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Near-infrared spectroscopic cathodoluminescence imaging polarimetry on silicon photonic crystal waveguides

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Abstract

1

We measure polarization- and wavelength-resolved spectra and spatial emission 2 intensity distributions from silicon photonic crystal waveguides in the near-infrared 3 spectral range using spectroscopic cathodoluminescence imaging polarimetry. A 30 4 keV electron beam, incident along the surface normal of the sample, acts as an ultra-5 broadband and deeply subwavelength excitation source. For photonic crystal waveg-6 uides with a broad range of design parameters, we observe a dominant emission inten-7 sity distribution that is strongly confined to the waveguide. For a period of 420 nm 8 and a hole radius of 120 nm, this occurs at a wavelength of 1425 nm. The polarization-9 resolved measurements demonstrate that this feature is fully linearly polarized along 10

the waveguide axis. Comparing the modal pattern and polarization to calculations of the electric field profiles confirms that we measure the odd TE waveguide mode of the system. This result demonstrates that the electron beam can couple to modes dominated by in-plane field components in addition to the more commonly observed modes dominated by out-of-plane field components. From the emission directionality, we conclude that we sample a leaky portion of the odd waveguide mode.

17 Keywords

¹⁸ Cathodoluminescence, photonic crystal waveguide, polarimetry, near-infrared

Photonic crystals, materials with a periodically varying dielectric function, can manip-19 ulate the propagation of light in a controlled way. They create a photonic band gap that 20 prevents light from propagating in certain directions for certain frequencies.¹⁻⁵ The photonic 21 band gap can lead to a strong confinement of light, and engineered defects allow the creation 22 of photonic crystal cavities and waveguides. Photonic crystal cavities can have long photon 23 lifetimes and small mode-volumes,^{6–8} leading to strong light-matter interactions and enabling 24 applications such as low threshold lasers.^{9–12} Photonic crystal waveguides are strongly dis-25 persive, and can slow light down, which also leads to enhanced light-matter interactions.^{13–21} 26 This strong dispersion allows such waveguides to serve as many components and building 27 blocks in photonic integrated circuits, such as splitters, switches or multiplexers.^{18,22–25} To 28 fully exploit the many applications of photonic crystal waveguides, it is essential to measure 29 the propagation and confinement of light at a subwavelength scale. This cannot be achieved 30 by conventional microscopy techniques. Near-field scanning optical microscopy (NSOM), 31 which uses subwavelength probes or apertures to detect or scatter the near field of these 32 structures,^{26–30} has enabled measurements of the field components of the optical near field 33 just above the waveguide.^{31,32} 34



Cathodoluminescence (CL) spectroscopy is an alternative technique that can be used

to study nanophotonic structures, coupling to and probing the field distributions inside. 36 A high-energy electron beam is used as a nanoscale optical excitation source in which the 37 time-varying electromagnetic field of the electron couples to the local optical modes of the 38 system as it traverses the sample.^{33–35} This mechanism, which is fully described by Maxwell's 39 equations, is fundamentally similar to that of the oscillating electric field of a laser beam 40 coupling to optical excitations. In CL, the light scattered from these optical modes to the 41 far field is detected. The short interaction time of the electron with the structure (a few 42 fs) results in a broadband excitation spectrum (typically several µm, down into the deep 43 UV). The high excitation resolution of CL is only limited by the extent of the electric field 44 about the electron trajectory and the spread of the beam in the sample. This allows one to 45 explore the radiative local density of states (LDOS) at deeply subwavelength scales.^{34,36} The 46 electron forms a noninvasive probe of the optical properties inside the material. Recently, 47 it has become possible to measure the full polarization distribution of CL emission as a 48 function of angle by using polarimetry.³⁷ These properties have made CL a powerful, deeply 49 subwavelength characterization technique,^{38–44} allowing measurements of the confinement 50 and dispersion of plasmonic and dielectric photonic crystal cavities in the visible spectral 51 range.^{34,45–47} 52

