Light propagation in multilayer metamaterials
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Applications and outlook

This Chapter provides an overview of ideas that originate from the research projects presented in the previous chapters of this thesis. The flat lens experimentally realized in Chapter 4 operated in the ultra-violet spectral range. Here we show that by changing the layer materials and thicknesses, a flat lens operating in the infrared may be realized, with an electrically tunable transmission. Furthermore, by studying the internal wave propagation through metal dielectric multilayer structures, as was done in Chapter 3, we show how we can use a hyperbolic metamaterial to design a special cavity geometry that very efficiently localizes light. Finally, we design a multilayer geometry that acts as a broadband angular filter, operating in the visible range. This structure filters incident light on angle of incidence and polarization, and might be applied to enhance the performance of light emitting diodes.

6.1 Flat lens operating in the near-infrared telecom band

6.1.1 Introduction

In Chapter 4 a metal/dielectric multilayer stack was designed that showed angle-independent negative refraction of energy, enabling a flat lens operating in the UV. Negative refraction is a general phenomenon that relies on having a significant amount of field localized in the metallic regions, with the permittivity of the metal being negative. As such, the phenomenon of negative refraction, and with appropriate design also flat lensing, can be obtained for any wavelength at which the metal permittivity is negative, provided that absorption losses are not too high.
To illustrate this, we design a flat lens operating in the near-infrared. This spectral range is important for telecommunication applications, as very long signal propagation lengths are attainable due to favorable material properties of both semiconductors (e.g. Si and Ge) and dielectrics (e.g. glass optical fibers), enabling integrated optical circuits [108]. Incorporating flat lenses in photonic integrated circuits may enable novel forms of on-chip optical signal processing.

To design an infrared flat lens, we first consider the noble metals Ag and Au. As shown in Fig. 6.1 they have an very large negative real part (a) of the permittivity in the IR, as well as a relatively large imaginary part (b). Because of the strongly negative real part of the permittivity, fields will not penetrate deep into the metallic layer, and therefore the interaction with the metal is small. Additionally, due to the large imaginary part, any field that is localized in the metallic layer will be strongly absorbed, preventing efficient light propagation in the lens.

![Figure 6.1: Real (a) and imaginary (b) part of the permittivity for different metallic materials. Optical constants for Ag and Au have been taken from [109]. The optical constants of the other materials are from [110].](image)

Recently research has been directed at alternative materials with a moderate negative real part of the permittivity, in combination with a relatively small imaginary part [110, 111]. Figure 6.1 shows the permittivities of TiN, ZrN, and the transparent conductive oxides aluminum-doped zinc oxide (AZO), gallium-doped zinc oxide (GZO) and indium tin oxide (ITO) [112]. At the telecom band, near $\lambda_0 = 1550$ nm, AZO is the material with the lowest imaginary part and has a small negative real part: $\varepsilon_m = -0.689 + 0.269i$. We will combine this metallic material with a dielectric $\varepsilon_d = 2.5^2$, which is comparable to TiO$_2$, to design a flat lens.
6.1 Flat lens operating in the near-infrared telecom band

6.1.2 IR Flat lens demonstration

To design a multilayer flat lens operating at $\lambda_0 = 1550$ nm, we calculate the isofrequency contour (IFC) $k_{Bl}(k_x)$ in the same way as was done in Chapter 4 for the UV spectral range. We perform this calculation for a range of layer thicknesses $d_m$ and $d_d$, corresponding to the metal and dielectric layers respectively. In order to provide a comprehensible figure of merit, we calculate the deviation of $k_{Bl}(k_x)$ with the ideal $k_z(k_x) = \pi/a - \sqrt{k_0^2 - k_x^2}$, where $a$ is the unit cell size. We determine the deviation by integrating the absolute difference between $k_{Bl}(k_x)$ and $k_z(k_x)$ between $k_x = 0$ and $k_x = k_0$, as given by Eq. 4.2.

