Probing light emission at the nanoscale with cathodoluminescence

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We measure polarization- and wavelength-resolved spectra and spatial emission intensity distributions from silicon photonic crystal waveguides in the near-infrared spectral range using spectroscopic cathodoluminescence imaging polarimetry. A 30 keV electron beam acts as an ultra-broadband and deeply subwavelength excitation source. For a photonic crystal waveguide with a period of 420 nm and a hole radius of 120 nm, we observe a dominant emission intensity distribution that is confined to the waveguide for a wavelength of 1425 nm. The polarization-resolved measurements demonstrate that this feature is fully linearly polarized along the waveguide axis. Both the modal pattern and polarization correspond to the odd TE waveguide mode of the system, which is confirmed by good qualitative agreement with calculations of the modal field profiles. From the emission directionality, we conclude that we sample a leaky portion of the odd waveguide mode and that it is not fully guided within the photonic crystal waveguide.
9 NIR spectroscopic CL polarimetry on silicon photonic crystal waveguides

9.1 Introduction

Photonic crystals, materials with a periodically varying dielectric function, can manipulate the propagation of light in a controlled way. They create a photonic band gap that prevents light from propagating in certain directions for certain frequencies [12, 16, 319–321]. Photonic crystal cavities can reach very high Q-factors to achieve strong light-matter interactions [15, 322, 323] and can be used for low threshold lasers [47, 324, 325]. Photonic crystal waveguides can serve as building blocks in photonic integrated circuits, such as splitters, switches, and multiplexers [326–328]. The modes in such waveguides are strongly dispersive and can slow down light, enhancing light-matter interactions [13, 14, 328–333]. To fully exploit the many applications of photonic crystal waveguides, it is essential to measure the propagation and confinement of light at a subwavelength scale. This cannot be achieved by conventional microscopy techniques. Near-field scanning optical microscopy (NSOM), which uses subwavelength probes or apertures to detect or scatter the near field of these structures [334–339], has enabled measurements of the field components of the optical near field just above the waveguide [77, 340, 341].

Here, we use cathodoluminescence (CL) spectroscopy to study silicon photonic crystal waveguides in the near-infrared (NIR) spectral range, coupling to and probing the field distributions inside the waveguide. In CL, a high-energy electron beam is used as a nanoscale optical excitation source in which the time-varying field of the electron couples to the local modes of the system as it traverses the sample [92, 124] (see Chapter 3). In CL, light scattered from these modes to the far field is then detected. The short interaction time of the electron with the structure (a few fs) results in a broadband excitation spectrum. The high excitation resolution of CL is only limited by the extent of the electric field about the electron trajectory and the spread of the beam in the sample. This allows one to explore the radiative local density of states (LDOS) at deeply subwavelength scales [105, 124]. Recently, it has become possible to measure the full polarization distribution of CL emission as a function of angle by using polarimetry [132, 259]. These properties have made CL a powerful, deeply subwavelength characterization technique [101, 102, 139, 179, 181, 182, 185, 194, 196], allowing measurements of the confinement and dispersion of plasmonic and dielectric photonic crystal cavities in the visible spectral range [124, 136, 195, 342].

In this article, we apply spectroscopic cathodoluminescence imaging polarimetry in the NIR spectral range to study the confinement and polarization of propagating photonic crystal waveguide modes. These structures possess different band structures for TE and TM polarization and support two modes for TE polarization, denoted as even and odd [321, 343, 344]. We demonstrate that CL imaging polarimetry enables direct identification and spatial mapping of the modal field distributions in the photonic crystal waveguides. The measurements show good agreement with calculations of the modal field intensities. We find that the CL emission is dominated by the odd TE waveguide mode. The results presented here
demonstrate the ability of CL to measure the spatial, spectral and polarization dependence of emission from complex nanophotonic structures in the near-infrared spectral range.

9.2 Experiment

Silicon photonic crystal waveguides (PCWGs) were fabricated on silicon-on-insulator (SOI) wafers with a 220 nm thick silicon layer on top of a 1 µm silica layer on a silicon substrate. Electron beam lithography was used to pattern the waveguides, followed by reactive ion etching to etch through the top silicon layer. A wet HF etch was used to remove part of the silica layer and obtain a suspended PCWG. Reference measurements in the visible and near-infrared spectral ranges demonstrate that a residual silica layer remains, since we observe characteristic silica defect-related emission peaks. Two different samples were studied; here we only discuss sample 1, showing data for sample 2 in the Supporting information. Figure 9.1(a) shows a SEM image of one of the PCWGs on sample 1 examined here, with a length of 90 µm and a total width of the photonic crystal section of 10 µm (25 periods). The PCWG is composed of a hexagonal array of holes with one missing row of holes (W1 waveguide) [321, 344, 345]. Five waveguides were made on sample 1 with the same period a=420 nm and hole radii varying in the range ∼105–125 nm. Figure 9.1(b) shows a close-up of the waveguide section for the most studied structure (denoted as WG2), which has a period a=420 nm and a hole radius r=120 nm.

The TE band structure of WG2 is shown in Figure 9.1(c), calculated using the MPB software [346]. TE polarization corresponds to electric fields that are oriented in the plane of the waveguide slab at z=0. The gray bands represent modes that make up a continuum below and above the photonic band gap, which opens up between normalized frequencies of ∼0.25–0.32, corresponding to free space wavelengths of ∼λ_0=1300–1700 nm. The discrete bands at the lower right are index-guided bands [321]. These are confined by total internal reflection in the slab in all directions since the waveguide itself has a higher average permittivity than the surrounding environment. The band structure is very sensitive to the period, hole size and slab thickness [347].