In this article, we apply spectroscopic cathodoluminescence imaging polarimetry in the 53 near-infrared (NIR) spectral range to study the confinement and polarization of propagating 54 photonic crystal waveguide modes. More specifically, we examine how the electron beam 55 couples to the electromagnetic eigenmodes of the system. CL emission is typically dom-56 inated by modes with primarily out-of-plane electric field components (hereafter referred 57 to as out-of-plane or TM modes). Modes with primarily in-plane electric field components 58 (hereafter referred to as in-plane or TE modes) are usually not significant. These structures, 59 however, possess different band structures for TE and TM polarization and support two well 60 defined modes for TE polarization, denoted as even and odd.^{5,48,49} We demonstrate that 61 CL imaging polarimetry enables direct identification and spatial mapping of the modal field 62

distribution in the photonic crystal waveguides. The CL emission is dominated by the odd TE waveguide mode, with measurements showing good agreement with calculations of the modal field intensities. Using photonic crystal waveguides as a well-known model system, we demonstrate the direct excitation of in-plane TE modes by the electron beam. We show that the excitation process involves a complex combination of coupling of the electron beam to multiple field components of the propagating TE modes.

⁶⁹ Experiment

Silicon photonic crystal waveguides (PCWGs) were fabricated on silicon-on-insulator (SOI) 70 wafers with a 220 nm thick silicon layer on top of a 1 µm silica layer on a silicon substrate. 71 Electron beam lithography was used to pattern the waveguides, followed by reactive ion 72 etching to etch through the top silicon layer. A wet HF etch was used to remove part of the 73 silica layer and obtain a suspended PCWG. Reference measurements in the visible and NIR 74 spectral ranges demonstrate that a residual silica layer remains, since we observe character-75 istic silica defect-related emission peaks. Two different samples were studied; here we only 76 discuss sample 1, showing data for sample 2 in Figure S1 of the Supporting Information. 77 Figure 1(a) shows a SEM image of one of the PCWGs on sample 1 examined here, with a 78 length of 90 μ m and a total width of the photonic crystal section of 10 μ m. The PCWG is 79 composed of a hexagonal array of holes with one missing row of holes (W1 waveguide).^{5,49,50} 80 Five waveguides were made on sample 1 with the same period a=420 nm and hole radii 81 varying in the range $\sim 105-125$ nm. Figure 1(b) shows a close-up of the waveguide section 82 for the most studied structure (denoted as WG2), which has a period a=420 nm and a hole 83 radius r=120 nm. 84

The TE band structure of WG2 is shown in Figure 1(c), calculated using an open-source MIT Photonic Bands (MPB) frequency domain mode-solver.⁵¹ TE polarization corresponds to electric fields that are primarily oriented in the plane of the waveguide slab (fully so only ⁸⁸ in the vertical plane of symmetry z=0). The gray bands represent modes that make up a ⁸⁹ continuum below and above the photonic band gap, which opens up between normalized ⁹⁰ frequencies of ~0.25–0.32, corresponding to free space wavelengths of ~ $\lambda_0=1300-1700$ nm. ⁹¹ The discrete bands at the lower right are index-guided bands,⁵ confined by total internal ⁹² reflection in the slab. The band structure is very sensitive to the period, hole size and slab ⁹³ thickness.⁵²

Removing rows of holes leads to allowed modes within this band gap,^{48–50,53} that are 94 confined vertically by index-guiding (total internal reflection), but horizontally by the band 95 gap of the photonic crystal. For a single row of missing holes there are two TE waveguide 96 modes in the band gap: an even mode with a symmetric field distribution and an odd mode 97 with an anti-symmetric distribution for the in-plane transverse electric field component.^{13,48} 98 The even mode has been studied intensely due to its anomalous dispersion and vanishing 99 group velocity over a large range of wavevectors when approaching the edge of the Brillouin 100 zone.^{13,14,18,19} The odd mode is less well studied, but also displays slow light over a broad 101 range of wavevectors (see Figure 1(c)). The dashed line in the figure represents the light line 102 in air; modes to the left will be leaky and modes to the right are guided in the waveguide 103 slab. 104

