Towards -1 effective index with one-dimensional metal-dielectric metamaterial: a quantitative analysis of the role of absorption losses

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Abstract: We propose a theoretical study of the optimization of one dimensional metal-dielectric metamaterials in order to approach -1 effective optical index. Taking into account actual values of dielectric constants of metal (silver) and dielectrics (HfO2, GaP), and taking advantage of the dispersion relation of Bloch modes, we get a silver/HfO₂ metamaterial with suitable parameters that possesses a near -1 effective optical index for all angles of incidence at a visible wavelength for H-polarized light (i.e. the magnetic field is parallel to the interfaces). The absorption losses of materials appear to be a crucial factor that affects the effective properties of the metamaterial. We show that the losses not only decrease the transmission of the stack, but also change the negative refraction effect. Then, we propose another silver/GaP structure design that is less sensitive to losses. When considering finite thickness structures, and with adequate thickness for the terminating layers, it is possible to achieve a high transmittance of the structure. A near -1 effective index and high transmittance metal-dielectric metamaterial may pave the way to the realization of negative refraction in the visible or ultraviolet wavelength range.

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1. Introduction

Negative refraction was originally suggested by V.G. Veselago in a pioneering work devoted to the study of left-handed (LH) materials (homogenous material whose permittivity and permeability are both negative) [1]. In a seminal paper, Sir J. Pendry predicted that in addition to producing a negative refraction effect, a LH material would make it possible to build a perfect lens that is a lens not limited by the Rayleigh criterion [2]. Obviously, such a result has attracted an important attention from the scientific community.

Although nature does not provide us with such a material, at least in the optical range, nowadays negative refraction has been experimentally verified in some metamaterials [3, 4]. There are also many articles reporting theoretical and experimental study of the negative refraction in photonic crystals (PCs) [5-7]. However it is still a formidable challenge to create metamaterials that have suitable properties in the optical range of wavelength.

A different approach has been suggested: for the H-polarization case a metallic layer, in the electrostatic limit, may act as a perfect lens [2]. Using such a simple structure super resolution has been experimentally exhibited [8-10].

Recently, several groups have reported studies of the negative refraction and subwavelength imaging using one-dimensional metal-dielectric metamaterials (1DMD) [11-14]. Obviously, 1D metamaterials are easier to fabricate and can achieve negative refraction in optical or even ultra-violet wavelength. Moreover, it has been shown that they could have better properties than a single layer [11].

In this letter, we show that with proper design, nearly -1 effective index for all angles of incidence at a visible wavelength can be achieved using this 1DMD metamaterial. When the influence of the dissipation of the metallic and dielectric layers is considered, not only the transmission is decreased, but also the negative refraction angle (and thus the effective index) is affected.

2. Lossless materials

The structure of 1DMD is shown in Fig. 1, it is composed of alternating layers of metal and dielectric, periodic with respect to the *z*-axis, and invariant along the x and y directions.



Fig. 1. 1DMD metamaterial with a symmetric arrangement. The dashed line shows the unit cell.

Firstly, for the sake of simplicity, we consider a lossless Drude model to describe the dielectric function of the metallic layers, $\varepsilon_2 = 1 - \omega_p^2 / \omega^2$, ω_p is the bulk plasma frequency of the metal (with $\lambda_p = 2\pi c / \omega_p = 250 \text{ nm}$). A parametric study has led us to choose $\varepsilon_1 = 4.6$, $d_1 = 37.5 \text{ nm} (0.15 \lambda_p)$, $d_2 = 25 \text{ nm} (0.1 \lambda_p)$, and assume that the permeability is constant ($\mu_1 = \mu_2 = 1$). Note that we assume a $\exp(-i\omega t)$ time dependency. In the following, we will consider a symmetric unit cell as it has been shown that it allows obtaining higher transmittance [14].



Fig. 2. (a). Band structure of 1DMD metamaterial. The purple zones represent the pass bands. The green dashed line represents the light line in free space. The black solid line indicates the frequency at which $n_{eff} = -1$. (b) EFCs for the second band, the labels indicate the frequencies

in unit of $2\pi c/d$. Black curve: EFC of free space for $\omega = 0.375 \times 2\pi c/d$.

For this structure, we have computed the band structure and equal frequency contours (EFCs) using transfer matrix formalism (see Fig. 2) [5]. In present paper, we only consider the H-polarization case.

Following the analysis developed in Ref. [15], the dispersion relation of 1DMD is given by:

$$\cos(K_z d) = \cos(\alpha_1 d_1) \cos(\alpha_2 d_2) - \frac{\alpha_1^2 \varepsilon_2^2 + \alpha_2^2 \varepsilon_1^2}{2\alpha_1 \alpha_2 \varepsilon_1 \varepsilon_2} \sin(\alpha_1 d_1) \sin(\alpha_2 d_2)$$
(1)

where K_z is the z-component of the Bloch wave vector and k_x its x-component, $d = d_1 + d_2$, $\alpha_i = \sqrt{k_0^2 \varepsilon_i \mu_i - k_x}$, (i = 1, 2), and $k_0 = \omega/c = 2\pi/\lambda$ is the modulus of wave vector in free space. The existence of a propagative Bloch mode requires $|\cos(K_z d)| \le 1$.