Removing rows of holes leads to allowed modes within this bandgap [343–345, 348], that are confined vertically by index-guiding (total internal reflection), but horizontally by the band gap of the photonic crystal. For a single row of missing holes there are two TE waveguide modes in the band gap: an even mode with a symmetric field distribution and an odd mode with an anti-symmetric distribution for the in-plane electric field component perpendicular to the propagation direction [329, 343]. The even mode has been studied intensely due to its anomalous dispersion and vanishing group velocity at the edge of the Brillouin zone [13, 326, 328–330, 332]. The odd mode is less well studied, but also displays slow light over a broad range of wavevectors. The dashed line in the figure represents the light
Figure 9.1 – (a) Scanning electron micrograph of one of the silicon photonic crystal waveguides on sample 1 studied here. A 90 µm long, 10 µm wide, and 220 nm thick waveguide with a hexagonal lattice of holes is suspended above a substrate of silica on silicon. (b) Close-up micrograph of waveguide WG2, with a period of a=420 nm and a hole radius of r=120 nm. (c) Band diagram of the waveguide from (b), for TE polarization, showing a selection of modes. The gray lines denote modes that are in the continuum of available modes above and below the photonic band gap. Within the band gap we distinguish an even (blue) and odd (red) waveguide mode. The black dashed line corresponds to the light line of air. (d) Schematic of the cathodoluminescence spectroscopy system. The 30 keV electron beam excites the sample, a parabolic mirror collects the emitted radiation and directs it to an optical setup where we can focus the light onto a fiber connected to a NIR spectrometer. We can also filter the emitted beam with a slit and measure the full polarization state using a QWP and linear polarizer. The coordinate system is also shown, with the PCWGs oriented along the y-axis for all measurements in the main text.

In addition to TE modes, the photonic crystal possesses TM modes, with an electric field perpendicular to the waveguide slab at z=0. Such modes are usually excited efficiently by CL, since the moving electron acts as a vertically polarized source. In Figure 9.9 of the Supporting information we show the band structure for line in air; modes to the left will be leaky and modes to the right are guided in the waveguide slab.
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TM polarization. We find that there is a small photonic band gap for wavelengths in the range $\sim \lambda_0=1100–1200$ nm with two waveguide modes within. In the spectral range of the TE band gap, the TM band structure exhibits a continuum of modes. Modes inside or near the band gap are usually localized to the waveguide, while modes in the continuous bands are more delocalized over the photonic crystal [321, 343]. The PCWGs studied here are specifically designed for high quality TE modes rather than TM modes. There are thus multiple possible sources of emission, for both TE and TM polarization, when exciting these Si PCWGs with swift electrons.

Figure 9.1(d) shows a schematic representation of the CL setup [124, 128, 183]. The 30 keV electron beam excites the sample and a parabolic mirror collects the subsequent emission and directs it onto a fiber connected to a NIR spectrometer. The small size of the electron probe and precise scanning capabilities of the SEM allow us to perform spectrally- and spatially-resolved scans of the PCWGs. We also measure the spectrally-resolved polarization of the emission by adding a movable, vertical slit to the optical path. In general, the polarization of the emitted radiation can change as it reflects off the mirror, due to its curved shape. The slit selects the central part of the mirror and thus conserves the emission polarization [129, 130], integrating over zenithal angles for a narrow range of azimuthal angles. We perform measurements for different positions of the slit and orientations of the waveguide with respect to the mirror to determine the polarization state and emission directionality (see Supporting information). We combine a quarter-wave plate (QWP) and linear polarizer (Pol.) to determine the Stokes parameters, which fully describe the polarization state of the emitted light [131, 132]. This allows for the separation of polarized and unpolarized light, as well as the retrieval of different field components and the relative phase difference between them [131]. The Methods Section describes the experimental setup and measurement protocol in more detail. For the measurements described in the main text, all waveguides are oriented along the y-axis, as defined by the coordinate system in Figure 9.1(d).

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Figure 9.2 shows 2D spatial CL intensity maps from WG2, at wavelengths of $\lambda_0=1170$ nm (a), $\lambda_0=1185$ nm (b), $\lambda_0=1400$ nm (c), and $\lambda_0=1425$ nm (d), all averaged over a 20 nm bandwidth. Combining the raw data with the spectral response of the system and in-situ beam current measurements allow us to determine the CL emission probability (number of photons emitted per incoming electron, per unit bandwidth of nm$^{-1}$) [119]. We additionally correct the data for the dark response of the detector as well as for signal from the remaining silica and the silicon substrate, which contributes a broadband response and a peak at $\lambda_0=1275$ nm. To do so, we use a reference spectrum measured in one of the holes, which has no contribution from the waveguide or photonic crystal modes. In the Supporting information, we show additional measurements for a sample with a different period (Figure 9.6),
for the input section of WG2 (Figure 9.7) and for WG2 in the visible spectral range (Figure 9.8).

The measurements at $\lambda_0=1170$ nm and $\lambda_0=1185$ nm (Figures 9.2(a,b)), exhibit an overall similarity, with high intensity at the inner edges of the holes lining the waveguide and darker spots along the waveguide at positions in between four holes. These two positions are denoted as A and B in Figures 9.2(a,c). Figure 9.2(b) exhibits a distinct enhanced intensity at the edges of the holes outside of the waveguide, compared to Figure 9.2(a). Figures 9.2(c,d) show data at $\lambda_0=1400$ nm and $\lambda_0=1425$ nm, displaying a high intensity at the inner edges of the holes lining the waveguide, which wrap around the hole edges more than for the data at shorter wavelengths. The center of the waveguide exhibits high intensity features
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at positions that were dark for $\lambda_0=1170$ nm and $\lambda_0=1185$ nm. At $\lambda_0=1425$ nm these peaks are most intense, while the region around the waveguide has a lower relative intensity than for $\lambda_0=1400$ nm. The fact that the signal for $\lambda_0=1425$ nm is very strongly confined to the waveguide suggests it is related to a waveguide mode.

