Hyperbolic surface wave propagation in mid-infrared metasurfaces with extreme anisotropy

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Abstract

Hyperbolic metasurfaces are characterized by an extreme anisotropy of their effective conductivity tensor, which may be induced at visible frequencies by sculpting metals at the subwavelength scale. In this work, we explore practical implementations of hyperbolic metasurfaces at mid-infrared wavelengths, exploiting devices composed of metals and high-index semiconductor materials, which can support the required field confinement and extreme anisotropy required to realize low loss hyperbolic surface waves. In particular, we discuss the role of broken symmetries in these hybrid metasurfaces to enable large and broadband hyperbolic responses spanning the entire mid-infrared wavelength range (3–30 µm). Our findings pave the way to the development of large scale nanophotonic devices to manipulate mid-infrared light, with applications in nonlinear optics due to the high field confinement, light routing at the nanoscale, thermal control and management, and sub diffraction imaging.

1. Introduction

While mostly used for far-field applications [1], metasurfaces have become of paramount importance also to control the guided propagation of electromagnetic (EM) waves on engineered surfaces for a wide range of applications [2–4]. An example of the extreme features enabled by metasurfaces for guided wave propagation is the phenomenon of hyperbolic surface wave propagation, which supports highly confined light with extreme enhancement of the local density of states. These surface waves are characterized by hyperbolic iso-frequency contours (IFCs) [5, 6], with strikingly different features compared to the closed IFCs that characterize surface waves supported by conventional materials and impedance surfaces. The open nature of hyperbolic IFCs implies extremely large light–matter interactions placed close to the surface. In addition, the group and phase velocities of hyperbolic surface waves are perpendicular to each other, offering peculiar propagation features, well suited for sub-diffraction imaging and negative refraction [7–10]. Compared to hyperbolic metamaterials [11], which provide similar features but in the bulk, hyperbolic metasurfaces (HMS) offer the additional advantages of reduced losses, since the wave propagates at the interface with free-space, and easier access to their features, both in terms of coupling to localized emitters and of accessing the hyperbolic modes from the exterior of the sample. The prominence of HMS has also led to a range of new applications, for example controlling the Coulomb force between atoms, enhancing EM interactions for radiation enhancement, light trapping, chemical sensing and Purcell enhancement [12–18]. For these reasons, HMS have been extensively studied in recent years both theoretically and experimentally in different frequency bands [5, 19–26].

To explore the possible implementations of HMS in different ranges of frequencies, we first recall that HMS are realized by tailoring the effective surface conductivity tensor $\sigma_{\parallel}$,
we present we propose the idea of broken symmetry in arrays of dimer gratings, and we show that when the
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we show the role of ultrathin gold stripes in fabrication, integration and tunability. The rest of the paper is organized as follows: in section mechanism to realize hyperbolic surface wave propagation in the mid-infrared range, more amenable to
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access to broadband extreme control of nanoscale mid-infrared light. Our work paves the way to a new
metal-backed dielectric substrate it is possible to tailor efficiently hyperbolic surface wave propagation and
conductivities compared to semiconductor composites \[ anisotropy of the lattice structure \[ naturally provide hyperbolic polariton propagation in the bulk around its phonon resonances, due to the
remained elusive, until recently thanks to the realization that phonon resonances can naturally provide
hyperbolic response of the surface \[ At near-infrared frequencies, patterned plasmonic surfaces have been explored \[ Visible range HMS were theoretically proposed and experimentally demonstrated exploiting these plasmonic phenomena in \[ and \[ respectively.

Despite significant past efforts and interest in these topics, HMS in the THz and mid-infrared range have remained elusive, until recently thanks to the realization that phonon resonances can naturally provide extreme anisotropy and hyperbolic responses in this regime. For instance, it has been shown that hBN can naturally provide hyperbolic polariton propagation in the bulk around its phonon resonances, due to the anisotropy of the lattice structure \[ Hyperbolic surface waves were enabled by patterning hBN in the form of subwavelength nanostrips \[ , or with patterned aluminum-doped ZnO, which exhibits a plasmonic response in the mid-infrared range \[ In parallel, unpatterned $\alpha$-MoO$_3$ has been recently found to naturally support in-plane phonon polariton propagation in the form of hyperbolic surface waves \[ , and twisted bilayers of this material were shown to enable reconfigurable surface wave propagation \[ , in which the twist angle can actually control the degree of hyperbolic response and even tune the response from elliptical to hyperbolic \[ .