In addition to TE modes, the photonic crystal possesses TM modes, with an electric field 105 perpendicular to the waveguide slab at z=0. Such modes are usually excited efficiently by 106 CL,³³ since the moving electron acts as a vertically polarized source. In Figure S4 of the 107 Supporting Information we show the band structure for TM polarization. We find that there 108 is a small photonic band gap for wavelengths in the range $\sim \lambda_0 = 1100 - 1200$ nm with two 109 waveguide modes within. In the spectral range of the TE band gap, the TM band structure 110 exhibits a continuum of modes. Modes inside or near the band gap are usually localized to 111 the waveguide, while modes in the continuous bands are more delocalized over the photonic 112 crystal.^{5,48} The PCWGs studied here are specifically designed for high quality TE modes 113 rather than TM modes, so the former will typically exhibit a higher LDOS. There are thus 114

¹¹⁵ multiple possible sources of emission, for both TE and TM polarization, when exciting these
¹¹⁶ Si PCWGs with swift electrons.

Figures 1(d,e) shows calculations of the electric field intensity distributions for the odd 117 (d) and even (e) TE polarized modes at $\lambda_0 = 1450$ nm, using the MPB code. We calculate 118 the E_x , E_y and E_z field components as a function of position and wavevector within a 119 small frequency range, then integrate over all k and field components. For simplicity, these 120 calculations are all 2D, performed at z=0 so E_z is strictly 0 as well, but this does not affect 121 the relevant features of these in-plane modes (see Figure S5 of the Supporting Information 122 for 3D calculations of E_z). All 2D calculations are normalized to the same overall maximum 123 (obtained for TE at $\lambda_0 = 1500$ nm, not shown here) and the holes are masked (the intensity 124 inside the holes is set to zero) to better compare the results to the measurements. For more 125 details about the calculation procedure, see the Methods Section. We observe that both 126 odd (Figure 1(d)) and even (Figure 1(e)) modes display sharp high intensity features along 127 the center of the waveguide. The odd mode, however, exhibits a more localized, distinct 128 and bright modal distribution pattern. These two modes are differentiated by the symmetry 129 of the in-plane field component transverse to the waveguide propagation direction, which 130 becomes clear when examining the real or imaginary amplitudes (not shown here) but not 131 apparent for the field intensity presented here. The modes are, however, also dominated by 132 different field components (see Figure S7 of the Supporting Information). 133

¹³⁴ Calculations for TM polarization in the range $\lambda_0 = 1430 - 1500$ nm are shown in Figure S4 ¹³⁵ of the Supporting Information, but exhibit no sharp features such as the ones on display for ¹³⁶ TE polarization.

Figure 1(f) depicts a schematic representation of the CL setup. ^{34,37,54} 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 142 emitted radiation can change as it reflects off the mirror, due to its curved shape. The slit 143 selects the central part of the mirror and conserves the emission polarization, ^{55,56} integrating 144 over zenithal angles for a narrow range of azimuthal angles. We perform measurements for 145 different positions of the slit and orientations of the waveguide with respect to the mirror to 146 determine the polarization state and emission directionality (see Supporting Information). 147 We combine a quarter-wave plate (QWP) and linear polarizer (Pol.) to determine the Stokes 148 parameters, which fully describe the polarization state of the emitted light.^{37,57} This allows 149 for the separation of polarized and unpolarized light, as well as the retrieval of different field 150 components inside the structure and the relative phase difference between them.⁵⁷ Measuring 151 the emission polarization thus allows the mapping of the electric field components. The 152 Methods Section describes the experimental setup and measurement protocol in more detail. 153 For the measurements described in the main text, all waveguides are oriented along the 154 y-axis, as defined by the coordinate system in Figure 1(f). 155

