Backward surface waves at photonic crystals

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We investigate wave propagation with opposite energy and phase velocity at the surface of a two-dimensional photonic crystal. We introduce a surface defect based on a terminating row rich in material. We show how this type of defect induces surface modes with dispersion that can be flexibly manipulated. We observe the formation of single or multiple surface bands coming from the upper periodic band with a negative or a positive band slope. We perform a numerical experiment, realizable at mid- and near-infrared frequencies, which unambiguously verifies in a direct fashion the forward or backward type of propagation of the excited surface wave. Our numerical results demonstrate the existence of backward-propagating surface waves stemming from bands with a negative slope. This study may aid the design of subdiffraction plasmon based guiding devices.

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The advent of photonic crystal (PC) materials1–2 spurred a lot of interest toward the existence of surface modes at the interfaces of such materials.3–6 These modes remain localized around the PC surface in a manner similar to surface plasmons on metal slabs.7 The first experimental observation of such photonic crystal surface waves came by Robertson et al.3 In the experiment, the authors employed a standard attenuated total reflection setup, widely used for surface-plasmon observations on metals.8 The majority of the subsequent theoretical studies focused on the existence of such surface modes in various PC structures. It was found that the frequency and in many cases even the mere existence of PC surface waves are strongly influenced by the way the periodic PC is terminated.2,4,5 Nevertheless, the initial acute interest for PC surface modes had somewhat subsided until recently. The need to understand and engineer PC surface phenomena,3–6 one aspect of the PC surface-wave propagation remains unexplored. In negative index metamaterials, uniform15 or composite16–18 energy and phase propagate in opposite direction, a phenomenon known as backward wave propagation.19,20 Recent studies showed that under certain conditions,21 photonic crystals can behave in many respects like the Veselago15 negative index medium,22–24 thus supporting backward wave propagation. A backward type of propagation inside a PC or other left-handed media can be identified experimentally only indirectly by observing the transmitted field distribution through a material-wedge structure.23,25 It is certainly most interesting to search for backward-propagating PC surface modes. First, the directionality of the modes is pertinent to surface-plasmon-based guiding structures26 and related optical devices. But more importantly, the possibility of the electromagnetic field detection around the PC surface with a local probe enables the direct demonstration of the backward wave propagation phenomenon.

In this paper, we investigate numerically the existence of backward surface waves at the surface of a photonic crystal. We propose an experimental setup, realizable at both microwave and visible frequencies, which unambiguously verifies in a direct fashion the type of PC surface-wave propagation (forward or backward). We create the PC surface mode through a defect row located at the PC surface.26,27 We employ a surface defect consisting of a one-dimensional lattice with a basis of two or more elements. Such complex type of defect, with structural elements identical to the bulk-PC sites, holds many advantages. In fact, it involves many modifiable parameters to permit flexible manipulation of the surface mode and provides routes for PC-surface-mode dispersion engineering. Furthermore, patterning these types of surface defects on mid- and near-infrared PC structures28,29 is much easier than patterning a surface row with specific termination.2–5

We search for surface modes at the surface of a square two-dimensional PC, consisting of cylindrical alumina (=9.3) pillars in air, with radius r=a/6, with a being the lattice constant. We take the electric field to be parallel to the pillars [E (TM) polarization]. We employ a two-dimensional finite difference frequency domain (FDFD) technique based on the solution of Helmholtz’s equation on a spatial grid lattice.31 The application of Bloch boundary conditions yields a solvable N×N system of equations, where N represents the total number of grid points within the numerical lattice. This system can be transformed into a generalized eigenvalue equation problem. The eigenvalues provide the dispersion relation ω(kx), where kx represents the wave vector along the PC surface and perpendicular to the pillars. Conversely, the eigenvector for a specific eigenvalue, ω(kx),
inset of Fig. 1. We find one PC-surface-mode band indicated corresponding supercell used in the FDFD method in the left dimer, composed of pillars identical to the pillars of the bulk formed by substituting each site on the upper PC row with a squared in the lower inset of Fig. 1. Indeed, we observe high we also plot the spatial distribution of the electric field /H20849 computational space is discretized with a grid cell and bottom PC row. In all the subsequent calculations, the specific value of the wave vector /H20648 mode lies below the lightline and within the band gap. For a second band of the periodic PC. As expected, the surface gives the field profile of the corresponding mode. We note that the presence of the surface breaks the translational symmetry in the normal direction. Accordingly, we must consider a supercell\(^5\) that spans the entire FDFD computational domain. This supercell consists of only one unit cell along the lateral direction, where translational symmetry still applies. Nevertheless, several PC sites (including the defect) embedded in air should be taken along the normal direction. The number of sites, as well as the length of the air space on the top and bottom of the terminating PC sites, must be sufficient\(^32\) to disallow any mode coupling between the top and bottom PC row. In all the subsequent calculations, the computational space is discretized with a grid cell \(a/21 \times a/21\) large.