We emphasize that the mid-infrared wavelength range is of great interest for chemical sensing, since it is the frequency range where the natural absorption response of several gas or liquid species lies \[ and both plasmonic and photonic metasurfaces in THz have been largely adopted for noninvasive spectroscopy, and improving sensing properties using toroidal moments \[ Moreover, the atmospheric transmission window lies mostly within this same frequency range, enabling access to thermal applications \[ While the mentioned approaches to realize hyperbolic propagation in this frequency range were based on phonon resonances of natural materials, metasurface approaches may provide more flexibility in terms of target frequency of operation and in tailoring the overall response. In this sense, patterned metasurfaces may provide an interesting yet unexplored opportunities to realize HMS also in this frequency range.

One of the main reasons that little studies have been presented so far is that metals at mid-infrared frequencies do not support appreciable plasmonic phenomena, since their real part of permittivity is too negative, Re($\varepsilon$) < $-1000$ \[ Therefore, the required condition for conductivity tensor in (1) cannot be achieved. Yet, the low loss of metals in this frequency range enables large field enhancements, well suited for nonlinear applications \[ . Needless to say, metallic metasurfaces have higher electrical and thermal conductivities compared to semiconductor composites \[ , which is an important advantage for various applications, e.g. thermal camouflage \[ .

Here we show that, by proper design schemes of three different metasurfaces engineered on a metal-backed dielectric substrate it is possible to tailor efficiently hyperbolic surface wave propagation and access to broadband extreme control of nanoscale mid-infrared light. Our work paves the way to a new mechanism to realize hyperbolic surface wave propagation in the mid-infrared range, more amenable to fabrication, integration and tunability. The rest of the paper is organized as follows: in section 2 we present high aspect ratio (AR) trenches made of metallic and dielectric gratings that show low-loss hyperbolic IFC. In section 3 we propose the idea of broken symmetry in arrays of dimer gratings, and we show that when the intracell spacing in the dimer is small enough the supported odd mode is characterized by hyperbolic IFCs over the entire mid-infrared range. Finally, in section 4 we show the role of ultrathin gold stripes in supporting hyperbolic surface waves.

\[
\bar{\sigma} = \begin{pmatrix}
\sigma_{xx} & \sigma_{xy} \\
\sigma_{yx} & \sigma_{yy}
\end{pmatrix}
\]  

(1)
2. Coupled optical waveguide arrays with high aspect ratios

High AR metallic structures have been extensively studied to realize EM wave absorbers and sensors, both theoretically and experimentally [48–50]. Here, we study these structures for their exotic surface wave propagation features. To start, we consider the structure shown in figure 1(a), a 2D metallic grating, i.e. extended to infinity along the y direction, with slit width w, height h and period p. The AR of this structure is \( \text{AR} = (p - w)/h \). We assume an AlN substrate with relative permittivity of \( 9 - 0.04i \), but other low-loss semiconductor materials may be also used, with thickness t and terminated by another metallic plane. The metal/dielectric metastructure can be seen as a dense array of coupled optical waveguides, with guided modes localized in the dielectric substrate. We use gold as the metal throughout the paper, with relative permittivity retrieved from experimental data [42], and we study the surface wave propagation at the metal/air interface on the top surface. Since this structure offers a strongly capacitive response for electric fields polarized along the x direction, and an inductive response in the y direction, we expect it to support hyperbolic surface waves over a broad frequency range. The presence of the substrate enables excitation of these modes, which then couple to the high AR slits to establish the hyperbolic response.

We performed an eigenmode analysis at the mid-infrared wavelength \( \lambda_0 = 6.5 \mu\text{m} \) and retrieved the IFC of this structure (see the caption for the optimized dimensions). The IFC shows the real part of the orthogonal wavenumbers \( k_x \) and \( k_y \) normalized to the free-space wave number \( k_0 \), and the results are shown by the solid black line in figure 1(b), while a cross section cut of the light cone is plotted in dashed blue. The hyperbolic topology of the surface modes can be easily identified from the IFC. They lie outside the light cone, ensuring that they are highly confined to the surface of the air metal interface. In addition, near the \( \Gamma \) point (\( k_y = 0 \)) the IFCs can be written as

\[
\frac{k_x^2}{k_0^2} - \frac{k_y^2}{k_0^2} = -1,
\]

defining a hyperbola. Figure 1(c) shows the ratio between the real and imaginary parts of the propagation constant varying \( k_x \), which determines the effect of loss [51]. For our design, this ratio approaches values from 14 to 26 as \( k_x \) changes from 0 to \( \pi/p \), implying a relatively long propagation distance for these hyperbolic modes, even in the limit of highly confined propagation. It is interesting to observe that this figure of merit grows as the fields get more confined to the surface, i.e. for larger wave numbers.