The features at $\lambda_0=1170$ nm and $\lambda_0=1185$ nm occur in the upper band of the TE band structure (see Figure 9.1(c)), that represent modes that are delocalized over the waveguide and surrounding holes [321, 343], as seen in Figures 9.2(a,b). In addition to the TE modes, the TM modes can also be responsible for this measured emission. As Figure 9.9 of the Supporting information shows, there is a small TM photonic band gap for wavelengths in the range $\sim \lambda_0=1100$–$1200$ nm with two waveguide modes within. The emission patterns at $\lambda_0=1400$ nm and $\lambda_0=1425$ nm occur in the middle of the TE photonic band gap, where the even and odd waveguide modes are present. For TM polarization these wavelengths are in the continuum of modes below the band gap, where one expects modes that are more delocalized from the waveguide, unlike the patterns observed here that are quite strongly confined to the waveguide. In order to distinguish between TE and TM modes, we perform polarization-resolved measurements and calculations of the different electric field components.

Figure 9.3 shows calculations of the electric field intensity distributions (summed over all $\omega$ and $k$ within the given frequency range) for the odd and even TE polarized modes at $\lambda_0=1450$ nm, using the MIT Photonics Band (MPB) code. For more details about the calculation procedure, see the Methods Section.

Figure 9.3 – Calculation of the modal intensity distributions of the two waveguide modes in the photonic band gap shown in the band structure diagram of Figure 9.1, for $\lambda_0=1450$ nm. (a) displays the odd mode and (b) the even mode. We calculate the $E_x$, $E_y$ and $E_z$ field components as a function of position and wavevector within a small frequency range, then integrate over all $k$ and field components to obtain $\sum |E|^2$. The modal field intensities are normalized to the maximum intensity for all polarizations and wavelengths (obtained for TE at $\lambda_0=1500$ nm, not shown here). We note the strong difference in intensity between the two modes. The white circles show the positions of the holes.
Excellent agreement is observed between the data and the odd TE waveguide mode. TM-polarized calculations in the range $\lambda_0=1430–1500$ nm are shown in Figure 9.9 of the Supporting information, but exhibit no sharp features such as the ones on display in the measurements. Calculations in the range of the TM band gap ($\lambda_0=1100–1200$ nm) were not possible due to computational constraints related to higher order modes in the vertical direction.

The electron beam principally couples to field components that are parallel to the electron trajectory. For electrons propagating along $z$, this should lead to preferential coupling to the TM modes, yet we clearly observe TE modes. Our 2D calculations for TE polarization are performed at $z=0$, where $E_z$ is strictly zero. The membrane does have a finite thickness, however, so $E_z$ has nonzero components for other heights [321]. We can, for example, expect vertical components at the edges of the holes [77]. Considering the high intensity in the middle of the waveguide, the even mode is symmetric with respect to the center, for the in-plane field component perpendicular to the waveguide axis, so it is expected to remain in-plane. The odd mode however is anti-symmetric, exhibiting a field gradient and a pole at the very center where the field switches sign. This flip in the fields can be accompanied by a nonzero $E_z$ component in the center for different heights, explaining why we preferentially measure the odd mode.

Another source of coupling between the electrons and the TE modes is the fact that scattering of the incident electrons inside the silicon membrane leads to a spread in their propagation directions, allowing for direct coupling to in-plane field components [124]. The scattering increases for lower electron energies, which should result in stronger coupling to the in-plane components. We do indeed observe higher intensities from the modal peaks using 10 keV instead of 30 keV (not shown here), indicating that the broadening electron distribution increases the coupling to TE modes.

### 9.4 Spectroscopic polarimetry

To further confirm the TE nature of the measured modes, we study the polarization-filtered spectral response of the waveguide. First, we show in Figure 9.4 the CL spectra at the inner edge of the hole lining the waveguide (position A in Figure 9.2(a), in red) and in the center of the waveguide between four holes (position B in Figure 9.2(c), in blue). Both positions are dominated by a peak at $\lambda_0 \sim 1425$ nm. The spectrum for position A also exhibits smaller peaks at $\lambda_0 \sim 1225$ nm and 1175 nm, for which the CL distribution was plotted in Figures 9.2(a,b).

The modal structure of PCWG is extremely sensitive to small changes in the geometry, which is demonstrated in Figure 9.4(b), where we have measured the spectra for five different waveguides (WG1–WG5) with increasing hole sizes, all measured for excitation position A. We observe a clear redshift of the spectral features for decreasing hole size. We note a variability in the intensity as well as an
increasing contribution of a second peak on the blue side of the main emission peak, for decreasing hole size. The inset of Figure 9.4(b) shows the main peak resonance wavelength as a function of the hole radius, as determined from SEM images. A \( \sim 20 \) nm change in hole radius leads to a \( \sim 80 \) nm shift in the resonance wavelength, underlining the extreme sensitivity of the modal fields to geometrical parameters [347].

To measure the polarization-resolved spectra, we first place the movable slit with a width of 3 mm in the optical path. We find that both peaks at \( \lambda_0 \sim 1175 \) nm and \( \lambda_0 \sim 1425 \) nm in the spectra from Figure 9.4(a) exhibit maximum intensity in the middle of the mirror, for orthogonal orientations of the waveguide relative to the
mirror, indicating that the emission direction is close to the surface normal. We can now use polarimetry to determine the polarization state of the emitted radiation. More details on the implementation can be found in the Methods Section and the Supporting information.