¹⁵⁶ Near-infrared spatially-resolved cathodoluminescence

Figure 2 presents 2D spatial CL intensity maps from WG2, at wavelengths of $\lambda_0 = 1170$ nm (a), 157 $\lambda_0 = 1185 \text{ nm (b)}, \lambda_0 = 1400 \text{ nm (c)}, \text{ and } \lambda_0 = 1425 \text{ nm (d)}, \text{ all averaged over a 20 nm bandwidth}.$ 158 Combining the raw data with the spectral response of the system and in-situ beam current 159 measurements allow us to determine the CL emission probability (number of photons emitted 160 per incoming electron, per unit bandwidth of nm^{-1}).⁵⁸ We additionally correct the data for 161 the dark response of the detector as well as for signal from the remaining silica and the silicon 162 substrate, which contributes a broadband response and a peak at $\lambda_0 = 1275$ nm. To do so, we 163 use a reference spectrum measured in one of the holes, which has no contribution from the 164 waveguide or photonic crystal modes. In the Supporting Information, we show additional 165 measurements for a sample with a different period (Figure S1), for the input section of WG2 166

¹⁶⁷ (Figure S2) and for WG2 closer to the visible spectral range (Figure S3).

The measurements at $\lambda_0 = 1170$ nm and $\lambda_0 = 1185$ nm (Figures 2(a,b)), exhibit an overall 168 similarity, with high intensity at the inner edges of the holes lining the waveguide and darker 169 spots along the waveguide at positions in between four holes. These two positions are denoted 170 as A and B in Figures 2(a,c). Figure 2(b) exhibits a distinct enhanced intensity at the edges 171 of the holes outside of the waveguide, compared to Figure 2(a). Figures 2(c,d) show data 172 at $\lambda_0 = 1400$ nm and $\lambda_0 = 1425$ nm, displaying a high intensity at the inner edges of the holes 173 lining the waveguide, which wrap around the hole edges more than for the data at shorter 174 wavelengths. The center of the waveguide exhibits high intensity features at positions that 175 were dark for $\lambda_0 = 1170$ nm and $\lambda_0 = 1185$ nm. At $\lambda_0 = 1425$ nm these peaks are most intense, 176 while the region around the waveguide has a lower relative intensity than for $\lambda_0 = 1400$ nm. 177 The fact that the signal for $\lambda_0 = 1425$ nm is very strongly confined to the waveguide suggests 178 it is related to a waveguide mode. 179

The features at $\lambda_0 = 1170$ nm and $\lambda_0 = 1185$ nm occur in the upper band of the TE band 180 structure (see Figure 1(c)), that represent modes that are delocalized over the waveguide 181 and surrounding holes,^{5,48} as seen in Figures 2(a,b). In addition to TE modes, TM modes 182 could also be responsible for this measured emission. As Figure S4 of the Supporting In-183 formation demonstrates, there is a small TM photonic band gap for wavelengths in the 184 range ~ λ_0 =1100–1200 nm with two waveguide modes within. The emission patterns at 185 $\lambda_0 = 1400 \text{ nm}$ and $\lambda_0 = 1425 \text{ nm}$ occur in the middle of the TE photonic band gap, where the 186 even and odd waveguide modes are present. For TM polarization these wavelengths are in 187 the continuum of modes below the TM band gap, where one expects modes that are more 188 delocalized from the waveguide, unlike the patterns observed here that are strongly confined 189 to the waveguide. Comparing the measurements to the calculations of the modal field distri-190 butions in Figures 1(d,e), excellent agreement is observed between the data and the odd TE 191 waveguide mode, while calculations for TM polarization exhibit a very different and weaker 192 response (Figure S4 of the Supporting Information). This indicates that the out-of-plane 193

electron beam is coupling most strongly to an in-plane mode, which seems counter-intuitiveat first.