When surface waves propagate mainly along the y direction i.e. \( k_x \rightarrow 0 \), they experience the lowest coupling with neighboring slits, and the mode behaves almost as a conventional surface plasmon polariton (SPP) traveling at the interface between an infinite plasmonic material and free space. Indeed, the wavenumber of a conventional SPP [52]

\[
k_{\text{spp}} = k_0 \sqrt{\frac{\epsilon + 1}{\epsilon + 2}} \approx (1.0003 + 0.0001i) k_0
\]

where \( \epsilon \) is the metal permittivity, is in close agreement with the hyperbolic dispersion at \( k_x \rightarrow 0 \), but with larger loss due to the metal patterning, associated with the field confinement in the slits, which enhances the absorption compared to an unpatterned vacuum–metal interface [49]. One difference between the structured HMS and an ideal HMS is its nonlocality, i.e. the dependence of the effective conductivity on the wavevector, \( \sigma_{ij}(k_x, k_y) \), with \( i, j \) accounts for the principal axes. As a result, the IFCs are not perfect hyperbola over the whole range of \( k_x \), instead they become flatter for larger \( k_x \), as shown in figure 1(b). This is expected, since at the band edge the derivative of the band curve needs to be flat, due to the periodicity of the structure.
is the speed of light, located above the surface as shown in figure 2(a). The choice of a confined dipole source enables launching a large number of high-\(k\) waves, which are supported by the open IFCs shown in figure 1(b). The simulation for this setup displays hyperbolic surface waves characterized by four main beams/lobes originated at the source location \([5]\), as shown in the normalized log scale distribution of the induced electric field in figure 2(b). The fringes appear in a direction parallel to the wave vector \(k\), and perpendicular to the power flow and direction of propagation, given by the vector \(S\), as indicated in the figure. This property reveals that the wavevector \(k\) is perpendicular to the Poynting vector \(S\), one of the exotic features of the hyperbolic response. The beams propagate at angles corresponding to the IFCs shown in figure 1(b).

The structure shown in figure 2(b) has a slit width \(w = 50\) nm, and height \(h = 2000\) nm, yielding an AR 40:1. We next consider lower AR HMS for facilitating fabrication, testing two other configurations with ARs of 20:1, with a shorter \(h = 1000\) nm (figure 2(c)), and 10:1, with also a larger slit width \(w = 100\) nm (figure 2(d)). The lower AR leads to more coupling with spurious substrate modes, which are isotropic in nature, but overall, the hyperbolic mode is still well visible in these configurations.

3. Broken symmetry in coupled optical waveguide arrays

While the design studied in the previous Section does support hyperbolic surface wave propagation, it requires high ARs, which may be difficult to fabricate. Here we study another route towards hyperbolic surface wave propagation based on broken symmetry in coupled optical waveguide arrays with much smaller ARs. To shed some insights into the nature of this response, we employ coupled mode theory (CMT) to analyze a 2D periodic array of coupled optical waveguides with period \(p/2\) in the \(x\) direction and again invariant in the \(y\) direction. When we introduce a small translational shift in the \(x\) direction for each second waveguide, the resulting array contains supercells with double period, each containing two identical waveguides (a dimer), as shown in figure 3(a). Due to broken symmetry, each unit cell supports two eignemodes, defined by the supported current distributions as even and odd modes. The inset of figure 3(a) shows a sample geometry in which the green region denotes the dielectric substrate with permittivity \(\varepsilon = 9.4 - 0.04i\) and the yellow regions represent gold. For this structure, the calculated normalized current distributions \(I_j\) and electric field \(E_x\) for odd and even modes at the I’ point \((k_x = 0)\) are shown in figures 3(b) and (c), respectively. It is evident from the electric field distribution that the even mode is mostly localized inside the dielectric substrate, and decays very strongly in the air region above the dimer, as shown in figure 3(c). However, the odd mode fields have much more extent into the air region above the dimer, still decaying in the far-field. This property will be shown later as a useful asset for exciting surface modes above the substrate that will be mainly dominated by the odd mode. Additionally, given the same incident field exciting either the odd or even mode, the enhancement of the odd mode fields is larger than the enhancement for the even mode. This feature shows that odd mode is easier to excite than the even mode, and therefore it will dominate the near-field.