We display the Stokes parameters for excitation position A on WG2 oriented along the y-axis in Figure 9.4(c). $S_0$ corresponds to the total intensity, where we have not corrected for the emission from the substrate. $S_3$ determines the ellipticity and handedness of the polarization and we find that $S_3 \approx 0$ for all wavelengths. This demonstrates that the slit is well-aligned to the center of the parabolic mirror since we expect that only the curvature of the mirror will contribute to that component. $S_2$, which indicates the orientation of the principal axes of linearly polarized light, is also close to 0 over all wavelengths. All of the polarized contribution is contained in $S_1$, meaning that the polarization is fully linear and either horizontal ($S_1 > 0$) or vertical ($S_1 < 0$). Horizontal polarization corresponds to emission polarized along the y-axis and vertical polarization corresponds to emission polarized along either the z-axis or the x-axis of the coordinate system (see Figure 9.1). We find that the dominant peak at $\lambda_0$=1425 nm is polarized along the waveguide orientation (y-axis for data shown here). In fact, measurements using different orientations of the waveguide (see Figure 9.10 of the Supporting information) demonstrate that all of the measured peaks are fully polarized in-plane rather than along the z-axis. This indicates that none of them are due to TM modes, since those are polarized out-of-plane.

Using polarimetry allows us to separate the polarized (in red) and unpolarized (in gray) contributions to the spectra from Figure 9.4(c). Compared to the total intensity $S_0$ we can clearly see that a majority of the signal, including the small peak at $\lambda_0 \sim 1275$ nm, is unpolarized. We can ascribe this unpolarized emission to the luminescence from the substrate. The peaks in the polarized contribution all correspond to modal features in Figure 9.2 (for both excitation positions A and B).

Figure 9.4(d) compares spectra without the slit (blue), with the slit (green), and the polarization-filtered spectra (red). The main peaks at $\lambda_0 \sim 1175$ nm and $\lambda_0 \sim 1425$ nm are well-preserved in all cases, only decreasing in intensity by up to a factor of two. Given that we only collect emission from the 3 mm wide slit, compared to the 23 mm width of the mirror, this implies that the emitted radiation is relatively directional towards the surface normal.

Figures 9.5(a,b) show measurements of the polarization-filtered CL emission intensity distributions from WG2, at $\lambda_0$=1425 nm, for x and y polarization. Clearly, the emission is polarized along the waveguide axis y. Figures 9.5(c,d) show the calculated modal field intensity distributions (summed over $k$) at $\lambda_0$=1450 nm for the $E_y$ (c) and $E_x$ (d) components. We observe good qualitative agreement between the calculations and the measurements, especially for the $E_y$ component, while the calculated $E_x$ intensity is more intense than the x-polarized data. At this wavelength the mode is very close to the light line, but is still guided. The emission directionality towards the surface normal ($k \sim 0$) suggests that there is a contribution from the leaky part of the odd mode that can radiate out.
Figure 9.5 – Polarization-filtered 2D excitation maps of WG2, showing the CL emission probability as a function of the electron beam position for a center wavelength of $\lambda_0=1425$ nm, averaged over a 20 nm bandwidth. Only a linear polarizer was used here. The polarization is horizontal along the waveguide (along $y$) for (a) and vertical (along $x$) for (b) and the two are shown on the same intensity scale. (c) Calculation of the $E_y$ field intensity for the odd waveguide mode at $\lambda_0=1450$ nm and the corresponding calculation for $E_x$ (d), integrated over $k$ within the frequency range, both shown on the same scale normalized to the overall total maximum intensity for all the calculations. We show $E_y$ (e) and $E_x$ (f) on the same scale for the odd mode calculated at $\lambda_0=1500$ nm, integrated (within the frequency range) over a range of $k$ close to 0, above the light line. The distributions for $k$ below the light line can be seen in Figure 9.11 of the Supporting information.
For this reason we also calculate the field profiles at $\lambda_0=1500$ nm, where the dispersion relation of odd mode intersects the frequency window of the calculation for regions of $k$ both above the light line (close to $k=0$) and below the light line. The modal intensity distributions for $k$ above the light line show very good agreement with the data, as we can observe in Figure 9.5(e) for the $E_y$ intensity and in Figure 9.5(f) for the $E_x$ intensity. The intensity profiles for $k$ below the light line differ more from the measured emission profiles (see Figure 9.11 of the Supporting information). Comparing the measurements to the calculations, we find that the intensity distributions and relative intensities (for both polarizations) show agreement for both calculations, but there is clearly a better match with the leaky distributions at $\lambda_0=1500$ nm. The discrepancy in wavelength between measurement and calculation can be attributed to variations between the measured and calculated geometrical parameters, which we have shown to very strongly impact the resonance wavelength. We note that the calculations are not designed to determine field profiles in the leaky region above the light line, since they do not take into account nonzero values of $k_z$, which necessarily exist for leaky modes that radiate out of the waveguide to free space. Calculations in other systems that do fully take leaky contributions into account have shown that the mode can retain its overall field profile, even if it does becomes more lossy [257, 258]. In our case this is advantageous, as the mode is radiating out of the structure more freely, allowing us to measure it directly.

### 9.5 Conclusions

In conclusion, we have applied spectroscopic cathodoluminescence imaging polarimetry in the near-infrared spectral range to identify waveguide modes in silicon photonic crystal waveguides. These waveguides are designed to have highly confined modes inside the photonic band gap for TE polarization. Accordingly, the most striking feature that we observe is the odd TE waveguide mode of the structure, which exhibits a highly localized emission intensity distribution. Using spectroscopic polarimetry we demonstrate that this mode is fully linearly polarized along the direction of the waveguide. This is supported by calculations of the electric field intensities which show good qualitative agreement with both the measured intensity distributions and polarization. The vertically-polarized electron beam can couple to this in-plane mode as a result of nonzero contributions from the out-of-plane field component at different heights within the waveguide. A redistribution of the electron trajectories due to scattering also plays a role. The emission peak corresponding to the odd waveguide mode is directional towards the surface normal, indicating that we sample a leaky part of the waveguide mode that radiates out of the structure. Overall, we have demonstrated that spectroscopic cathodoluminescence imaging polarimetry is a powerful tool to measure light confinement and propagation in photonic crystal waveguides.
9.6 Methods