The electron beam principally couples to field components that are parallel to the electron 196 trajectory.³³ For electrons propagating along z, this should lead to preferential coupling to 197 the TM modes, yet we clearly observe patterns identical to TE modes. Our 2D calculations 198 for TE polarization are performed at z=0, where E_z is strictly zero. The membrane does have 190 a finite thickness, however, so E_z has nonzero components for other z-coordinates.⁵ We can, 200 for example, expect vertical components at the edges of the holes.³² To verify this we have 201 performed a set of 3D MPB calculations, determining the modal fields for different values of 202 z. We display the calculated E_z in Figure S5 of the Supporting information, showing that 203 the hole edges indeed exhibit a distinct E_z component. Considering the high intensity in 204 the middle of the waveguide, the even mode is symmetric with respect to the center, for 205 the transverse in-plane field component (perpendicular to the waveguide axis), so there is no 206 field gradient across the central axis and the electric field is expected to remain in-plane. The 207 odd mode however is anti-symmetric for the transverse in-plane field component, exhibiting 208 a field gradient across the central axis and a node at the very center where the field switches 209 sign. This flip in the fields is accompanied by a nonzero E_z component in the center for 210 different (nonzero) z-coordinates, explaining why we preferentially measure the odd mode. 211 This is also confirmed by Figure S5, showing that the odd mode has nonzero values of E_z 212 along the waveguide center while E_z of the even mode is close to zero and the odd mode also 213 has a higher intensity overall than the even mode. The E_z intensity locally reaches ~15 % 214 of the maximum value of the total intensity for the odd mode and ~ 5 % for the even mode. 215 Another source of coupling between the electrons and the TE modes is the fact that 216 scattering of the incident electrons inside the silicon membrane leads to a spread in their 217 propagation directions, allowing for direct coupling to in-plane field components.³⁴ The scat-218 tering increases for lower electron energies, which should result in stronger coupling to the 219 in-plane components. We do indeed observe higher intensities from the modal peaks using 220

²²¹ 10 keV instead of 30 keV (not shown here).

Both the 3D distribution of the electric fields with locally significant E_z components aligned with the incident electrons and electron scattering inside the silicon slab allowing for alignment with the E_x and E_y components play a role in exciting the in-plane TE modes in the PCWG slab. Although TM modes should still have a better overlap with the electron beam, the band structure is dominated by a continuum of modes. For TE, however, there is a clear band gap with well defined waveguide modes that can stand out, as they have a higher local density of states than the delocalized TM modes.

²²⁹ Spectroscopic polarimetry

To further confirm the TE nature of the measured modes, we need to study the polarizationfiltered spectral response of the waveguide. We begin by examining non-filtered spectra in Figure 3(a), which presents the CL spectra at the inner edge of the hole lining the waveguide (position A in Figure 2(a), in red) and in the center of the waveguide between four holes (position B in Figure 2(c), in blue). Both positions are dominated by a peak at $\lambda_0 \sim 1425$ nm. The spectrum for position A also exhibits additional smaller peaks at $\lambda_0 \sim 1225$ nm and 1175 nm, for which the CL intensity distribution was plotted in Figures 2(a,b).

The modal structure of PCWGs is sensitive to small changes in the geometry, which is 237 demonstrated in Figure 3(b), where we have measured the spectra for five different waveg-238 uides (WG1–WG5) with increasing hole sizes, all measured for excitation position A. We 239 observe a clear redshift of the spectral features for decreasing hole size. We note a variability 240 in the intensity as well as an increasing contribution of a second peak on the blue side of 241 the main emission peak, for decreasing hole size. The inset of Figure 3(b) shows the main 242 peak resonance wavelength as a function of the hole radius, as determined from SEM im-243 ages. A ~ 20 nm change in hole radius leads to a ~ 80 nm shift in the resonance wavelength, 244 underlining the sensitivity of the modes to geometrical parameters.⁵² 245

