Materials Physics and Mechanics 13 (2012) 1-8 Received: March 13, 2012

EFFECTS OF ELECTROMAGNETIC INTERACTION IN PERIODIC ARRAYS OF SINGLE-WALL METALLIC CARBON NANOTUBES

Igor S. Nefedov

Aalto University, School of Electrical Engineering

SMARAD Center of Excellence, P.O. Box 13000, 00076 Aalto, Finland

e-mail: igor.nefedov@aalto.fi

Abstract. We demonstrate that periodic arrays of single-wall metallic carbon nanotubes (CNTs) exhibit electromagnetic wave properties which are strongly different that possessed by single CNTs. The distinctive feature of CNT arrays is a hyperbolic dispersion of electromagnetic waves, propagating in these structures. Electromagnetic interaction between carbon nanotubes leads to dramatic slowdown of eigenwaves in CNT arrays.

1. Introduction

Interest to electromagnetic high-frequency properties of carbon nanotubes is caused by their potential applications in nanoelectronics [1], nanoantennas [2-4], polarizers [5], free electron lasers [6], devices for THz sensing and imaging [7]. Carbon nanotubes (CNTs), possessing metallic properties, are of special interest for nanoelectronics due to their high conductivity at THz frequencies compared to metal nanowires [2]. By this reason, their applications seem to be promising in THz and infrared ranges due to noticeable lower losses compared to other conductive materials.

One of the most important electromagnetic property of metallic CNTs is a capability to support propagation of strongly delayed surface waves [8, 9]. It is caused by a very high kinetic inductance of thin single-wall CNTs [10] and it makes electromagnetic (EM) wave propagation in CNTs strongly different compared to transmission lines, made of usual bulk metals. For description of electromagnetic properties of metallic CNTs, very often the model of impedance cylinder and effective boundary conditions is used [9]. The model of impedance cylinder takes into account quantum properties of CNTs via the complex surface frequency-dependent conductivity. This model was applied for theoretical study of CNT transmission lines and interconnects [1], structures composed of closely packed bundles of parallel identical metallic CNTs [11]. In [12] it was applied for studying two-dimensional periodic arrays of single-wall metallic CNTs.

In this paper we describe briefly the numerical model of the periodic CNT array and demonstrate that electromagnetic waves in this structure are characterized by a hyperbolic dispersion. The hyperbolic dispersion means that isofrequency surfaces are open and extend to infinity in the space of wave vectors. The most important physical consequence of this is that waves with any large wave vectors can propagate in media, characterized by the hyperbolic dispersion. It means that waves with large wave vector components, which are the evanescent (exponentially decaying) waves in usual media, can propagate in hyperbolic media (media with the hyperbolic dispersion). Wide class of media and structures belong to hyperbolic media (HM). In 1960-th a couple of works, related to waves in an anisotropic plasma, characterized by the hyperbolic dispersion, were published (see bibliography in [13]).

Some general wave properties of uniaxial media with different signs of components of the permittivity tensor, such as a power, radiated by a source, were described in [14]. The hyperbolic dispersion is inherent in the TEM (Transverse ElectroMagnetic) wave in periodic multi-conductor lines (wire media) (straight line, characterizing its dispersion is the limiting case of hyperbola), waves in some periodic pin structures and periodic planar networks, composed of transmission lines (all structures, listed above and their dispersion diagrams were described in [15]), waves in tangentially magnetized ferrite slabs [16]. A capability of HM to support propagation ob backward waves and such a phenomena as a negative refraction was discussed in [17]. Now very often HM are referred as *indefinite media.* This term was introduced by D. Smith [18]. Hyperbolic media can be used for a hyperlensing, providing a resolution beyond the diffraction limit [19]. Some promising applications are based on dramatic increase of density of states in these media that allows the control of spontaneous emission [20, 21]. The nature of this phenomenon can be understood if to consider two hyperboloids, corresponding to different frequencies in the space of wave vectors. One can see that the phase space volume enclosed between hyperboloids is infinite. The hyperbolic dispersion for aligned carbon nanotubes composites was predicted in framework of the mean-field theory by Mikki and Kishk [22]. For two-dimensional periodic arrays of metallic CNTs it was shown using full-wave Green's function method [12] and the effective medium theory [23, 24]. Novel physical effect such a giant radiation heat transfer through the gap, filled with carbon nanotubes, was predicted in [25].

