Optical negative-index bulk metamaterials consisting of 2D perforated metal-dielectric stacks

Shuang Zhang,1 Wenjun Fan,1 N. C. Panoiu,2 K. J. Malloy,1 R. M. Osgood,2 and S. R. J. Brueck1

1 Center for High Technology Materials and Department of Electrical and Computer Engineering, University of New Mexico, Albuquerque, NM 87106, USA
2 Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY, 10027, USA
brueck@chtm.unm.edu

Abstract: Numerical simulations of a near-infrared negative-index metamaterial (NIM) slab consisting of multiple layers of perforated metal-dielectric stacks exhibiting a small imaginary part of the index over the wavelength range for negative refraction are presented. A consistent effective index is obtained using both scattering matrix and modal analysis approaches. Backward phase propagation is verified by calculation of fields inside the metamaterial. The NIM figure of merit, \[ -\left(\frac{\text{Re}(n)}{\text{Im}(n)}\right) \], for these structures is improved by \~10x compared with previous reports, establishing a new approach to thick, low-loss metamaterials at infrared and optical frequencies.

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References and links

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1. Introduction

More than 40 years ago, Veselago proposed the existence of many unconventional phenomena for media with negative refractive indices, including the application of a negative-index metamaterial (NIM) slab as an imaging lens [1]. Recently, Pendry took a further step and showed that a NIM slab can magnify the evanescent fields and work as a diffractionless, “perfect” lens [2]. Based on Pendry’s theory, super lenses overcoming diffraction limits have been experimentally demonstrated [3, 4]. These results, as well as the first experimental demonstration of an artificial NIM in the microwave region [5], have led to numerous experimental and theoretical efforts.

In the last two years, there has been much progress towards the realization of NIMs at optical frequencies. This has included numerical studies of infrared magnetic metamaterials [6] and NIMs [7, 8] and experimental demonstrations of THz, mid-infrared and near-infrared magnetic metamaterials [9-13] as well as near-infrared NIMs [14, 15]. However, to date, the experimentally demonstrated near-IR NIMs exhibit large Im(n), which makes them unsuitable for many applications. As a result, a figure of merit, \(-\frac{\text{Re}(n)}{\text{Im}(n)}\), has been introduced [14] to allow comparison between different NIM structures. To reduce the loss and enhance the transmission, structures similar to that in [14] were parametrically evaluated and optimized numerically [16] and later experimentally verified [17-19]. As shown in Ref. [14], a thin metamaterial (<\lambda) slab consisting of a metal/dielectric/metal layer stack with a periodic array of holes exhibits a negative refractive index in the vicinity of its quasi-static LC resonances. This thin metamaterial slab can be considered as a basic NIM building block that can be used to construct a much thicker metamaterial (~\lambda). The evolution of the optical properties of a metamaterial as a function of the number of unit cells is an interesting question in its own right as well as providing insight into the design of NIMs [20].

As shown in Ref. [16, 21], an array of paired metallic stripes oriented along the direction of magnetic field vertically separated by a dielectric layer can exhibit a magnetic (LC tank circuit) resonance with a negative effective permeability over a limited wavelength range. The resonance wavelength has a linear relation to the stripe linewidth. Adding an array of metallic stripes along the direction of electric field to this magnetic structure results in metal/dielectric/metal films with a square 2D array of holes perforating the multiple layers.
Reduced surface plasma frequencies in perforated metal films have been proposed and experimentally verified [22, 23]. Thus, a moderately negative permittivity can be achieved, which, in combination with the magnetic response, leads to a negative refractive index. The schematic of the thick metamaterial structure simulated in this paper is shown in Fig. 1 with geometric parameters corresponding to the single-layer (thin building block) simulation reported in [16].

![Schematic of a metamaterial consisting of multiple unit cells.](image)

**Fig. 1.** Schematic of a metamaterial consisting of multiple unit cells. The geometric parameters are: 801-nm pitch along orthogonal in-plane directions and a linewidth of the metal gratings along the direction of magnetic field of 500 nm and that along the electrical field of 200 nm. The thickness of the air/Au/dielectric/Au/air unit cell is 5/30/60/30/5 nm.