To measure the polarization-resolved spectra, we first place the vertical movable slit 246 with a width of 3 mm in the optical path. We find that both peaks at $\lambda_0 \sim 1175$ nm and 247 $\lambda_0 \sim 1425$ nm in the spectra from Figure 3(a) exhibit maximum intensity in the middle of the 248 mirror, for orthogonal orientations of the waveguide relative to the mirror, indicating that the 249 emission direction is close to the surface normal. We can now use polarimetry to determine 250 the polarization state of the emitted radiation, which allows the retrieval of the electric field 251 orientations inside the structure. We assume the interface does not significantly alter the 252 field orientations for emission close to the surface normal. For these measurements we do 253 not separately subtract the signal from the substrate. More details on the implementation 254 can be found in the Methods Section and the Supporting Information. 255

We display the Stokes parameters for excitation position A on WG2 oriented along the y-256 axis in Figure 3(c). S0 corresponds to the total intensity, where we have not corrected for the 257 emission from the substrate. S3 determines the ellipticity and handedness of the polarization. 258 We do not expect circularly polarized emission from the structure, but for linearly polarized 259 emission the measured reflection off of the curved surface of the mirror can lead to a circular 260 component. This is only negligible if the slit that spatially filters the emission is positioned 261 at the center of the parabolic mirror, where the emitted and reflected rays lie in the same 262 plane as the surface normal of the mirror. In that case the problem reduces to classical 263 Fresnel reflection where the s- and p-polarizations (horizontal and vertical) are conserved. 264 We find that $S3\approx 0$ for all wavelengths, demonstrating that the slit is well aligned. S2, which 265 indicates the orientation of the principal axes of linearly polarized light, is also close to zero 266 over all wavelengths. All of the polarized contribution is contained in S1, meaning that 267 the polarization is fully linear and either horizontal (S1>0) or vertical (S1<0). Horizontal 268 polarization corresponds to emission polarized along the y-axis and vertical polarization 269 corresponds to emission polarized along either the z-axis or the x-axis of the coordinate 270 system (see Figure 1). We find that the dominant peak at $\lambda_0 = 1425$ nm is polarized along the 271 waveguide axis (y-axis for data shown here). A TM mode predominantly has an out-of-plane 272

electric field, i.e. along the z-axis and would therefore be measured as a vertical polarization 273 for any orientation of the waveguide. In-plane TE modes, with electric field components 274 typically along the waveguide axis or orthogonal to it, will be along either the x- or y-axes for 275 carefully aligned orthogonal orientations of the waveguide. Their emission will be measured 276 up as a horizontal polarization for one orientation and vertical for the other orthogonal 277 orientation. Experiments using such orthogonal orientations of the waveguide (see Figure S6 278 of the Supporting Information) result in orthogonal horizontal/vertical polarizations for all 279 of the measured peaks. This demonstrates that all of the features are related to TE and 280 not to TM modes, confirming once again that the electron beam can couple to in-plane 281 excitations. 282

Using polarimetry allows us to separate the polarized (in red) and unpolarized (in gray) contributions to the spectra from Figure 3(c). Compared to the measured total intensity S0 we can clearly see that most of the signal, including the small peak at $\lambda_0 \sim 1275$ nm, is unpolarized. We ascribe this unpolarized emission to the luminescence from the substrate. The peaks in the polarized contribution all correspond to modal features in Figure 2 (for both excitation positions A and B) and demonstrates the power of polarimetry to filter out these unpolarized contributions to obtain clear resonances with a high contrast.

Figures 4(a,b) show measurements of the polarization-filtered CL emission intensity dis-290 tributions from WG2, at $\lambda_0=1425$ nm, for x and y polarization. Clearly, the emission is 291 polarized along the waveguide axis y. Figures 4(c,d) show the calculated modal field inten-292 sity distributions (summed over k) at $\lambda_0=1450$ nm for the E_y (c) and E_x (d) components. 293 We observe good qualitative agreement between the calculations and the measurements, es-294 pecially for the E_y component, while the calculated E_x intensity is more intense than the 295 x-polarized data. At this wavelength the mode is guided, but it is close to the light line. The 296 emission can still escape, due to scattering from roughness and imperfections for instance. 297 The emission directionality towards the surface normal $(k \sim 0)$ suggests, however, that the 298 mode can radiate out directly, indicating that the leaky part of the odd mode contributes to 290

300 the measured emission.