**Cathodoluminescence measurements:** The measurements were performed in a FEI XL-30 SFEG (10–30 keV electron beam, ∼30–46 nA current) equipped with a home-built CL system [124, 128, 183]. An aluminium parabolic mirror collects the emitted light and directs it outside of the microscope to an optical setup. We can measure the spectrum in the $\lambda_0=350–1000$ nm spectral range with a liquid-nitrogen-cooled back-illuminated silicon CCD array (Princeton Instruments Spec-10 100B) and in the $\lambda_0=900–1600$ nm spectral range with a liquid-nitrogen-cooled InGaAs photodiode array (Princeton Instruments OMA V). Due to the readout noise of the individual pixels, we smooth the spectra with a moving filter over a 2 nm bandwidth. We correct for the system response of the setup by using transition radiation from single crystal aluminium as a reference [119]. A Faraday cup integrated in the sample holder measures the current of the electron beam, which in combination with the system response allows us to determine the CL emission probability. A quarter-wave plate (QWP, Thorlabs AQWP10M-1600) and linear polarizer (Pol., Moxtek PUBB01A50M) are used together to measure the full polarization state of the emitted radiation [132]. To measure the polarization we place a 3 mm wide slit in the beam path followed by the QWP and Pol., which offers a good balance between signal intensity and polarization contrast [129, 130]. Because we focus all of the light passing through the slit onto the spectrometer, the measured polarization is momentum averaged over the zenithal angles that are collected. A series of six measurements for different combinations of the QWP and Pol. (horizontal/90°, vertical/0°, 45°, 135°, right- and left-handed circular) determine the Stokes parameters, which fully describe the polarization state of the light. For all spectral measurements we collect a dark reference spectrum where we blank the electron beam, subtracting this from the data in the post-processing stage. Measurement errors can occur due to drift of the electron beam across the sample, bleaching or contamination leading to a reduction in the measured intensity, as well as fluctuations in the current and optical alignment of the mirror.

**Calculations:** To calculate the modal fields of the photonic crystal waveguide, we calculated the eigenfrequencies and complex field amplitudes $E(r)$ using the MIT Photonics Band (MPB) code [346], which is a plane-wave method that uses periodic boundary conditions to calculate the eigenfrequencies and eigenmodes of our PCWGs. The band structure diagrams were calculated with the full 3D version. In order to conserve computational resources, we implemented a 2D version of the calculation using an effective index approximation to determine the field profiles. The effective index of the slab was chosen to be that of a 220 nm thick slab of silicon with the refractive index appropriate for each frequency range considered (for example for wavelengths around $\lambda_0=1450$ nm, we used 3.484). This procedure yields an effective index of 2.873 for TE modes and 1.831 for TM modes at $\lambda_0=1450$ nm. We determine the eigenvalues between 99 % and 101 % of the desired frequency. The $E_x$, $E_y$, and $E_z$ field profiles (or eigenmodes) are calculated on a rectangular grid of
points separated by a/16, ensuring that the eigenfrequencies are converged to better than 0.1%. The modes are normalized such that \( \int_{\text{unit cell}} \epsilon(r) * |E(r)|^2 \, dr = 1 \). The calculations are performed for wavevectors in the first irreducible Brillouin zone, after which we use symmetry arguments to add the fields for different wavevectors with the correct weighting factor, over the full first Brillouin zone. Essentially, we sum the field intensities over all wavevectors of the modes that occur within the frequency range of the calculation. The total field intensity is then determined by summing over all three field components. All of the resulting field intensity distributions are normalized to the maximum total intensity value for all wavelengths and polarizations (TE at \( \lambda_0 = 1500 \text{ nm} \)).

9.7 Supporting information

9.7.1 Reproducibility for different geometrical parameters

The measurements in the main text were all performed on sample 1, containing waveguides with a 420 nm pitch and slightly different hole sizes, which shifted the resonance by \( \sim 4 \text{ nm} \) per nanometer change in hole radius. To study how robust the measured features are to other changes in the geometry, we examine a second sample with a much smaller period, \( a = 300 \text{ nm} \) instead of 420 nm. The hole size is variable again, with a radius between 94 nm and 107 nm. Figure 9.6 shows the experimental results in the NIR for sample 2. We first examine 2D spatial scans of the PCWG with a hole radius of \( r = 94 \text{ nm} \), finding distinct emission patterns for wavelengths much shorter than for the previous sample, namely \( \lambda_0 = 925 \text{ nm} \) for Figure 9.6(a) and \( \lambda_0 = 1140 \text{ nm} \) for Figure 9.6(b). The double row of bright spots at \( \lambda_0 = 925 \text{ nm} \) is very different from any pattern measured on the other sample, which can be related to different dispersion, especially since there are more possible modes in the vertical direction of the slab at these short wavelengths. This measurement highlights the deeply subwavelength resolution of CL, since we can resolve this pattern so clearly at this scale. For a wavelength of \( \lambda_0 = 1140 \text{ nm} \) we find the same emission distribution as the dominant mode at \( \lambda_0 = 1425 \text{ nm} \) for WG2. The resonance wavelength of this peak shifts with hole size as in the previous sample, reaching \( \lambda_0 = 1080 \text{ nm} \) for a hole radius of \( r = 107 \text{ nm} \). This demonstrates that the main features of these PCWGs scale with both period and hole size, as expected.