2. Numerical model

Let us consider EM waves, propagating along a two-dimensional volumetric array of infinitely long metallic zigzag CNTs, having the radius r and forming hexagonal lattice with the constant d, see Fig. 1. We assume that all nanotubes possess metallic properties. This is some kind of idealization since usually, in a process of nanotubes fabrication, about one-third of all possible single-wall nanotubes exhibit metallic properties and the remaining two-third act as semiconductors. However, this is a realistic assumption in view of recent studies of single-wall CNTs [26-28]. For eigenwaves in arrays of infinitely long carbon nanotubes we take the space-time dependence of fields and currents as $\exp(j\omega t-\beta z-\mathbf{k}_\perp \cdot \mathbf{r}_\perp)$ where $\mathbf{k}_\perp$ is the wave vector of Floquet-Bloch waves propagating in plane of periodicity $\mathbf{r}_\perp$ (the z-axis is directed along carbon nanotubes). Carbon nanotubes are classified by the dual index (m,n) and for zigzag CNTs n=0. If m=3q, zigzag CNTs possess metallic properties. The radius of such a nanotube can be expressed via m and it equals to $r=\sqrt{3}\, mb/2\pi$ where b=0.142 nm.

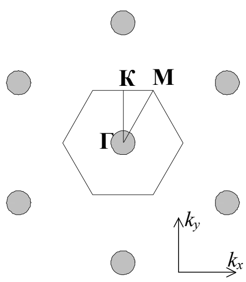

Fig. 1. Hexagonal lattice in space of wave vectors.

As a model of the individual metallic zigzag nanotube, we take impedance cylinder, characterized by the complex dynamic conductivity. For frequencies below the optical transition band the following simple expression for the axial conductivity can be used [9]:

$$\sigma_{zz} \cong -j\frac{2\sqrt{3}\,e^2\Gamma_0}{m\,\pi\hbar(\omega - j\nu)}, \qquad m = 3q, \tag{1}$$

where e is the electron charge, Γ_0=2.7 eV is the overlapping integral, $\tau=1/\nu$ is the relaxation time. We neglect the azimuthal currents at the carbon nanotube surface compared to axial one which is fully justified for parameters of CNTs chosen below and, consequently, the axial component of the magnetic field H_z. This approximation is adequate because of the strong anisotropy of the CNT conductivity [9] resulting from quantum effects. It follows from (1) that the surface impedance per unit length reads

$$z_i = \frac{1}{2\pi r\sigma} = \frac{m\hbar^2\nu}{4\sqrt{3}\,e^2\Gamma_0 r} + j\omega\frac{m\hbar^2}{4\sqrt{3}\,e^2\Gamma_0 r} = R + j\omega L. \tag{2}$$

The inductance L has a quantum nature and it is actually the kinetic inductance [29]. Namely the positive imaginary part of the surface impedance, i.e. the kinetic inductance, determines such a property of CNTs as a capability to support propagation of strongly delayed waves. The same relates to graphene in the intraband region [30].

The dependence of electric field on transversal coordinates x,y can be presented in the form of Floquet-Bloch waves propagating in the plane of periodicity $\mathbf{r}_\perp = x\mathbf{x}_0 + y\mathbf{y}_0$ ($\mathbf{x}_0$ and $\mathbf{y}_0$ are unit vectors of corresponding coordinate axes), so

$$\mathbf{E}(x,y,z) = \sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\mathbf{E}_{ln}e^{-j(\alpha_l x + \gamma_{ln} y + \beta z)}. \tag{3}$$