![Figure 6.2](image_url)

**Figure 6.2:** a, Deviation from ideal spherical IFC as a function of metal $d_m$ and dielectric $d_d$ layer thickness for a AZO/TiO$_2$ metamaterial at $\lambda_0 = 1550$ nm. b, IFC of the optimum geometry (blue) with: $d_m = 410$ nm and $d_d = 58$ nm. c, Result of a Green's tensor calculation showing the $|E(x,z)|$ spatial field amplitude calculated for a horizontal dipole placed above a slab of 5 unit cells of the optimum geometry. An elongated image is observed of the dipole.

Figure 6.2a shows the calculated deviation as a function of $d_m$ and $d_d$. An optimum configuration is found with $d_m = 410$ nm and $d_d = 58$ nm, for which the deviation between ideal and calculated IFC is smallest. Figure 6.2b shows the IFC $k_{Bl}(k_x)$ (blue) corresponding to this optimum geometry, compared to the ideal spherical curve $k_z(k_x)$ (red). There are deviations between the IFC and the ideal case (red), which are especially pronounced at $k_x > 3 \mu m^{-1}$, corresponding to an angle of approximately $48^\circ$. To demonstrate the imaging characteristics of a flat lens based on negative refraction in this multilayer structure, we consider a horizontal dipole source placed at $(x,z) = (0,-5)$ nm below a multilayer structure formed by 5 unit cells of this optimized geometry. Using Green's tensor calculations we can then determine the field profile on the other side of this multilayer stack. Fig. 6.2c shows the spatial field distribution above the surface at $z = 2.34 \mu m$; as is clear, a focus is being formed above the infrared flat lens, corresponding to the image of the dipole source. The focus exhibits strong lateral confinement, with a FWHM of 1.7 $\mu m$.  

81
6 Applications and outlook

6.1.3 Tunable flat lens

The use of a transparent conductive oxide (TCO) as a constituent of the flat lens design enables several new functionalities, as the permittivity of TCOs can be tuned locally by applying a positive electric bias [113]. An electric field across the TCO leads to a charge accumulation layer near the TCO/insulator interface. As the permittivity of AZO is described by a Drude model, a change in carrier density corresponds to a local change in permittivity.

![Diagram of tunable flat lens design](image)

**Figure 6.3:** (a) Tunable infrared flat lens design. Four unit cells of AZO/TiO$_2$ are considered, with an alternatingly positive and negative bias applied to the AZO, leading to an accumulation layer at the positively biased AZO interfaces. Blue corresponds to the biased AZO, where dark blue indicates the accumulation layers, and green layers are the TiO$_2$. (b) Real and (c) imaginary part of the permittivity of ITO at $\lambda_0 = 1550$ nm, taken from [113]. The linear function fitted to the real part of the permittivity has a slope of $-5.9/V$.

Next, we investigate if the optical response of the flat lens can be changed dynamically by applying an electric bias. To this end, we imagine connecting subsequent AZO layers to either a positive or negative bias. Figure 6.3a shows the proposed multilayer design. For simplicity, in the following we will model the accumulation layer as a step-function, where the permittivity of the AZO within 5 nm of the interface is modulated by the potential. In reality, the charge accumulation depth profile will have an exponential shape. Note that no change in permittivity was experimentally observed for a negative bias [113]. Figure 6.3b,c shows the real and imaginary part of the permittivity of ITO at $\lambda_0 = 1550$ nm in the accumulation layer for varying potential, as experimentally observed by spectroscopic ellipsometry in [113]. A linear function fitted to the real part of the permittivity in Fig. 6.3b has a slope of $-5.9/V$. In the following we will apply this relation to the real part of the...
experimental values of the permittivity of AZO, while keeping the imaginary part at the unperturbed value.

Figure 6.4: a, Absolute value of the electric field calculated along the optical axis above an AZO/TiO$_2$ flat lens operating in the infrared. The object is a horizontal dipole, placed 5 nm below the flat lens at $(x, z) = (0, -5)$ nm. The field amplitude is calculated above the lens surface (at $z = 1.872 \mu$m, dashed line), for modulations of the permittivity: $\Delta \varepsilon_m = 0$ (red), $\Delta \varepsilon_m = -5$ (green) and $\Delta \varepsilon_m = -10$ (blue). b, Image calculated when there is no potential on the flat lens. c, Image when the permittivity in the accumulation layer is modulated with $\Delta \varepsilon_m = -10$.