To evaluate the dispersion of this surface, we can write the CMT equations for the \(n\)th waveguide mode, 
\[
u_n^{(c,o)} = U_n e^{-jk_n^{(c,o)}z} e^{-\beta_n x}, \quad \text{where } k_n^{(c,o)} \text{ is the propagation constants for the even/odd mode with superscript}.
\]
(e) / (a), and $k_x$ is the wavenumber in the transverse $x$ direction, with its value is limited to the first Brillion zone, i.e. $-\pi/p < k_x < \pi/p$. The CMT equation reads

$$
\frac{d}{dy} u_{n}^{(e,o)} \approx k_{y_0}^{(e,o)} u_{n}^{(e,o)} + \kappa^{(e,o)} (u_{n+1}^{(e,o)} + u_{n-1}^{(e,o)}).
$$

(4)

Here we assume only nearest-neighbor coupling for each waveguide, with symmetric real coupling coefficient $\kappa$ for both sites $n-1$ and $n+1$, as shown in figure 3(a). We solve this problem for frequency $f$, for which the even/odd mode has propagation constant $k_{y_0}^{(e,o)}$ at the $\Gamma$ point ($k_x = 0$). The solution to this equation is

$$
k_{y_0}^{(e,o)} = k_{y_0}^{(e,o)} + 2\kappa^{(e,o)} \cos k_x p.
$$

(5)

For even modes, the coupling coefficient is positive, $\kappa^{(e)} > 0$, while it is negative for $\kappa^{(o)} < 0$, similar to the case of a 1D array of nanoparticles supporting guided modes [53], when the excited dipoles in the particles are transverse to the propagation direction (even mode), or when the dipoles are longitudinal to it (odd mode). Interestingly, due to the negative coupling coefficient of the odd mode, the resulting dispersion is hyperbolic near the $\Gamma$ point. A hyperbolic response based on negative coupling in waveguide arrays has been recently reported in [54]. However, this was done using periodic perturbations of the waveguide in the $y$ direction [54], whereas here we use broken symmetry in the array as a viable solution that makes it easier the fabrication and analysis.

We numerically calculated the IFCs for the even and odd modes supported by the geometry in figure 3(b) using full-wave simulations at the wavelength of $\lambda_0 = 6.5$ $\mu$m. The IFCs for the even and odd modes are shown in figure 3(c), additionally we plot the results from CMT in equation (5) using as fitting parameters the coupling coefficients $\kappa^{(e,o)}$ and $k_{y_0}^{(e,o)}$. The results show excellent agreement, manifesting the hyperbolic response for odd surface waves as predicted.

In order to show the nature of hyperbolic surface wave propagation on this metasurface, we excite it with a $z$-oriented electric dipole placed above the metasurface and calculate the response using full-wave simulations. In figure 4(a), the red arrows indicate the Poynting vector flow, showing that the power propagating along the principal axes ($x,y$) is almost vanishing in this case, and the beams are split into four clear directions with wavefronts perpendicular to the power flow, similar to figure 2(b). The $E_z$ component is plotted in the figure, with the inset zooming in the region close to the source right underneath the metallic pattern. In this region, we notice that the source also excites the even mode, which is however characterized by propagation mainly canalized along $x$, consistent with the flat dispersion in figure 3(c). In contrast, in the field above the metasurface, the contribution from the even mode is negligible, consistent with the modal configurations found in figures 3(b) and (c). This feature allows us to clearly access only the odd mode associated with a hyperbolic response.
It is interesting to study the response of the metasurface for different wavelengths in the mid-infrared range in order to understand the modal dispersion and the overall bandwidth over which we can expect a hyperbolic response. We calculated the IFCs at different wavelengths in figure 5(a). Indeed, across the whole mid-infrared range the IFCs of the odd mode are hyperbolic. Their hyperbolicity, defined by the curvature around the Γ point, increases for shorter wavelengths, which is expected because the normalized grating vector at the Brillouin edge becomes smaller, so there is more room for an increased $k_y$ component, still satisfying the dispersion relation of the dielectric substrate. This increased hyperbolicity makes the surface more suitable for negative refraction applications required for nanofocusing of surface waves.