We first explore a type of a surface defect which can be formed by substituting each site on the upper PC row with a dimer, composed of pillars identical to the pillars of the bulk PC and oriented along the lateral direction. We show the corresponding supercell used in the FDFD method in the left inset of Fig. 1. We find one PC-surface-mode band indicated with the solid line in the figure. The straight line represents the lightline, and the dashed lines the limits of the first and second band of the periodic PC. As expected, the surface mode lies below the lightline and within the band gap. For a specific value of the wave vector \(k_\parallel\) indicated with the arrow, we also plot the spatial distribution of the electric field squared in the lower inset of Fig. 1. Indeed, we observe high field values and confinement around the surface. It should be noted that our FDFD calculations reveal that the surface mode shown in Fig. 1 is pulled down from the second band (air band). On the other hand, we checked that defects arising from a material deficient\(^33\) upper row in the same type of periodic PC are pushed up from the first band (dielectric band). In other words, PC surface modes act like bulk-PC defects with the addition or removal of material. The surface band shown in Fig. 1 arises from the addition of alumina at the surface and is thus analogous to semiconductor donor states.\(^2,34\)

It is interesting to examine how the surface band shown in Fig. 1 can be tuned. In the corresponding dimer type of defect, the distance between the defect row and the rest of the bulk PC equals one lattice constant, \(a\). We can modify this distance or alter the separation between the two pillars composing the dimer defect or both. Our calculations show that as the separation between the dimer cylinders increases, the surface band drops in frequency until it touches the upper limit of the first band. For large \(k_\parallel\), the mode practically coincides with the periodic PC band edge.\(^35\)

Now, we investigate the surface-band behavior as the distance between the dimer defect and the periodic PC shortens. To be specific, we take the defect-PC separation equal to \(a/2\) and find a surface band with negative slope similar to the one shown in Fig. 1 but also a second nonmonotonic band at lower frequencies. If we decrease further the separation to \(a/3\), we find again two bands: one with negative slope like the one in Fig. 1 and one with positive slope appearing at higher frequencies. We plot the results in Fig. 2 for the latter case along with the supercell taken in the FDFD method. Note that the defect row in this case has touched the first row of the periodic PC. Thus, it forms a composite defect together with the first bulk-PC row. That is to say, this striking behavior of the surface band stems from a three-pillar defect, as seen in the supercell of Fig. 2. We also depict the field distributions for two different modes lying in the respective bands specified by the arrows in the figure. The spatial profile shown corresponds to the square of the magnitude of the electric field. The mode belonging to the lower PC-surface-mode band with negative slope has a substantially different configuration from the mode for the higher PC-surface-mode band with positive slope. We note that it is also entirely possible to excite laterally propagating (guided) waves.
through a single array of alumina-rod dimers or trimers, even
without the presence of the underlying periodic PC. These
modes are analogous to waveguide modes through silver
without the presence of the underlying periodic PC. These
through a single array of alumina-rod dimers or trimers, even
or even the number of related surface-mode band
that we can induce a change in the frequency location, slope,
defect. By rotating the dimer axis around the surface, we find
that they also depend on the orientation of the dimer
dispersion.