Figure 6.4 shows the calculated electric field amplitude above the tunable flat lens, resulting from a horizontal dipole placed just below the multilayer structure at $(x, z) = (0, -5)$ nm. The electric field is calculated as a function of separation from the multilayer surface $z$, with $x = 0$. The lens consists of 4 unit cells corresponding to a surface at $z = 1.872 \mu$m. The profile is calculated for three values of modulation of the permittivity in the accumulation layers: $\varepsilon_m = -0.689 + 0.269i$ (red), $\varepsilon_m = -5.689 + 0.269i$ (green) and $\varepsilon_m = -10.689 + 0.269i$ (blue) respectively, corresponding
to voltages between 0 and 2 V (Fig. 6.3b). As can be seen, the peak in field amplitude at the focal point is modulated with 12%. The peak amplitude shifts 600 nm towards the flat lens interface. To illustrate the effect on the overall imaging performance of the flat lens, we show the image formed by the flat lens with no permittivity modulation in Fig. 6.4b, and with a permittivity modulation of $\Delta \epsilon_m = -10$ in Fig. 6.4c. The main effect visible is the reduction in amplitude, and the shift of the focal position towards the lens.

In the above, we have assumed strong permittivity changes of $\Delta \epsilon_m = -10$, based on the experimental data of [113]. Given such a strong modulation, the observed effect in imaging properties of the flat lens is relatively modest. We attribute this to the fact that the permittivity is only modulated close to the interface, while the light propagating through the flat lens interacts with the entire layer stack. A stronger interaction might be expected when light is coupled exclusively to surface waves [114]. Nonetheless, the design proposed here shows significant electrically controlled modulation in transmitted intensity, that could be used to modulate optical signals in a photonic integrated circuit operating in the infrared.

### 6.2 Hyperbolic metamaterial cavity

#### 6.2.1 Introduction

As described in Chapter 4, propagation of light in hyperbolic metamaterials (HMMs) is described by permittivities of opposite sign for two orthogonal propagation directions. This extreme anisotropy leads to fascinating optical properties. Wave components with extremely high wavevectors, which are usually evanescent in vacuum, can propagate through a HMM. This is because the hyperboles in the dispersion relation (see Fig. 6.5a) only flatten off when $k_z$ becomes comparable with $\pi/a$, where $a$ is the unit cell size. Most hyperbolic metamaterial designs have an extremely small unit cell, which allows propagation of light with very high wavevectors.

Hyperbolic metamaterials can be used to fabricate nanoscale cavities [89, 115, 116], for which an anomalous scaling law is observed; the cavity resonance frequency is independent of cavity size. This phenomenon is exploited to fabricate deeply sub-wavelength cavities. So far, the details of internal wave propagation in these cavities have not been discussed to the best of our knowledge. Here, we predict a very fascinating relation between the internal wave propagation characteristics and the HMM cavity geometry.

The inspiration for this prediction comes from a very different research field; physical oceanography. It has been shown that internal gravity wave propagation in a uniformly stratified fluid is described by a hyperbolic dispersion relation, which implies that waves propagate in a direction with a fixed angle to the vertical [117, 118]. Interestingly, by appropriately designing a cavity with stratified water, it has been observed that following multiple internal reflections, these waves will eventu-
ally follow one specific path (an "attractor"), regardless of the original position and
direction of the wave. Given how light propagates through a hyperbolic metamate-
rial, we expect a very similar phenomenon to occur for wave propagation through
a hyperbolic optical metamaterial.