One can see from Fig. 2(b), that at frequency $\omega = 0.375 \times 2\pi c/d$, the EFC is almost circular (indicating that the metamaterial can be considered as an isotropic medium or more precisely as a uni-axial material as we consider only one case of polarization) and n_{eff} can be well defined at this frequency. Note that the circular EFC is not centered at the origin but on the point $(k_x = 0, K_z = \pi/d)$ [see Figs. 2(b)]. However, if the interface delimiting the structure is perpendicular to the z-axis, then this position of the EFC has no effect on the refractive properties of the structure. Also note that the EFC's radius decreases when the frequency increases, this indicates that the group velocity ($\mathbf{v}_s = \mathbf{grad}_k(\omega)$) is in the opposite direction of the wave vector, and thus shows negative refraction behavior.

We found that for $\omega = 0.375 \times 2\pi c/d$ ($\varepsilon_2 = -0.778$), the radius of EFC is almost equal to that of the EFC of the free space. Thus, the effective index n_{eff} of this stack is nearly -1 at this frequency.

In order to analyze the negative refraction effect of 1DMD structure, we did some numerical experiments to show the field when a Gaussian beam illuminates the 1DMD metamaterial slab (a structure with a finite thickness). Note that in the considered model, the Gaussian beam is limited only along one direction, thus the incident magnetic field is given by the following relation:

$$H_{iv} = \int_{\infty}^{\infty} dk_x \exp[i(k_x x + k_{iz} z)]\phi(k_x)$$
⁽²⁾

where

$$\phi(k_x) = \frac{g}{2\sqrt{\pi}} \exp[-g^2 (k_x - k_{ix})^2 / 4]$$
(3)

The incident beam centered about $k_i = \hat{x} k_{ix} + \hat{z} k_{iz} = \hat{x} k_0 \sin \theta_i + \hat{z} k_0 \cos \theta_i$, θ_i is the incident angle, g represents the width of the waist, in the following simulation work, we choose $g = 2\lambda$.

As an example, we consider a five periods structure (total thickness is 312.5 nm, with 125 nm of metal) surrounded by free space. Figure 3 shows the time-averaged power density calculated using the transfer matrix method [16]. The Gaussian beam is incident from left with resp. angle of 30° and 45° [resp. Figs. 3(a) and 3(b)]. The beam is refracted at the interface according to Snell's law (similarly to a homogenous material with n_{eff} close to -1). The transmittance is significant in a wide range of incident angle (see Fig. 8, for the lossless silver/HfO₂ structure, *i.e.* the black solid curve). The arrows in the figure are the loci of the maximum incident, refracted and transmitted light.



Fig. 3. Time-averaged power density distribution for negative refraction of a Gaussian beam by a 5-periods stack (H polarization). (a) incident angle 30° (b) incident angle 45° . The arrow line in the map shows the locus of the maximum incident, refracted and transmitted fields. We use arbitrary units for the power density in all the maps.

From the field map, we have evaluated the refraction angle as being respectively 30.1° and 45.0° when the incident angle is 30° and 45° . It is in accordance with the results deduced from the dispersion relationship: respectively 30.4° and 45.5° [see Fig. 2(b)]. This confirms that the effective index of this stack is close to -1.

3. Effects of the absorption losses on the negative refraction

In order to take into account realistic material parameters, we now consider the losses in the metal and dielectric layers. At the operating wavelength ($\lambda = 333.4$ nm), the dielectric constants for silver is $\varepsilon_{silver} = -0.778 + 0.3i$ [17], the dielectric layer is assumed to be HfO₂ ($\varepsilon_{HfO2} = 4.6 + 0.016i$) [18]. We study the complex band structure of this metamaterial, the real component corresponds to the wave number (one can check that the average energy flow direction is given by $\mathbf{v}_g = \mathbf{grad}_{real(\mathbf{k})}(\omega)$), while the imaginary part determines the absorption [19].



Fig. 4. (a). The red dashed curve is the real component of the Bloch vector of 1DMD stack with losses. The black and blue curves are the same as Fig.2 (b), i.e. for lossless materials. The dot line illustrates the conservation of the parallel component of the wave vector. (b) Imaginary component of the Bloch vector. The red dashed curve represents the case with losses and the black case with lossless materials.