Here $\mathbf{E}_{ln}$ are amplitudes of spatial harmonics. For the hexagonal lattice

$$\alpha_l = k_x + \tfrac{2\pi l}{d}, \quad \gamma_{ln} = k_y + \tfrac{2\pi(2n-l)}{d\sqrt{3}},$$

and for the square lattice γ_{ln} is replaced by γ_n and

$$\alpha_l = k_x + \tfrac{2\pi l}{d}, \quad \gamma_n = k_y + \tfrac{2\pi n}{d},$$

where k_x and k_y are the components of the wave vector, belonging to the first Brillouin zone. Then we use the following representation of electric field induced by currents on the surface of CNT:

$$\mathbf{E}(\mathbf{r}_\perp) = \frac{\eta}{jk\varepsilon_{\mathbf{h}}}\int_L \overline{\overline{G}}(\mathbf{r}_\perp, \mathbf{r}'_\perp)\cdot\mathbf{J}(\mathbf{r}'_\perp)\,dl, \tag{4}$$

where $\mathbf{r} = \mathbf{r}_\perp + z\mathbf{z}_0$, k and η are the wavenumber and the wave impedance in free space, respectively, $\varepsilon_{\mathbf{h}}$ is the permittivity of the host medium, L is the contour of the single carbon nanotube. Dyadic Green's function has the form

$$\overline{\overline{G}}(\mathbf{r}_\perp, \mathbf{r}'_\perp) = \left[(\nabla_\perp - j\beta\mathbf{z}_0)(\nabla_\perp - j\beta\mathbf{z}_0) + k^2\varepsilon_h\overline{\overline{I}}\right]G(\mathbf{r}_\perp, \mathbf{r}'_\perp), \tag{5}$$

where $\overline{\overline{I}}$ is the unit dyadic, and scalar Green's function has form

$$G(x,y\,|\,x',y') = -\frac{1}{A_c}\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\frac{e^{-i(\alpha_l\bar{x}+\gamma_n\bar{y})}}{g_{ln}}, \tag{6}$$

where A_c is the area of unit cell which equals $d^2\sqrt{3}/2$ for the hexagonal lattice and we have denoted $\bar{x} = x - x'$, $\bar{y} = y - y'$, $\alpha_l = k_x + q_l$, $\gamma_n = k_y + q_n$, $q_s = \frac{2\pi s}{d}$, $g_{ln} = k^2\varepsilon_{\mathbf{h}} - \alpha_l^2 - \gamma_n^2 - \beta^2$.

Due to the strong anisotropy of the CNT conductivity, one can neglect the azimuthal current at the nanotube surface. We can neglect the non-homogeneity of the current distribution on the contour of the nanotube due to its extremely small radius, so $\mathbf{J}(\mathbf{r}'_\perp) = \mathbf{z}_0 J_z$. Then the vector integral relation (4) is reduced to the scalar form for the z components of electric field and current. The electric field at the CNT surface can be expressed via the current as $E_z(\mathbf{r}_\perp \in L) = \frac{J_z}{\sigma}$. Thus, we obtain the integral equation with respect to the current density $J_z(\mathbf{r}_\perp)$. Integrating this equation over the contour of CNT we come to the dispersion equation:

$$\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\left|J_0\left(r\sqrt{\alpha_l^2+\gamma_n^2}\right)\right|^2\frac{\beta^2-k^2\varepsilon_h}{g_{ln}} = j\frac{d^2\varepsilon_h k}{2\pi r\eta\sigma}, \tag{7}$$

where $J_0(x)$ is the zero order Bessel's function. After solving Eq. (7) numerically we can find relations between k, k_x, k_y, β, i.e. calculate dispersion of eigenwaves, propagating in CNT arrays in any direction. Conversion of series depends the lattice constant d and for examples, considered in this paper, sufficient accuracy is achieved when the maximal number of spatial harmonic is taken to be 50-70.

3. Waves in two-dimensional periodic arrays of carbon nanotubes

Dispersion diagram in the form of slow-wave factor (the ratio of speed of light in vacuum to the phase velocity) over the transversal wave vector plane is shown in Fig. 2. The zigzag CNT (21,0) is taken as an example, so $r\approx 0.822$ nm. Calculations were implemented at 27 THz. The slow-wave factor for the surface wave in a single CNT with such a radius equals to 70 and is shown by the dashed line.