We examine further the properties of the dimer defect and
find that they also depend on the orientation of the dimer
defect. By rotating the dimer axis around the surface, we find
that we can induce a change in the frequency location, slope,
or even the number of related surface-mode band(s). Our
numerical results imply that a dimer oriented perpendicularly
to the surface induces a surface mode with positive band
slope that is pulled down from the air band. Surface bands
reported thus far, which emanate from a material deficient
terminating row, are pushed up from the dielectric band and
have a positive band slope. Here, we found two distinct cases
of PC-surface-mode bands which emanate from a dimer sur-
face defect oriented laterally and normally, respectively.
Both these surface bands drop from the air band but their
respective slopes have opposite signs. Correspondingly, there
is no correlation between the kind of surface band (donor or
acceptor) and the respective slope of the band. However, the
electric field maps of the surface modes in all these different
cases reveal a noteworthy correlation. This is illustrated in
Fig. 3 for four different cases. Figure 3(a) depicts the electric
field corresponding to the surface-mode band of Fig. 1. Fig-
ure 3(b) depicts the electric field for a surface mode emanat-
ing from a dimer defect oriented perpendicularly to the PC
surface. The field depicted in Figs. 3(c) and 3(d) corresponds
to the lower and upper respective surface bands, which arise
from the trimer-type defect of Fig. 2. We observe that the
electric field of a positive-band-slope donor surface mode
flips sign when crossing the mid-defect plane. On the con-
trary, the electric field of a negative-band-slope donor
surface mode retains its sign when crossing the mid-defect
plane. It is not surprising that surface-mode field profiles
with evenlike and oddlike symmetries in respect to the inter-
face lead to bands with a different band slope. Actually, the
band slope can be expressed as a function of the electric field
with the aid of the $k \cdot p$ perturbation method.21,37 We found in
general that evenlike modes can favor a strong negative con-
tribution in such an expression, thus yielding a negative band
slope. This is not the case with oddlike modes, which lead
accordingly to a positive band slope.

In periodic PCs, previous studies21,23 demonstrated that a
negative band slope leads to a backward-propagating
Floquet-Bloch wave. In particular, the Floquet-Bloch mode
gains consistently a constant phase while traveling from one
unit cell to the next, throughout the photonic lattice.21 The
sign of this phase coincides with the sign of the correspond-
ing band slope and signifies a parallel (when positive) or
antiparallel (when negative) relation between phase and en-
ergy velocities (for isotropic dispersion in wave vector
space). To our knowledge, it has not been thus far demon-
strated how the slope of a PC surface band relates with the
type of propagation (forward or backward). In order to in-
vestigate, we propose the following experiment described in
the schematics of Fig. 4. We implement such experiment in
the two-dimensional finite difference time domain (FDTD)
method with perfect matched layer (PML) absorbing bound-
ary conditions.39

We place a 45° isosceles Plexiglas prism on top of the
photonic crystal face with the surface defect. A Gaussian
beam with a wide waist is launched from the top right side of
the prism and creates an evanescent wave that can excite the
surface mode. We employ a pulsed signal with central fre-
quency tuned to be around the midgap of the periodic PC
(i.e., $\frac{\omega}{c}=0.41$). Subsequently, we monitor the time evolu-
tion of the electric field at different detector points. We then
apply a fast Fourier transform (FFT) to the signal at each of
these points and normalize it by the respective spectrum of
the source. The first detector consists of one point placed just
above the middle of the left side of the Plexiglas prism, as
seen in Fig. 4. In the absence of any surface states, we would
expect a normalized intensity strength of about 0.90.41 Now,
This means that a signal detected by the second set of detectors created by the input beam points toward the left and must be enhanced along the surface normal. The parallel wave vector $k_{\parallel}$ of Fig. 4 can be realized in corresponding systems operable in microwave or infrared and visible frequencies. A monopole antenna or a scanning near-field optical microscopy (SNOM) tip can serve as the localized detector probes in each side of the photonic crystal.

