimental demonstration of effective medium approximation breakdown in deeply subwavelength alldielectric multilayers," Phys. Rev. Lett. 115, 177402 (2015).
- 14. R. J. Pollard, A. Murphy, W. R. Hendren, P. R. Evans, R. Atkinson, G. A. Wurtz, A. V. Zayats, V. A. Podolskiy, "Optical nonlocalities and additional waves in epsilon-near-zero metamaterials," Phys. Rev. Lett. **102**, 127405 (2009).
- 15. B. M. Wells, A. V. Zayats, V. A. Podolskiy, "Nonlocal optics of plasmonic nanowire metamaterials," Phys. Rev. B: Condens. Matter Mater. Phys. 89, 035111 (2014).
- P. Ginzburg, D. J. Roth, M. E. Nasir, P. Segovia, A. V Krasavin, J. Levitt, L. M. Hirvonen, B. Wells, K. Suhling, D. Richards, V. A. Podolskiy and A. V. Zayats, "Spontaneous emission in non-local materials," Light: Science & Applications 6, e16273 (2017).
- 17. B. Wells, Zh. A. Kudyshev, N. Litchinitser, and V. A. Podolskiy, "Nonlocal Effects in Transition Hyperbolic Metamaterials," ACS Photonics 4, 2470-2478 (2017).
- 18. M. Garnett, "Colors in metal glasses and in metallic films," Philos. Trans. R. Soc., A 3, 385-420 (1904).
- 19. H. N. S. Krishnamoorthy, Z. Jacob, E. Narimanov, I. Kretzschmar, V. M. Menon, "Topological transitions in metamaterials," Science 336, 205 (2012).
- N. Vasilantonakis, G. A. Wurtz, V. A. Podolskiy, A. V. Zayats, "Refractive index sensing with hyperbolic metamaterials: strategies for biosensing and nonlinearity enhancement," Opt. Express 23, 14329–14343 (2015).
- 21. Z. Jacob, I. I. Smolyaninov, E. E. Narimanov, "Broadband Purcell effect: Radiative decay engineering with metamaterials," Appl. Phys. Lett. **100**, 181105 (2012).

 22. E. M. Purcell, "Spontaneous emission probabilities at radio frequencies," Phys. Rev. B **69**, 674 (1946).
- T. U. Tumkur, J. K. Kitur, C. E. Bonner, A. N. Poddubny, E. E. Narimanov, M. A. Noginov, "Control of Förster energy transfer in the vicinity of metallic surfaces and hyperbolic metamaterials," Faraday Discuss 178, 395 (2015).