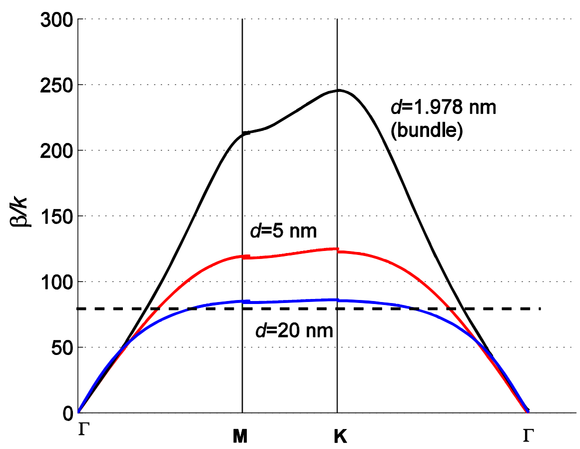

Fig. 2. Real part of the slow-wave factor Re(β/k) calculated for different lattice constants d.

It is remarkable, that the slow-wave factor strongly depends on the transversal wavenumber. Namely, at the Γ-point ($|\mathbf{k}_\perp|=0$) $\beta/k=1$, but for larger $|\mathbf{k}_\perp|$ the slow-wave factor can strongly exceed this value for the single CNT. This result is in agreement with [11] where bundles of closely packed metallic CNTs were considered, and it was found that the slow-wave factor for azimuthally symmetric guided waves decreases with increase of the number of nanotubes tending to unit. It takes place even for the ratio $d/2r \approx 12$ (blue curve) where the term "closely packed" is not applicable. Evidently, this feature is inherent in azimuthally symmetric waves in large quantity of electromagnetically coupled CNTs (which is infinite in the considered case) independently on their assembling. Reduction of the lattice period causes increase of the electromagnetic interaction between nanotubes resulting in increase of β/k. The most dense packing of CNTs in arrays takes place in bundles, where the distance between nanotubes is 0.334 nm, so the lattice constant d =1.978 nm. In this case the maximal value $\beta/k \approx 250$ is achieved near the K-point.

Fig. 3 illustrates relation between directions of the phase velocity and the group velocity of EM waves in CNT arrays. In this example calculations were implemented for the square lattice for simplicity. A vector of the phase velocity $\mathbf{v}_p$ has the same direction as the wave vector in $\mathbf{k}$-space $\mathbf{k}(k_x,\beta)$, which starts from the origin of the coordinate system and finishes at some point of an isofrequency. The vector of the group velocity $\mathbf{v}_g=\mathrm{grad}_\mathbf{k}(\omega)$ is orthogonal to the isofrequency at the point, corresponding to the wave vector. It is remarkable that the group velocity is almost orthogonal to the phase velocity. However, due to a discontinuity of the CNT array, the isofrequency differs from the hyperbola already if $k_x d>0.7$ [23] and becomes qualitatively different from it under a large transversal wave vector component, see Fig. 2. In three-dimensional $\mathbf{k}$-space a surface of dispersion is a cone [12]. It follows a very important consequence from the hyperbolic dispersion: namely, a slab of vertically-standing finite-thickness carbon nanotubes supports propagation of backward waves [24], i.e. waves whose phase and group velocities have opposite directions.

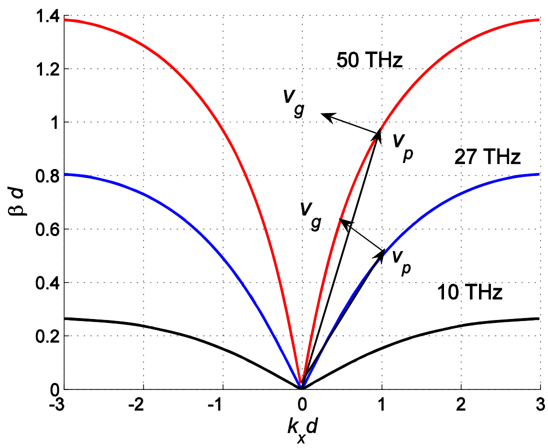

Fig. 3. Isofrequencies in the plane of wave vectors. The lattice constant d=15 nm.