Figure 4 shows the complex Bloch vector of 1DMD metamaterial taking into account losses. The real component is distorted when compared with the dispersion curve for the lossless case, especially when the incident angle is increased (large values of k_x). The red arrow indicates the refraction direction (35.6°) with an incident angle of 45° for absorptive materials, whereas the blue arrow indicates the refraction direction in the lossless case. Thus, the angle of refraction is greatly affected by the presence of losses.

In Fig. 4(b), for propagative waves (*i.e.* $-1 < k_x/k_0 < 1$), note that the imaginary part of the Bloch wave vector is null when considering lossless materials while not when absorption is not zero, this obviously results in a decrease of transmission.



Fig. 5. Identical to Fig. 3(b) but with losses in the metallic and dielectric layers.

The time-averaged power density distribution in Fig. 5 confirms the influence of the losses discussed above. The refraction angle calculated according to the field distribution is about 31°. The little difference with the angle deduced from the dispersion relation could be attributed to the fact that, first, we consider a finite thickness metamaterial and, also, to the finite width of the Gaussian beam and thus its non-null angular width.

As the losses obviously influence the refraction angle and transmittance in the metamaterial mentioned above (Silver/HfO₂ metamaterial), we tried to find another structure (Silver/GaP metamaterial) that is less sensitive to loss, and still possesses a near -1 effective optical index.

From mathematical studies, it appears that the suitable transformation providing the relationship between non absorptive and absorptive dielectrics is the so-called "complex dilation" [20, 21]. In practice, this transformation consists in performing a phase-variation for the dielectric constant of silver and GaP. Consequently, if this phase-variation is small, then the effect of losses is expected to be small also. From these arguments, we designed a structure with the dielectric constant of silver ε_{silver} such that the ratios $|\text{Im}(\varepsilon_{silver})/\text{Re}(\varepsilon_{silver})|$

and $|\text{Im}(\varepsilon_{GaP})/\text{Re}(\varepsilon_{GaP})|$ are as small as possible.

The metamaterial is made of silver and GaP layers and the operating wavelength has been found to be 459 nm, $\varepsilon_1 = \varepsilon_{silver} = -5.19 + 0.23 i$ (the data is measured in our lab, in order to be much closer to the experimental process), $\varepsilon_2 = \varepsilon_{GaP} = 14.6 + 0.1 i$ [22] and $d_1 = 46.7$ nm, $d_2 = 26.7$ nm. Figure 6 shows the dispersion curve of this metamaterial (EFC).



Fig. 6. Identical to Fig. 4, but for the silver/GaP metamaterial.

Although, the dispersion curve is not perfectly circular (but rather an ellipse), it is less affected by the presence of losses. The real part of the Bloch wave vector is almost not changed in a wide range of parallel wave vector components, thus the refraction angle is almost not changed. For the incident angle of 45° , the refraction angle deduced from the dispersion relation are 39.8° for the lossless structure and 38.1° for the lossy metamaterial. Moreover, the imaginary part is smaller than the one of previous structure that implies a lower level of absorption.

Since the period of this type of metamaterial is thicker than the period of the silver/HfO₂ metamaterial, we consider a 4-periods stack in order to have a similar total thickness (the total thickness of metal is 186.8 nm, the total thickness of dielectric is 106.8 nm and the total thickness of the metamaterial slab is 293.6 nm). Figure 7 shows the time-averaged power density distribution with an incident angle equal to 45° . One can see that the refraction angle change is hardly visible when considering losses or not. The calculated refraction angle is 39.2° for the metamaterial without losses, and 33.3° with losses which is comparable to the values obtained from the dispersion relation.



Fig. 7. Time-averaged power density distribution of negative refraction with the 4-periods silver/Gap metamaterial without or with losses as the angle of incidence is 45°.



Fig. 8. Transmittance of silver/HfO₂ and silver/GaP metamaterials. The solid curves are for 5periods silver/HfO₂ metamaterial, the dashed curves are for 4-periods silver/GaP metamaterial. The black two are the results without loss, the red are with losses.

Figure 8 shows the transmittance through the two different metamaterials (silver/HfO₂ and silver/GaP) with respect to the parallel wave vectors k_x . Comparing the transmittances of the two types of metamaterials shows that it is almost unity in a wide range of k_x when losses are not considered. However, when losses are taken into account, the transmittance is less sensitive to the angle of incidence for the silver/GaP metamaterial.

4. Conclusion

In conclusion, we have shown that near -1 effective index can be achieved using 1DMD metamaterials with a proper choice of parameters. Considering realistic material parameters, we have presented a study of the complex band structure and shown that the absorption losses in metallic layers not only decrease the transmittance, but also change the negative refraction angle in the metamaterial (and thus its effective optical index). Then, we have proposed another 1DMD metamaterial less sensitive to the losses. Therefore a near -1 effective index 1DMD stack with high transmittance can be realized using classical film deposition fabrication technology.