We have performed the numerical FDTD experiment described above for the defect cases of Figs. 1 and 2. We plot the Fourier transformed signal arriving at the first detector in Figs. 5(a) and 6(a), respectively. Correspondingly, the signals recorded by the second and third sets of detectors are shown in Figs. 5(b) and 6(b). The exact location and size of the two line detectors in each set, at each side of the photonic crystal, are also depicted. The vertical lines in the figures designate the frequencies of the surface modes predicted previously by the FDFD method. Notice the remarkable agreement between the dips in Figs. 5(a) and 6(a) and the calculated surface-mode frequency values. Also, the signal strength around these dips is quite close to the rough estimate we just made above. The small discrepancy is due to the beam divergence of the finite width Gaussian beam. Now, for the case of Fig. 1, we observe a strong signal recorded by the third set of detectors at the expected frequency providing firm evidence for backward wave propagation. The enhanced intensity value of this signal in comparison with the intensity of the input beam is a lensing type of effect. We have a wide cent wave to a narrow beam tight around the dimer-defect edge. Our numerical experiment outlined in the schematics of Fig. 4 can be realized in corresponding systems operable in microwave or infrared and visible frequencies. A monopole antenna or a scanning near-field optical microscopy (SNOM) tip can serve as the localized detector probes in each side of the photonic crystal.

We remind the reader that the PC-surface-mode band has negative slope in this case. This ascertains that similar to the case of the bulk PCs, a PC-surface-mode band with negative slope implies a backward-propagating surface wave. However, we also see in Fig. 5(b) that the second set of detectors also records a signal with strength about 5% the signal recorder by the third set of detectors. We alert the reader that by no means, this would imply a contribution of a
forward-propagating wave. After examining carefully the time evolution of all detected field, we see that all the results are caused by a superposition of a first signal caused by the initial beam, and a second signal caused by multiple reflections at the prism surfaces. It is the second signal which generates the fringes in the spectra of Figs. 5(a) and 6(a). A simple geometric ray tracing will show that this second signal contributes a $k_s$ same in magnitude but opposite in sign in respect to the original $k_i$. Therefore, a backward surface wave excited by this second signal would arrive in the second set of detectors, hence the corresponding small signal peak. Our arguments are supported by the relative magnitude of the two signals which is consistent with a rough estimate made from Fresnel-type formulas.\textsuperscript{45,46} Also, the results shown in Fig. 6 establish the backward (forward) wave propagation for the first (second) mode with the negative (positive) band slope for the cases of Fig. 2. Again, the smaller humps at the same frequency are from the second multireflected signal and should not be taken into account when determining the directionality of the surface wave.

To conclude, we have investigated a dimer defect for the surface of a two-dimensional photonic crystal consisting of the same pillars as the bulk PC. Many characteristics of this type of defect can be altered, such as separation between the dimer pillars, orientation in respect to the surface, etc., leading to flexibly engineered surface-wave bands. We identified two kinds of surface bands with a positive or a negative band slope. We have verified with a numerical experiment the existence of backward-propagating surface waves, arising from surface-wave bands with a negative band slope. Our suggested defect configuration can be implemented at corresponding structures operating at the near-IR and visible frequencies. Thus, we believe that it has potential for subdiffraction surface-plasmon-based waveguiding at these frequencies, which is recently attracting increasing attention.\textsuperscript{26,47,48}

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\bibitem{supercell_microwaves} The PC should be thick enough so that the field values in the last PC row are small in comparison with the field values in the top surface row. In addition, the air space on top and bottom of the PC should be sufficient to prevent the decaying fields emanating from the top defect row to hit the bottom of the PC. (The space directly above the top edge of the supercell continues directly above its bottom edge.)
\end{thebibliography}
The terminating upper row consists of infinite-height pillars of truncated cross section equal to $1/4$, $1/2$, and $3/4$ of the regular circular cross section.


An additional band may pull out from the second band as well but lies too close to the second PC band.


Making a rough estimate from Fresnel-type formulas, the electric field intensity at the exit of the prism should be about $(\frac{4n}{(n+1)})^2$, where $n=1.60$, represents the refractive index of the prism.


The photonic crystal edge is more than ten free space wavelengths away from the prism edge. This ensures that any near field stemming from the prism edge cannot directly influence the field in the vicinity of the PC edge.


A beam reflected from the second side of the prism would have an intensity $(n-1)^2/(n+1)^2 \sim 0.05$, smaller than the intensity of the beam arriving originally at the base of the prism.