4. Arrays of crossed carbon nanotubes

In this section we consider EM waves propagation in arrays of crossed carbon nanotubes. As a model we take two mutually orthogonal periodic CNT arrays, considered in previous sections. It consists of two-dimensional periodic arrays of carbon nanotubes, infinitely long in the x and y directions. Actually, it is a three-dimensional periodic structure, see Fig. 4. Let us apply first the effective medium model for description of this structure [23]. A periodic carbon nanotube array looks similarly to a wire medium (WM) which is an artificial medium formed by a lattice of well-conductive thin wires [31].

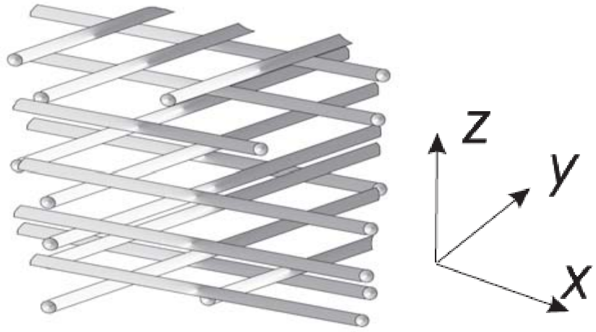

Fig. 4. Schematic view of crossed arrays of CNTs.

Each of crossed arrays can be described in terms of the uniaxial permittivity dyadic. Applying this model to both arrays we come to the following form

$$\overline{\overline{\varepsilon}} = \varepsilon_{zz}\mathbf{z}_0\mathbf{z}_0 + \varepsilon_t(\mathbf{x}_0\mathbf{x}_0 + \mathbf{y}_0\mathbf{y}_0), \tag{8}$$

where $\varepsilon_{zz}=\varepsilon_h$ and the transversal components in the case of identical arrays are expressed by the Drude formula

$$\varepsilon_t = \varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_h\left(1 - \frac{k_p^2}{k^2\varepsilon_h - j\xi k}\right), \tag{9}$$

where ξ is the loss coefficient [31]. Here the effective plasma wave number k_p for the square lattice is defined as [32]

$$k_p = \frac{\mu_0}{d^2L},$$

where μ_0 is the permeability of vacuum and L the inductance of the CNT in array, defined by formula (2). Generally, this inductance contains two serially included contributions, the kinetic inductance and the electromagnetic inductance [10]. However, for thin nanotubes the electromagnetic inductance can be neglected compared to the kinetic one that was shown for single CNTs near a ground plane [1, 10] and for CNTs, forming periodic arrays [23].

Actually, CNT arrays and WM possess strongly different properties, see [12]. It is caused by the spatial dispersion which takes place in WM [33] and is totally suppressed in arrays of single-wall CNTs [24]. Dispersion equation for the TM-waves (waves whose vector of the magnetic field is orthogonal to the wave vector)) propagating in the *xy*-plane reads

$$k^2\varepsilon_h - \frac{k_x^2}{\varepsilon_{yy}} - \frac{k_y^2}{\varepsilon_{xx}} = 0. \tag{10}$$

Obviously, the waves cannot propagate if $k<k_p$ because $\varepsilon_{xx}<0$ and $\varepsilon_{yy}<0$.

Different result is obtained in framework of the numerical model. The same formalism, as was used by us for *double wire medium* [34, 35] can be applied to the structure, formed of crossed CNT arrays. In opposite to the effective medium theory, Green's function method [34] predicts propagation of very slow waves in the *xy*-plane, see Fig. 5. This dispersion characteristic was calculated using formulas from [34], modified for the case of a finite, complex, conductivity of carbon nanotubes. The dispersion diagram looks similar to observed for the TM-waves in double WM. Relations between directions of the phase and the group velocities for both compared structures also are similar [35]. Note, that Green's function model was developed in assumption that wires (carbon nanotubes) are not connected. Similar array of connected wires does not support propagation of the TM waves in the plane of wires [36]. It is reasonable to expect that similar situation takes place for arrays of CNTs. Namely the effective medium theory should describe electromagnetic properties of arrays of mutually connected nanotubes, aligned in the *xy*-plane. At the same time, the model, based on Green's function method, describes an ideal structure, composed of mutually orthogonal, identical non-connected carbon nanotubes where all electromagnetically coupled nanotubes guide EM waves. In reality one can expect that a part of CNTs are mutually connected. At the same time, non-connected CNTs provide guiding of slow waves. Thus, considered above examples present two limiting cases and a real structure, containing simultaneously connected and non-connected carbon nanotubes, will reveal intermediate properties.