Figure 9.6(c) shows spectra for three characteristic positions of bright features in the spatial maps, denoted by C, D and E. We observe the same peaks at \( \lambda_0 = 1140 \text{ nm} \), \( \lambda_0 = 1100 \text{ nm} \) and \( \lambda_0 = 925 \text{ nm} \) for all three positions, but with varying relative intensities, as was already clear from the emission patterns. We can examine the polarization behavior for this waveguide in the same fashion as in the main text, finding similar behavior. When orienting the waveguide along the y-axis and measuring the Stokes parameters for excitation position E, we obtain the spectra shown in Figure 9.6(d). Similarly to Figure 9.4(c), S2 and S3 are close to 0, while S1 dominates the polarized intensity, with the main emission peak
corresponding to the modal pattern of the odd mode being strongly linearly (horizontally) polarized. The majority of the CL emission is due to an unpolarized contribution from the background, leaving a very clean polarized spectrum with an excellent signal-to-noise ratio. These measurements show that the PCWG3s reproducibly possess highly localized waveguide modes that are very strongly polarized and exhibit distinct emission profiles, both of which we can measure accurately with infrared spectroscopic CL imaging polarimetry.

### 9.7.2 Input waveguide and short NIR-wavelength measurements

The majority of the PCWG exhibits a periodically repeating response, but at the interface with the input waveguide, the symmetry of the periodicity is broken,
strongly modifying the band structure. Figure 9.7 displays a 2D spatial intensity distribution measurement on the input section of WG2, the structure most studied in the main text, with a period of 420 nm and a hole radius of 120 nm. We show the CL emission probability for $\lambda_0=1305$ nm (a), $\lambda_0=1440$ nm (b), and $\lambda_0=1480$ nm (c), averaged over a 20 nm bandwidth. At $\lambda_0=1440$ nm we clearly recognize the emission distribution of the odd mode measured at $\lambda_0=1425$ nm in Figure 9.2(d). The wavelength is slightly different here because the holes are a little smaller at the edges of the structure, which redshifts the resonances. For $\lambda_0=1305$ nm we distinguish a different modal pattern from the previous cases, with this time a bright feature along the middle of the waveguide directly between two holes. At $\lambda_0=1480$ nm we observe a pattern slightly similar to that at $\lambda_0=1440$ nm, but now there are alternating bright and dark spots along the center of the waveguide, with much rounder bright features. This last emission pattern actually resembles the calculated electric
field profile at $\lambda_0 = 1500$ nm for the high $k$ values shown in Figure 9.11(a).

In addition to the spectral measurements in the $\lambda_0 = 900$–1600 nm range presented above, we also measure in the $\lambda_0 = 400$–1000 nm range. Figure 9.8 shows the CL emission probability averaged over a 20 nm bandwidth, as a function of electron beam excitation position, for wavelengths of $\lambda_0 = 865$ nm (a), $\lambda_0 = 920$ nm (b), $\lambda_0 = 935$ nm (c), and $\lambda_0 = 990$ nm (d). We observe complex and distinct emission distributions even for wavelengths only 15 nm apart. At these shorter wavelengths there appear to be many higher order modes with very intricate modal patterns. These are beyond the scope of the research presented here, but the data attest to the high resolution attainable with CL as well as the broadband excitation and detection capabilities.

![Figure 9.8](image-url)

**Figure 9.8** – CL emission probability as a function of excitation position on WG2 (sample 1), measured for a center wavelength of $\lambda_0 = 865$ nm (a), $\lambda_0 = 920$ nm (b), $\lambda_0 = 935$ nm (c), and $\lambda_0 = 990$ nm (d). The emission probability is averaged over a 20 nm bandwidth.
9.7.3 TM polarized calculations

The measurements and calculations in the main text have focused on TE polarization, since the waveguides are specifically designed to have well-defined, high-quality modes for that polarization. The TM modes can also contribute to the emission properties however, so they should not be ignored. Figure 9.9(a) displays the band structure for TM polarization with the geometrical parameters used in the main text (period \(a=420\,\text{nm}\) and hole radius \(r=120\,\text{nm}\)). As in Figure 9.1(c), we show the normalized frequency \(\omega \times \frac{a}{2\pi c}\) as a function of the normalized wavevector \(k \times \frac{a}{2\pi}\) along the propagation direction of the waveguide. The dashed line indicates the light line in air. The continuum of modes dominates nearly the entire band.

![Band structure diagram for a waveguide with \(a=420\,\text{nm}\) and \(r=120\,\text{nm}\), corresponding to sample 1, WG2, for TM polarization. The frequency \(\omega\) and the wavevector \(k\) are shown in normalized units using the period \(a\). The gray lines denote modes that are in the continuum of available modes above and below the photonic band gap, which display two waveguide modes close to \(\lambda_0=1150\,\text{nm}\). The black dashed line indicates the light line in air. We calculate the total \(|E|^2\) field profiles, integrating over all available modes and \(k\) for \(\lambda_0=1430\,\text{nm}\) (b), \(\lambda_0=1450\,\text{nm}\) (c), and \(\lambda_0=1500\,\text{nm}\) (d). The intensities are normalized to the overall maximum intensity of all the calculations (as in the main text).](image-url)

**Figure 9.9**
9.7 Supporting information

diagram. Just below the continuum at high values of $k$ there is a discrete band related to total internal reflection inside the slab. Unlike the TE polarization, there is no large photonic band gap here that extends across a broad range of frequencies and wavevectors, but only a small gap between $\sim 1080$–$1170$ nm for high values of $k$ below the light line. Within this small gap we can distinguish two waveguide modes. These waveguide modes and band edges are in the same spectral range as the modal features observed in Figures 9.2(a,b), so those could be due to TM modes, but we cannot determine the field profiles in that spectral range to confirm this.