### 6.2.2 Internal wave propagation

In the following, we consider a HMM comprised of a stack of Ag and Ge thin films,
as in [89], with the layers stacked in the $z$ direction, and extended in the $x − y$
plane. For the Drude model given in that work, we find for a frequency of 220 THz
($\lambda_0 = 1363$ nm), $\varepsilon_{\text{Ag}} = -94.5 + 3.7i$, and we take $\varepsilon_{\text{Ge}} = 16$. Figure 6.5a shows the
calculated IFC for this multilayer stack, for a unit cell of $a = 10$ nm, and a metal
filling fraction of $\rho_{\text{Ag}} = 0.4$. The IFC is calculated for the center frequency at 220
THz (in green), and for a slightly lower frequency (red) and higher frequency (blue).
The black circle plotted around the origin represents the IFC for a plane wave in
vacuum at this frequency. If a dipole scatterer would be placed in the near field
of the HMM medium, its wave vector components that are evanescent in air could
couple into the HMM medium, and propagate inside the HMM. As an example,
waves with $k_x = 50 \mu m^{-1}$ are shown in Fig. 6.5a. The Poynting vector is indicated by
the arrows, and as can be seen, light propagates in the metamaterial with an angle
close to $\pm 45^\circ$ or $\pm 135^\circ$ with respect to the $z$-direction.

![IFC calculated for a hyperbolic Ag/Ge metamaterial with a unit cell size $a = 10$ nm, $\rho_{\text{Ag}} = 0.4$ at 220 THz. The Poynting vector is oriented at $\pm 45^\circ$ and $\pm 135^\circ$.](image)

If we now consider a cavity fabricated from this HMM, constructed by stacking
a limited number of unit cells in the $z$ direction, and by limiting the extension of the layers in the $x-y$ plane, light with high spatial frequencies will be confined to the cavity due to total internal reflection. Inside the cavity, light only propagates at specific angles, as determined from the corresponding IFC. A cross-section in the $x-z$ plane of the HMM cavity is shown in Figure 6.5b. The top row shows a square cavity, with a dipole source (red dot) placed at different positions above the cavity. As radiation can only propagate under certain angles, the cavity mode will always be rectangular in shape, as is clear from the ray tracing shown in the top row. If the dipole source is placed at a different position, the cavity mode will have a different rectangular shape accordingly.

When we adapt the cavity shape, by displacing the bottom-right corner inward, as shown in the middle row, we see that the radiation will collapse onto the cavity diagonal. Interestingly, in this case, the path light collapses onto is independent of dipole position: all light in the cavity will eventually be guided onto the diagonal path, called an attractor [118]. The bottom row shows a different cavity shape, with a different size aspect ratio than the cavity in the middle row, for which light collapses onto a rectangular path.

To visualize how waves propagate inside the HMM cavity, we perform a finite-difference time domain simulation of the propagation of light emitted by a horizontal dipole source placed at $(x, z) = (-75, 105)$ nm, for a cavity with corners at $(-100, -85)$, $(10, -85)$, $(100, 100)$ and $(-100, 100)$ nm, and Ag and Ge layers with a permittivity as given above. Figure 6.6a shows the simulated field profile

![Figure 6.6: a. Simulated field distribution in a Ag/Ge hyperbolic metamaterial cavity with corners at: $(-100, -85)$, $(10, -85)$, $(100, 100)$ and $(-100, 100)$ (positions in nanometers). A horizontal dipole source is placed at $(-75, 105)$. The Re($H_y(x, z)$) field component is shown. b. Ray tracing for this cavity geometry shows good agreement. Black (blue) lines; light emitted towards the right (left).](image)
Re($H_y(x, z)$) in the cavity. As can be seen, the field follows lines propagating at $\pm 45^\circ$ or $\pm 135^\circ$ to the normal, as expected. The individual Ag and Ge layers, stacked in the $z$ direction, can also be resolved in the figure from the modulation in field amplitude. As is clear from the figure, the field is strongly absorbed, such that only the first few reflections in the cavity are resolved. However, the field clearly follows the expected path, based on ray tracing as shown in Fig. 6.6b. Interestingly, there seems to be no phase advance as light propagates along a ray, as seen from the almost constant value of the field component. We explain this effect by noting that the orientation of $k$ and $S$ is almost exactly perpendicular (see Fig. 6.5a), so as the energy flows in the direction of $S$, only a small phase advance should be observed.