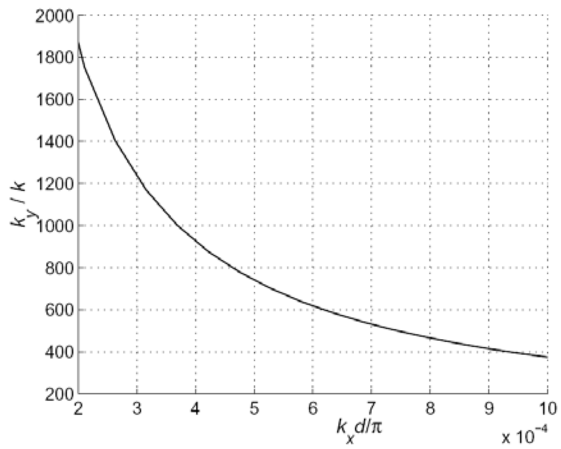

Fig. 5. Slow-wave factor versus $k_x\, d/\pi$. Propagation in *xy*-plane, *d*=25 nm.

5. Conclusions

In this work we have studied the electromagnetic-wave properties of two- and three-dimensional periodic arrays of single-wall metallic carbon nanotubes. It was shown that slow-wave factor of waves, propagating in single periodic arrays of CNTs, can be several times larger than in individual CNTs. At the same time, for arrays of crossed, mutually orthogonal non-connected CNTs this factor can reach very high values. Such a dramatic slowdown is caused by the periodicity and by the electromagnetic interaction between carbon nanotubes. We demonstrated that both studied structures belong to hyperbolic metamaterials which exhibit a number of novel phenomena. According to our estimations, the most promising for applications of CNT arrays seems to be the infrared range (at frequencies below interdand transitions in carbon nanotubes) [24].

This work has been partially funded by the Academy of Finland and Nokia through the Center-of-Excellence program.

References

[1] A. Maffucci, G. Miano, F. Villone // *Int. Journal of Circuit Theory and Applications* **36** (2008) 31.
[2] G.V. Hanson // *IEEE Trans. on Antennas and Propagation* **53** (2005) 3426.
[3] Y. Wang, K. Kempa, B. Kimball, J. B. Carlson, G. Benham, W.Z. Li, T. Kempa, J. Rybczynski, A. Herczynski, Z.F. Ren // *Appl. Phys. Lett.* **85** (2004) 2607.