### 2. Rigorous coupled wave analysis

Rigorous coupled wave analysis (RCWA) was used for the simulation [24]. Two methods were used to extract the refractive index of this structure. The first is the determination of the effective index from the complex coefficients of transmission and reflectance on a metamaterial slab (S-parameter approach). This method requires taking the inverse of a cosine function, which causes ambiguity due to its multiple branches. To resolve this ambiguity, metamaterials with a different number of unit cells are simulated; the branch that is consistent for a different numbers of unit cells is chosen as the root, as described in [25].

For light propagating in a periodic structure, an infinite number of modes exist for a given frequency (each mode is the linear combination of many Floquet plane waves based on the periodicity in the transverse directions). As the number of unit cells along the propagation direction is increased, the mode with the smallest imaginary part dominates the optical response [20]. Based on this consideration, a second method is used; in this the eigenvalues of the transfer matrix are solved for a single unit cell; the mode with the smallest decay dominates the optical response and an effective index associated with this mode is obtained.

In RCWA, the electromagnetic fields are expanded into a spatial Fourier series based on the transverse periodicities of the structure. Inside the structure the forward and backward propagating waves have spatial Fourier coefficients $A_{mn,i,\sigma}$ and $B_{mn,i,\sigma}$, where $m$ and $n$ are the diffraction orders in $x$ and $y$ directions, $i$ is the material index, and $\sigma$ the polarization. The electric field associated with the forward and backward propagation is a sum over all the spatial com-
ponents. For instance, the electric field of the forward propagating beams can be expressed as

\[ \vec{E}_{A,i,\sigma} = \sum_{m,n} A_{mn,i,\sigma} f_{mn}(x,y) \gamma_{i,mn} \]  \hspace{1cm} (1)

with

\[ f_{mn}(x,y) = \exp[j(\alpha_{m} x + \beta_{n} y)] \] \hspace{1cm} (2)

where \( \gamma_{i,mn} = \sqrt{\varepsilon \mu - \alpha_{m}^{2} - \beta_{n}^{2}} ; \) \( \alpha_{m} \equiv 2 \pi m / l_{x} ; \) \( \beta_{n} \equiv 2 \pi n / l_{y} \) and \( l_{x}, l_{y} \) are the periods of the structure in the \( x, y \)-directions. In the calculation, the same number of diffraction orders, \((2N+1)\), are kept in both directions [a total of \((2N+1)^{2}\) orders], with \( m \) and \( n \) ranging from \((-N)\) to \( N \). Up to 19 diffraction orders \((N = 9)\) were kept in each direction, good convergence was obtained with negligible differences between the simulations for \( N = 8 \) and \( N = 9 \).

Using RCWA, the transmission matrix can be obtained numerically for a periodic structure, which relates the coefficient vector \( A_{mn,0,\sigma} \) \( B_{mn,0,\sigma} \) (before the unit cell, index 0) and \( A_{mn,l,\sigma} \) \( B_{mn,l,\sigma} \) (after the unit cell, material index \( l \)) by,

\[ \begin{bmatrix} A_{mn,0,\sigma} \\ B_{mn,0,\sigma} \end{bmatrix} = \overline{M} \begin{bmatrix} A_{mn,l,\sigma} \\ B_{mn,l,\sigma} \end{bmatrix} \] \hspace{1cm} (3)

where \( \overline{M} \) is a transfer matrix of dimension \( 4(2N+1)^{2} \), which is evaluated based on the Fourier transform of the dielectric function along the transverse directions. Next, the solution for the eigenvalues of the \( \overline{M} \) matrix can be obtained as \( q \), where \( q \) ranges from 1 to \( 4(2N+1)^{2} \), only half of the eigenvalues with modulus larger than 1 represent the physical propagating modes (decaying at infinity), with each mode being a linear combination of all of the spatial harmon-
ics. When light propagates through many unit cells, only the mode with the smallest $|\gamma|$ (smallest decay) dominates. Thus, the effective index can be expressed as:

$$n' = -\text{Im} \log(\gamma) / (k_0 d) \quad \text{and} \quad n'' = \text{log}|\gamma| / (k_0 d)$$

In Eq. (4), $d$ is the thickness of a single unit cell along the propagation direction and $k_0$ is the wave vector in vacuum. The various terms are shown in Fig. 2.

![Graph](image)

Fig. 3. The magnitude of the transmission (a), (c) and reflectance (b), (d) for slabs consisting of 1, 2, 5, 6 and 10, 100 and 200 unit cells along the propagation direction.