Instead we calculate in Figure 9.9 the total electric field intensities for wavelengths of $\lambda_0 = 1430$ nm (b), $\lambda_0 = 1450$ nm (c), and $\lambda_0 = 1500$ nm (d). The intensities are normalized to the maximum total intensity for all wavelengths and polarizations, as in the main text, so that we can compare the values of the color scale. We find that for all wavelengths the field profiles do not show the high confinement and localization in or near the waveguide that is present in the TE calculations at these wavelengths. Indeed the intensities are actually lowest inside the waveguide. This is logical because in the band structure we are deep in the continuum of modes, which are typically delocalized over the entire photonic crystal and not confined to the waveguide. We can conclude that the measured emission patterns in this wavelength range agree with the TE calculations and not with the TM ones.

### 9.7.4 Implementation of spectroscopic polarimetry

Using polarimetry to measure spectra proves to be a powerful way to determine which spectral features are (strongly) polarized, what their polarization state is, and to separate them from unpolarized background contributions. This allows detailed analysis of the resulting polarized spectra which provides strong insight into the processes generating the radiation. Figure 9.10 describes in more detail how the spectroscopic polarimetry is implemented. The method is based on using a rotating-plate polarimeter composed of a quarter-wave plate (QWP) and linear polarizer (Pol.), taking six measurements for different settings of the polarimeter (horizontal/90°, vertical/0°, 45°, 135°, right- and left-handed circular). These can then be combined to determine the Stokes parameters ($S_0 = I_H + I_V$, $S_1 = I_H - I_V$, $S_2 = I_{45} + I_{135}$, and $S_3 = I_{RHC} - I_{LHC}$). Figure 9.10(a) displays these six measurements when exciting WG2 (aligned along the y-axis) at excitation position B (in the middle of the waveguide). We observe that below $\lambda_0 = 1400$ nm there is no difference between the six spectra, indicating the emission is unpolarized. The peak at $\lambda_0 = 1425$ nm however is very strongly horizontally polarized, being entirely visible for 90° and absent for 0° (so $S_1$ is large). The left- and right-handed measurements have very similar intensity ($S_3 \sim 0$), demonstrating there is no circular polarization, while the similarity between 45° and 135° ($S_2 \sim 0$) indicates that the orientation of the polarization is indeed fully horizontal.

To determine how polarized or unpolarized the emission is in an intuitive way, we can use the Stokes parameters to determine the different degrees of polariza-
Figure 9.10 – (a) CL emission probability for polarization-filtered spectra excited at position B (in the middle of the waveguide) on WG2, with the waveguide oriented along the y-axis. We show the six spectra corresponding to all the combinations of QWP and linear polarizer settings needed to determine the Stokes parameters (vertical/0°, horizontal/90°, 45°, 135°, left-handed circular and right-handed circular). (b) Degree of polarization as a function of wavelength determined from the spectra shown in (a). The degree of linear polarization (DOLP, red) is nearly indistinguishable from the total degree of polarization (DOP, black). (c) CL spectra excited at position B on sample 1, WG2 for vertical/0°/x polarization and horizontal/90°/y polarization for two different orientations of the waveguide, along x or y as defined by the coordinate system shown in Figure 9.1(d) of the main text. (d) Polarization-filtered spectra for excitation position A on sample 1 WG2 oriented along the x-axis. We show the Stokes parameters S0 (black), S1 (turquoise), S2 (blue) and S3 (green) as well as the polarized (red) and unpolarized (gray) contributions, as for Figure 9.4(c) of the main text. We note that S1 and the polarized contribution overlap for the shorter wavelengths.

Polarimetry measurements on Sample1 WG2 (a=420 nm, r=120 nm)

(a) Pos. B WG along Y
- Pol: 0
- 90
- 45
- 135
- LHC
- RHC

(b) Pos. B WG along Y
- DOUP
- DOLP
- DOCP
- DOP

(c) Pos. B
- Pol 0(X) WG along Y
- Pol 0(X) WG along X
- Pol 90(Y) WG along Y
- Pol 90(Y) WG along X

(d) Pos. A WG along X
- Unpolarized
- Polarized

Stokes parameters:
- S0
- S1
- S2
- S3

Cl Em. Prob. (10^-7 nm^-1)

Wavelength (nm)

Figure 9.10 – (a) CL emission probability for polarization-filtered spectra excited at position B (in the middle of the waveguide) on WG2, with the waveguide oriented along the y-axis. We show the six spectra corresponding to all the combinations of QWP and linear polarizer settings needed to determine the Stokes parameters (vertical/0°, horizontal/90°, 45°, 135°, left-handed circular and right-handed circular). (b) Degree of polarization as a function of wavelength determined from the spectra shown in (a). The degree of linear polarization (DOLP, red) is nearly indistinguishable from the total degree of polarization (DOP, black). (c) CL spectra excited at position B on sample 1, WG2 for vertical/0°/x polarization and horizontal/90°/y polarization for two different orientations of the waveguide, along x or y as defined by the coordinate system shown in Figure 9.1(d) of the main text. (d) Polarization-filtered spectra for excitation position A on sample 1 WG2 oriented along the x-axis. We show the Stokes parameters S0 (black), S1 (turquoise), S2 (blue) and S3 (green) as well as the polarized (red) and unpolarized (gray) contributions, as for Figure 9.4(c) of the main text. We note that S1 and the polarized contribution overlap for the shorter wavelengths.

Polarimetry measurements on Sample1 WG2 (a=420 nm, r=120 nm)

(a) Pos. B WG along Y
- Pol: 0
- 90
- 45
- 135
- LHC
- RHC

(b) Pos. B WG along Y
- DOUP
- DOLP
- DOCP
- DOP

(c) Pos. B
- Pol 0(X) WG along Y
- Pol 0(X) WG along X
- Pol 90(Y) WG along Y
- Pol 90(Y) WG along X

(d) Pos. A WG along X
- Unpolarized
- Polarized

Stokes parameters:
- S0
- S1
- S2
- S3

Cl Em. Prob. (10^-7 nm^-1)

Wavelength (nm)
and DOLP are nearly identical. Only the emission peak at \( \lambda_0 = 1425 \) nm and a broad feature for the highest wavelengths are strongly polarized. We are not certain about the nature of the polarized contribution at these highest wavelengths, but it can be related to polarized modes in the continuum of the upper band in the band structure which are not clearly separated.