The attenuation evident in Fig. 6.6a is caused by the absorption in the Ag layers, for which the imaginary part of the permittivity is very large. As noted in the previous section however, alternative materials such as transparent conductive oxides are available, which have much lower imaginary permittivity values in the IR. Furthermore, recent studies have shown that hexagonal boron nitride is a natural hyperbolic material in the mid-IR [119, 120], with a permittivity characterized by a negligible imaginary part. Such hyperbolic metamaterials would allow the waves to propagate much further in the cavity, leading to a stronger field enhancement along the attractor.

In the above, we have discussed the internal wave propagation inside a hyperbolic metamaterial. However, probing this internal field distribution in a three-dimensional cavity might prove difficult. A solution would be to use a hyperbolic metasurface, as was realized recently [86] in the form of a high quality Ag grating pattern. Such a hyperbolic metasurface provides an ideal platform to study the attractor in a hyperbolic metasurface cavity using the third dimension for optical experiments to probe the field pattern, using e.g. a near-field scanning optical microscope or cathodoluminescence microscopy. These techniques have a very high spatial resolution, enabling the observation of the attractor pattern in the cavity.

As can be seen in Fig. 6.6a, two rays leave the dipole, propagating at $\pm 135^\circ$ to the top surface normal, as expected. As was shown in [86], the direction of propagation in the hyperbolic metasurface is dependent on the polarization handedness, resulting in a plasmonic spin-Hall effect [121]. Similarly, the two rays visible in Fig. 6.6a should correspond to a different handedness. Reciprocally, this could entail that by exciting a rotating dipole in the near field of the hyperbolic metasurface cavity, all the energy is directly emitted in one direction determined by the polarization handedness, leading to a cavity mode which is non-degenerate. Therefore, this geometry allows us to very effectively harvest the evanescent components of a scattering element, and by tuning the exact cavity shape, the radiation profile can be steered. Accordingly, this platform can be used to route optical signals in a photonic integrated circuit.
6.3 Dielectric angular filter applied for light emission

6.3.1 Introduction

A well-known application of dielectric multilayers is in distributed Bragg reflectors (DBRs) [122], which act as mirrors for a specific wavelength range, depending on the material permittivities and layer thicknesses. Here, we discuss a special multilayer design that transmits TM-polarized light at the Brewster angle, while light with a different polarization and at different angles of incidence is reflected. Such an angular filter can be used to enhance the emission of light emitting diodes (LEDs) in a particular well defined angular range.

As a model system, we calculate the transmission coefficient of a multilayer structure consisting of 50 unit cells, where each unit cell has a defined size $a_0$, and the layers in the unit cell have: $\varepsilon_1 = 1$, $\varepsilon_2 = 2$, with $d_1 \sqrt{\varepsilon_1} = d_2 \sqrt{\varepsilon_2}$ and $d_1 + d_2 = a_0$. The transmission coefficient is calculated for TM polarized light as a function of wavelength and angle of incidence. Figure 6.7 shows the transmission coefficient $|t(\lambda_0, \theta_i)|$. We calculate the transmission coefficient for six different values of $a_0$, between 200 nm and 450 nm (a-f). Two observations are evident from the figure; first, there is a band of wavelength for which the multilayer stack shows high reflectance at normal incidence, and this band shifts to longer wavelength for larger values of $a_0$. Second, at the Brewster angle $\theta_{Br} = \tan^{-1}(\sqrt{\frac{\varepsilon_2}{\varepsilon_1}}) = 54.7^\circ$ (dashed white line), the transmission $|t| = 1$ for all wavelengths.

By creating a supercell structure, where multilayer stacks with a different unit cell size $a_0$ are combined, an angular filter may be achieved operating for a broad band of wavelengths [123]. For such a geometry all wavelengths are reflected for all angles of incidence, except for TM polarized light at the Brewster angle. As an example, we consider a multilayer stack formed by 6 supercells, where each supercell consists of 8 unit cells. The unit cell size in supercell $i$ is given as $a_i = a_0 r_0^{i-1}$, with rate $r_0 = 1.2$ and starting unit cell size $a_0 = 200$ nm for $i = 1 - 6$. In this case, the unit cell size $a_i$ is gradually adjusted between $a_1 = 200$ nm for the bottom supercell and $a_6 = 500$ nm for the top supercell. As before, the unit cell parameters are given by: $\varepsilon_1 = 1$, $\varepsilon_2 = 2$, with $d_1 \sqrt{\varepsilon_1} = d_2 \sqrt{\varepsilon_2}$ and $d_1 + d_2 = a_0$. Because the multilayer structure now consists of reflectors designed to reflect different wavelengths, a broadband angular filter is realized.