We first numerically calculate the transmission and reflectance for one, two, five, six, ten, 100 and 200 layers of unit cells with both the incident and exit media as air. The transmission and reflectance spectra are shown in Fig. 3. (Transmission and reflectance curves for 100 and 200 layers of unit cell are shown separately for clarity.) For a single unit cell (air/metal/dielectric/metal/air), the transmission shows a peak around 1.93 $\mu$m and a dip around 2 $\mu$m. With an increasing number of layers, the transmission at long wavelengths ($\lambda > 1.93 \mu$m) decreases rapidly and approaches zero, consistent with a simple metallic response away from resonance. For multiple unit cells at wavelengths below $\sim 1.95 \mu$m, $T$ and $R$ exhibit characteristic one-dimensional Fabry-Perot slab oscillations. As will be shown later, this is the negative index region. With the dimension of unit cell along the propagation being only 130 nm, the thickness of a slab with ten unit cells is only 1.3 $\mu$m, which is less than the 2.0-$\mu$m vacuum wavelength of interest. Nevertheless, as many as eight resonant peaks are observed over the pass band from 1.5 $\mu$m to 1.95 $\mu$m. As will be shown later, this large number of resonances is due to the large and varying absolute value of the effective index across the negative refraction region. Further increasing the number of metamaterial layers to 100 and 200 elimi-
nates the oscillation in transmission and reflectance curves and gives the asymptotic feature for a bulk, lossy metamaterial, as shown in Fig. 3(c) and Fig. 3(d). The transmission peak around 1.55 μm corresponds to the wavelength with the lowest loss. The reflectance is low at shorter wavelengths from 1.5 to 1.95 μm, while it increases rapidly at longer wavelengths, exhibiting metal-like properties.

Next, the effective indices of structures with different numbers of unit cells (except for 100 and 200 layers) are calculated using the complex coefficients of transmission and reflectance, as shown in Fig. 4. For a single unit cell, the real part of index is continuous and negative from 1.77 to 2.18 μm; the imaginary part shows a peak around 2 μm. For multiple unit cells, the negative refraction region starts at ~1.5 μm, the indices decrease quickly with wavelength to ~ -8 at 2 μm. Over this negative index range, the real part of index for two to ten layers agrees well and the imaginary part of index for five to ten layers converges nicely and is very small over the range from 1.5 to 1.7 μm (less than 0.1 for ten unit cells). As mentioned before, the inverse method involves finding the root of a multi-branched cosine function. As shown in Fig. 4, the real part of the effective index along branch 1 is consistent for different numbers of unit cells up to 2 μm, for wavelengths longer than 2 μm, branch 1 diverges for different layers. However, branch 2, as shown in Fig. 4, is consistent for different numbers of unit cells. This leaves a large discontinuity in the Re(n) at 2 μm. However, to meet the requirement that the refractive index be consistent for different number of unit cells of metamaterial, we need to accept these two branches for different wavelength regions. For wavelengths over 2 μm (branch 2 is chosen), the real part of index is almost zero and the imaginary part is much larger than the real part, exhibiting metallic properties. Compared to single unit cell, the imaginary part is small and featureless over this long wavelength range.
3. Modal analysis

A modal analysis was carried out to provide insight into the origins of this discontinuity. Using Eq. (4), both the real and imaginary parts of the refractive index for the two modes with the smallest decay are obtained, as shown in Fig. 5(a). The reason for the discontinuity is clear: the imaginary part of the first mode exceeds that of the second mode for wavelengths above 2 μm, and therefore, for a thick slab, the second mode becomes the dominant mode at longer wavelengths. The results obtained from the modal analysis are very consistent with those from the inverse method. In addition, the coupling efficiency of an incident beam into each mode is also important. As shown in Fig. 4, the effective index calculated for five to ten layers converges very well except for a narrow wavelength range around 2 μm where the two modes exhibit comparable losses, indicating that the fundamental mode is absolutely dominant over other modes over most of the frequency range. Furthermore, in Fig. 3, over the negative index region, the transmission is very large even for ten unit cells, indicating good coupling between a normal-angle incident beam with the negative index fundamental mode.

Next, we plot the figure of merit defined in Ref. [14], \[-\frac{\text{Re}(n)}{\text{Im}(n)}\], in Fig. 5(b). The largest value of 25 is achieved around 1.7 μm. Compared to that of a single unit cell [17], the optical properties of NIM slab consisting of multiple layer are much improved.