[4] S.A. Maksimenko, G.Y. Slepyan, A.M. Nemilentsau, M.V. Shuba // *Physica E* **40** (2008) 2360.
[5] L. Ren, C.L. Pint, L.G. Booshehri, W.D. Rice, X. Wang, D.J. Hilton, K. Takeya, I. Kawayama, M. Tonouchi, R.H. Hauge, J. Kono // *Nano Letters* **9** (2009) 2610.
[6] K.G. Batrakov, S.A. Maksimenko, P.P. Kuzhir, C. Thomsen //*Phys. Rev. B* **79** (2009) 125408.
[7] K. Fu, R. Zannoni, C. Chan, S.H. Adams, J. Nicholson, E. Polizzi, K.S. Yngvesson // *Appl. Phys. Lett.* **92** (2008) 033105.
[8] G.Y. Slepyan, S.A. Maksimenko, A. Lakhtakia, O. Yevtushenko, A.V. Gusakov // *Phys. Rev. B* **57** (1998) 9485.
[9] G.Y. Slepyan, S.A. Maksimenko, A. Lakhtakia, O. Yevtushenko, A.V. Gusakov // *Phys. Rev. B* **60** (1999) 17136.
[10] P. J. Burke // *IEEE Trans. on Nanotechnology* **3** (2002) 129.
[11] M. V. Shuba, S.A. Maksimenko, A. Lakhtakia // *Phys. Rev. B* **76** (2007) 155407.
[12] I. S. Nefedov // *Phys. Rev. B* **82** (2010) 155423.
[13] R.K. Fisher and R.W. Gould // *Phys. Rev. Lett.* **22** (1969) 1093.
[14] E. Arbel, L.B. Felsen, In: *Electromagnetic Theory and Antennas*, ed. E.C. Jordan (Pergamon Press, New York, 1963).
[15] R.A. Silin, V.P. Sazonow, *Slow-wave structure* (Staschera, Boston-SPA Eng., National-Landing Science and Technology, 1971). R.A. Silin, *Periodic Waveguides* (Phasis, Moscow, 2002), in Russian.
[16] V.N. Ivanov, N.P. Demchenko, I.S Nefedov, R.A. Silin, A.G. Schuchinsky // *Radiophysics and Quantum Electronics* **6** (1989) 577.
[17] I.V. Lindell, S.A. Tretyakov, K.I. Nikoskinen, S. Ilvonen // *Micr. and Opt. Techn. Lett.* **31** (2001) 129.
[18] D. R. Smith, D. Schurig // *Phys. Rev. Lett*. **90** (2003) 077405.
[19] Z. Jacob, L.V. Alekseyev, E.E. Narimanov // *Opt. Express* **14** (2006) 8247.
[20] Z. Jacob, J.-Y. Kim, G.V. Naik, A. Boltasseva, E.E. Narimanov, V.M. Shalaev // *Appl. Phys. B* **100** (2010) 215.
[21] M.A. Noginov, H. Li, Yu. A. Barnakov, D. Dryden, G. Nataraj, G. Zhu, C.E. Bonner, M. Mayy, Z. Jacob, E.E. Narimanov // *Optics Letters* **35** (2010) 1863.
[22] S.M. Mikki, A.A. Kishk // *IEEE Trans. Antenna and Propag*. **57** (2009) 412.
[23] I.S. Nefedov, S.A. Tretyakov // *Photonics and Nanostructures: Fundamentals and Applications* **9** (2011) 374.
[24] I.S. Nefedov, S.A. Tretyakov // *Phys. Rev. B* **84** (2011) 113410.
[25] I.S. Nefedov, C. R. Simovski // *Phys. Rev. B* **84** (2011) 195459.
[26] M. Kusunoki // *Chem. Phys. Lett.* **366** (2002) 458.
[27] L. Pfefferle, G. Haller, D. Ciuparu // *US Patent 7357983*.
[28] A.M. Nemilentsau, M.V. Shuba, G.Y. Slepyan, P.P. Kuzhir, S.A. Maksimenko, P.N. D'yachkov, A. Lakhtakia // *Phys. Rev. B* **82** (2010) 235424.
[29] P.J. Burke, S. Li, Z. Yu // *IEEE Trans. on Nanotechnology* **5** (2006) 314.
[30] G.W. Hanson // *J. Appl. Phys*. **103** (2008) 064302.
[31] W. Rotman // *IRE Trans. on Antennas and Propag*. **10** (1962) 82.
[32] J.B. Pendry, A.J. Holden, W.J. Stewart, I. Youngs // *Phys. Rev. Lett.* **76** (1996) 4773.
[33] P.A. Belov, R. Marques, S.I. Maslovski, I.S. Nefedov, M. Silveirinha, C.R. Simovski, S.A. Tretyakov // *Phys. Rev. B* **67** (2003) 113103.
[34] I.S. Nefedov, A.J. Viitanen, S.A. Tretyakov // *Phys. Rev. E* **71** (2005) 046612.
[35] I.S. Nefedov, A.J. Viitanen, S.A. Tretyakov // *Phys. Rev. B* **72** (2005) 245113.
[36] M. Hudlička, J. Macháč, I. Nefedov // *Progress in Electromagnetics Research* **65** (2006) 233.