Figure 6.8 shows the calculated transmission for TM-polarization as a function of wavelength and angle of incidence. As is clear, only light around the Brewster angle ($\theta = 54.7 \pm 10^\circ$) is transmitted through the structure. This band can be made narrower by using more supercells, and by changing the rate $r_0$ to a value closer to 1. Interestingly, light that is TE-polarized (Fig. 6.8b) is reflected for all wavelengths and all angles of incidence. This principle was experimentally demonstrated [123] for a SiO$_2$/Ta$_2$O$_5$ multilayer structure. We now repeat the calculations for the more realistic parameters $\varepsilon_1 = 1.5^2$ and $\varepsilon_1 = 2.5^2$, to show that this idea may be applied using different materials. Figure 6.8(c-d) shows the calculated transmission for TM and TE polarized light respectively, for $r_0 = 1.15$, $a_0 = 120$ nm, and a multi-
layer structure consisting of 8 supercells with 5 unit cells each. As can be seen, the stack again only transmits broadband light around the Brewster angle for TM-polarization.

### 6.3.2 Angular filter for light emission

One complication that arises when $\varepsilon_1 = 1.5^2$ is that the Brewster angle in such a multilayer system $\theta_{Br} = 59.0^\circ$ cannot be reached for propagating waves in air, as the maximum angle of propagation in the $\varepsilon_1$ medium will then be limited by refraction at the air-multilayer interface: $\theta_{max} = 41.8^\circ$. Therefore, light propagating through such a stack would suffer total internal reflection, and light incident from outside the multilayer stack would also be reflected. One solution to this problem is to suspend the multilayer structure in a fluid which is index matched to $\varepsilon_1$, contained
in a square holder, as is sketched in Fig. 6.8e, and demonstrated in Ref. [123].

Such a solution is not very practical if we want to use the angular filters to control the directionality of the emission of light emitting diodes for instance. However, emission of light in a light emitting diode usually takes place in a high index medium [124]. Therefore, by directly covering the LED with an angular filter, as is sketched in Fig. 6.8f, light will be able to couple to the Brewster angle. To prevent total internal reflection at the top interface, we propose a triangular outcoupler, index matched to the low index dielectric layer with $\varepsilon_1$, which maintains the angle of propagation, and steers beams of light in opposite directions at well-determined angles.

An interesting aspect of the multilayer structures is that all light not at the Brewster angle, or not TM-polarized, is reflected back to the LED. Scattering elements could be incorporated in the LED to redistribute light, such that initially reflected light is scattered into the Brewster angle, enhancing outcoupling at a fixed angle. Alternatively, if a material is used with a very high radiative emission, more exotic schemes such as photon recycling [125] might lead to further improved angular emission efficiency.
6.3 Dielectric angular filter applied for light emission

Figure 6.8: a,b, Transmission coefficient as a function of wavelength and angle of incidence for $\varepsilon_1 = 1$, $\varepsilon_2 = 2$. Shown is the transmission coefficient for TM (a) and TE (b) polarized light, for a supercell structure with $a_0 = 200$ nm and $r_0 = 1.2$. The Brewster angle is indicated by the vertical dashed line. c,d, Transmission for a stack with $\varepsilon_1 = 1.5^2$ and $\varepsilon_1 = 2.5^2$, again for TM (c) and TE (d) polarization. Here, $a_0 = 120$ nm and $r_0 = 1.15$. e, Experimental geometry used in [123], the multilayer stack is placed in an index matching fluid, and the sample is rotated with respect to the incident beam. f, Sketch of proposed geometry to control light emission using an integrated multilayer angular filter.