Fig. 5. (a) The effective indices of the two modes with the lowest decay rates. For wavelengths below ~ 2 μm mode 1 has the lowest loss and dominates the response. At longer wavelengths, mode 2 has a lower loss and becomes dominant. (b) The ratio of the real part to the imaginary part of effective index in the negative index region.
4. Field distributions

It is of interest to study the details of the light propagation inside the metamaterial. To do this, we first calculated the distribution of electric fields for the dominant mode (lowest decay) at several positions within a unit cell along the propagation direction. The phase of the electric field averaged over one transverse unit cell versus propagating distance for three different wavelengths, $\lambda=1.58$, 1.63, and 1.70 $\mu$m, are shown in Fig. 6(a). For all the three wavelengths, the phase decreases along the propagation, directly demonstrating the negative-index property. Furthermore, the absolute amount of phase change from $z=0$ to $z=130$ nm increases with increased wavelength, consistent with the effective index shown in Fig. 5. The magnitude and phase of the electric field at $z=65$ nm (the middle of the unit cell) are plotted in Figs. 6(b) and 6(c). As expected, the electric field is mainly confined to the inside of the rectangular aperture; the phase of electric field inside the aperture is more uniform than the magnitude. In both plots, the modulation at high spatial frequencies is due to the limited number of diffraction orders retained in the RCWA simulation.

Fig. 6. (a) Evolution of the phase of the average electric field along the propagation direction across a unit cell. (b), (c) Electric field amplitude and phase plots ($\lambda=1.7$ $\mu$m) at the center of the cell ($z=65$ nm) across a unit cell in the transverse plane. The white frames represent the location of the open aperture.
Fig. 7. The magnitude and phase of the magnetic field for a three-layer structure across one transverse unit cell at the middle of the structure (indicated by the dashed line) for wavelengths of 1.5, 1.7 and 2.1 μm.
Next, we simulated a structure consisting of three unit cells along the propagation direction. We plot the distribution of the magnetic field, both the magnitude and phase, across one transverse unit cell at the middle of the structure (indicated by the dashed line in Fig. 7) for three wavelengths, 1.5-, 1.7-, and 2.1-μm. For the shortest wavelength, \( \lambda = 1.5 \mu m \), which is far away from the metamaterial resonance around 1.9-2.0 μm, the magnitude of the magnetic field is slightly higher in the area beneath the metal pattern (region II and III indicated by Fig. 7) than that in the air aperture, while the phase of the magnetic field beneath the metal lines along the magnetic field \( H_y \) (defined as region II) is exactly \( \pi \) shifted from that in the air aperture (defined as region I) and in the area beneath the thin metal wires along the electrical field \( E_x \) (defined as region III), as shown in Figs. 7 (a) and 7 (b). Although the magnetic field in region III is as strong as that in region II, the area is much smaller, leading to an overall opposing magnetic field to that in region I. This directly verifies the existence of magnetic activity at this wavelength. Furthermore, this result confirms one point made in Ref. [16], i.e. the increase of metal linewidth along the electric field weakens the magnetic resonant strength. At the longer wavelength of 1.7 μm, which is closer to the resonance frequency, the magnetic field in region II and III is much larger than that in region I, leading to a stronger magnetic activity and more negative index than that at 1.5 μm, as shown in Figs. 7 (c) and 7 (d).

At an even longer wavelength, i.e. 2.1 μm, mode 2 becomes the dominant, low-loss, mode. The corresponding magnetic field distribution also shows very different features from that at 1.5 and 1.7 μm. The magnetic field in region II has the same phase as that in region I. While the magnetic field in region III opposes that in region I, it is much weaker. So the overall magnetic field in II and III is positive with respect to that in region I. In addition, the magnetic field at 2.1 μm is much smaller than that at 1.5 and 1.7 μm, mainly as a result of the large imaginary part of the refractive index at 2.1 μm.

5. Summary

In conclusion, we have numerically demonstrated a low loss negative-index metamaterial with a thickness much larger than the free space wavelength (for 100 and 200 layers) in the near-infrared region. Numerical study of the electromagnetic fields inside the metamaterial slab verifies backward phase propagation and strong magnetic activity in the negative index region. Further studies (not shown here) demonstrate that if the thin air gaps are eliminated, the results are essentially unchanged. Given the rapid progress in optical and interferometric lithography, in nanoimprinting and in nanoscale self-assembly techniques, fabrication of this structure should be feasible in the near future.

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