The worst-case scenario in terms of propagation loss is expected for propagation along the $y$ direction, i.e. for $k_x = 0$. In figure 5(b) we plot the ratio between real and imaginary parts of $k_y$ in this scenario. We find enhanced propagation at shorter wavelengths, much larger than what obtained at visible frequencies in HMS based on metallic gratings [6]. Compared to the previous design in section 1, the figure of merit in this design is significantly larger, as expected due to the reduced thickness of the metal, so that the mode resides more within the low-loss substrate, offering exciting opportunities for hyperbolic surface wave propagation, both in terms of bandwidth and resilience to loss.

4. Thin gold strips

Finally, we show a third metasurface geometry that can support hyperbolic surface wave propagation based on thin strips of gold. Structured nanostrips of graphene has been explored to realize HMS in the far-infrared spectrum, around the wavelength of 30 $\mu$m [5]. The advantage of graphene over metal resides in its electrical tunability using a variable gate voltage. However, the graphene conductivity under reasonable gating voltages is low compared to thin metallic strips in the mid-infrared regime [5], which makes thin metals more appealing for the design of HMS. For example, the conductivity of gold thin sheets with thickness $t$ can be written in terms of the Drude permittivity of gold as

$$\sigma_{\text{sheet}} = (i\omega\varepsilon_0 (\varepsilon_{\text{Drude}} - 1)) \times t [S]. \quad (6)$$
Graphene conductivity, on the other hand, is given by Kubo formula \([56]\), and for a chemical potential \(\mu_c = 0.3\) eV we obtain \(\sigma = (0.009 - 0.108i)\) [mS] at \(\lambda_0 = 6.5\) \(\mu m\). At the same wavelength, the conductivity of a thin sheet of gold with \(t = 2\) nm is \(\sigma_{\text{sheet}} = (2.4 - 9.6i)\) [mS], roughly 100 folds larger than the one of graphene, as shown in figure 6(a). To determine the optimal thickness of gold, we choose our wavelength of operation \(\lambda_0 = 6.5\) \(\mu m\) and evaluate the transmission in the setup shown in figure 6(b), comparing full-wave simulations, with the prediction using the conductivity model \(\sigma_{\text{sheet}}\). The results, shown in figure 6(c), show that the conductivity model can be applied up to a thickness of 5 nm, after which the gold layer becomes totally reflective and cannot support surface waves.

Next, we designed a metasurface consisting of parallel thin gold strips, as shown in the inset of figure 7(a). We simulated three different structures with fixed periodicity \((p = 400\) nm\) and filling factor (width of strip is fixed to \(w = 300\) nm) but variable thickness, \(t\). As seen in figure 7, a lower thickness enables larger \(k\) values but also increased loss. For a thickness \(t = 5\) nm, the IFCs display nearly flat propagation, corresponding to canalization of surface waves, i.e. they propagate in a diffraction-free path along the \(y\) axis. Another important feature of the proposed metasurface can be observed from the loss response as \(k_x\) increases. In contrast to the high AR metallic structures presented in section 1, the figure of merit here increases with larger \(k_x\), which can be justified evaluating the field for the two extreme values \(k_x \to 0, \pi/p\) as shown in the inset of figure 7(b). When \(k_x \to 0\), the field decays towards the surroundings of the thin strips at a much lower rate than when \(k_x \to \pi/p\), i.e. the field is more confined to the lossy metals when \(k_x \to \pi/p\), therefore causing larger losses.

5. Summary

In summary, we presented three different routes to realize HMSs in the mid-infrared band. The high AR metallic grating with small gap widths shows pronounced hyperbolic response and low loss. The dimer grating structure supports both anisotropic and hyperbolic modes, which can be selectively excited and routed in different directions. Additionally, we have shown an ultrabroadband response spanning across the entire mid-infrared range for this design. Finally, thin strips of gold separated by small gaps emulate the response of graphene HMS, extending it to the mid-infrared range, with a better resilience to loss. The gold strips support a broadly tunable IFC response and larger field confinement compared to other two designs,
which makes it interesting for various applications, provided that the required thickness can be implemented successfully in fabrication. In this work, we have considered conventional semi-conductors for the dielectric region in all the metasurface designs, and we expect that similar responses may be found exploiting multi-quantum well (MQW) substrates, as those recently used to enable metasurfaces with giant nonlinear responses [44]. We expect exciting opportunities stemming from combining the enhanced, broadband light–matter interactions associated with hyperbolic surface wave propagation demonstrated in this work with the giant nonlinearities available at mid-infrared frequencies in MQWs.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Conflict of interest

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