These measurements for the waveguide oriented along the y-axis, exhibiting horizontal polarization for the main emission peak at \( \lambda_0 = 1425 \) nm, indicate that it is in any case not a TM contribution with electric fields normal to the sample surface (along the z-axis). Additionally, polarization along the x-axis should, upon reflection by the mirror, become vertically polarized, which we do not observe. This leads us to conclude that the emission process we measure here is polarized along the waveguide axis (here the y-axis). To confirm this, we also perform measurements after rotating the waveguide by 90° so it is aligned with the x-axis of the coordinate system. Figure 9.10(c) compares spectra measured for horizontal and vertical polarization for the two waveguide orientations, when exciting WG2 at position B. We observe that when the waveguide is oriented along the x-axis, the polarization flips, as expected. In this case no peak is observed at \( \lambda_0 = 1425 \) nm for horizontal polarization (along y, 90°), instead a peak is clearly observed for vertical polarization (0°) which corresponds to polarization along x. This confirms that this emission peak is entirely polarized along the propagation direction of the waveguide, which agrees with the odd waveguide mode as shown in Figure 9.5 of the main text.

Figure 9.10(d) shows the Stokes parameters as well as the polarized and unpolarized intensities for excitation position A on WG2 oriented along the x-axis, which we can compare to the same measurement for the waveguide oriented along the y-axis (Figure 9.4(c)). As in the previous cases, we observe that the majority of the emission is unpolarized, S2 and S3 are close to 0 so that the polarized intensity very closely follows S1. The only difference is the sign of S1, which is positive for horizontal polarization and negative for vertical polarization. Comparing the peaks at \( \lambda_0 = 1175 \) nm and \( \lambda_0 = 1425 \) nm, we note that the first one is positive and the second one in negative. This is exactly the opposite in Figure 9.4(c), confirming the flip in polarization expected from the different orientation that was just discussed for Figure 9.10(c). It also confirms that the emission peaks at these two wavelengths indeed display an opposite polarization. Since the peak at \( \lambda_0 = 1175 \) nm does not exhibit vertical polarization for both waveguide orientations, it makes it less likely that it is caused by TM modes, which are dominated by the \( E_z \) field component.

### 9.7.5 Polarization of the even and odd waveguide modes

In Figure 9.5 of the main text, we compared the polarization-filtered measurements to electric field profiles of the odd waveguide mode for TE polarization. For \( \lambda_0 = 1500 \) nm, we found that two separate regions of wavevectors \( k \) contribute and that there is good agreement for the range of small \( k \) above the light line, where the mode is leaky. For comparison, we show here the normalized field intensi-
Figure 9.11 – Calculation of the $E_y$ (a) and $E_x$ (b) field intensities for the odd waveguide mode from Figure 9.1(c) of the main text, for $\lambda_0=1500$ nm. Here we show the field profiles, on the same scale, obtained after integrating over the range of $k$ values below the light line, as opposed to the range above the light line shown in Figures 9.5(e,f). We also show the field profiles of the even mode, summed over all contributing $k$, with $E_y$ (c) and $E_x$ (d) on the same scale, at $\lambda_0=1500$ nm. As before, the intensities are all normalized to the maximum total intensity of all the calculations.

Figure 9.11 – Calculation of the $E_y$ (a) and $E_x$ (b) field intensities for the odd waveguide mode from Figure 9.1(c) of the main text, for $\lambda_0=1500$ nm. Here we show the field profiles, on the same scale, obtained after integrating over the range of $k$ values below the light line, as opposed to the range above the light line shown in Figures 9.5(e,f). We also show the field profiles of the even mode, summed over all contributing $k$, with $E_y$ (c) and $E_x$ (d) on the same scale, at $\lambda_0=1500$ nm. As before, the intensities are all normalized to the maximum total intensity of all the calculations.

...ties summed over the range of $k$ below the light line, for the $E_y$ component (Figure 9.11(a)) and the $E_x$ component (Figure 9.11(b)). Similarly to the previous calculations, we show the two components on the same intensity scale, normalized to the maximum overall intensity obtained for all wavelengths and polarizations. We find bright features in the middle of the waveguide separated by dark sections for $|E_y|^2$ and enhanced intensity at the inner edges of the holes for $|E_x|^2$. Compared to the measurements in Figures 9.5(a,b), the qualitative agreement is not as good as for the field profiles in the leaky region, even though the latter are less accurate. The brightness in the center of the waveguide for $|E_y|^2$ is much more continuous than that shown here and $|E_x|^2$ is much darker than what we observe here. The total intensity (summed over all field components) does, however, show strong similarities with the measured emission profile at $\lambda_0=1480$ nm in Figure 9.7(c), suggesting the guided portion of the mode can play a role at slightly different wavelengths from those dominated by the leaky portion.
We found the same polarization and field profiles for the measurements and the odd waveguide mode, leading us to discount the even waveguide mode. Verifying the expected opposite symmetry and polarization of the modes allows us to confirm this. We show in Figures 9.11(c,d) that the even mode is dominated by $|E_x|^2$ (d) while $|E_y|^2$ (c) is dark, completely opposite to the measurements and the calculations of the odd mode. We only display the modal intensity distributions at $\lambda_0=1500$ nm, but find that for wavelengths of 1430, 1450 and 1550 nm there is very little difference in the field profiles and intensities.