For this reason we also calculate the field profiles at $\lambda_0 = 1500$ nm, where the dispersion 301 relation of odd mode intersects the frequency window of the calculation for regions of k both 302 above the light line (close to k=0) and below the light line. The modal intensity distributions 303 for k above the light line show very good agreement with the data, as we can observe in 304 Figure 4(e) for the E_y intensity and in Figure 4(f) for the E_x intensity. The intensity profiles 305 for k below the light line differ more from the measured emission profiles (see Figure S7 of 306 the Supporting Information). Comparing the measurements to the calculations, we find that 307 the intensity distributions and relative intensities (for both polarizations) show agreement 308 for both calculations, but there is clearly a better match with the leaky distributions at 300 $\lambda_0 = 1500$ nm. The discrepancy in wavelength between measurement and calculation can be 310 attributed to variations between the measured and calculated geometrical parameters, which 311 we have shown to strongly impact the positions of all resonances in the spectra. We note 312 that the calculations are not designed to determine field profiles in the leaky region above 313 the light line, since they do not take into account nonzero values of k_z , which necessarily 314 exist for leaky modes that radiate out of the waveguide to free space. Calculations in other 315 systems, however, that do fully take leaky contributions into account, have shown that the 316 mode can retain its overall field profile, even if it does becomes more lossy. 59,60 In our case 317 this is advantageous, as the mode is radiating out of the structure more freely, allowing us 318 to measure it directly. 319

³²⁰ CL spectroscopy proves to be a useful technique to measure modes in nanophotonic struc-³²¹ tures, comparable to NSOM for example. In the case of NSOM, the near field is mapped ³²² with a nanoprobe that is brought into the evanescent field of the light in the nanostructure. ³²³ As a result, different field components of both the electric and magnetic fields can be dis-³²⁴ tinguished, ^{31,32} allowing in-depth studies of confined modes at the nanoscale, including their ³²⁵ dispersion. However, the image formation is complex and the interpretation of the experi-³²⁶ mental results is non-trivial. The nanoprobes used to perform NSOM measurements can, in

certain cases, perturb the system, so care must be taken in the processing and interpretation 327 of the data. Another way to image confined modes is grating-assisted Fourier space imaging, 328 in which light from below the light-line is scattered to the far field by a secondary grating 329 and collected by a Fourier lens.^{61,62} This approach permits one to determine the dispersion 330 relation, symmetry, and interaction of confined modes, but the secondary grating can also 331 perturb the system similarly to the NSOM nanoprobes and adds additional complexity to 332 the fabrication. CL on the other hand is a noninvasive far field technique (the electrons 333 excite, but do not perturb, the electromagnetic modes), measuring light both from leaky 334 modes above the light line and from confined modes that scatter out due to defects. Unlike 335 NSOM it probes the fields inside the structure, instead of the evanescent near field. Or 336 rather, it does not directly measure the electric field, but the emission can be related to the 337 radiative LDOS³⁶ and the excitation resolution is truly nanoscale (~ 10 nm). 338

339 Conclusions

In conclusion, we have demonstrated that an electron beam can be used to excite the prop-340 agating TE modes of a Si photonic crystal waveguide, despite them being dominated by 341 in-plane field components. We applied, for the first time, spectroscopic cathodoluminescence 342 imaging polarimetry in the near-infrared spectral range to directly image the modal field dis-343 tribution and image the emission and polarization with nanoscale resolution. Accordingly, 344 the most striking feature that we observe is the odd TE waveguide mode of the structure. 345 which exhibits a highly localized emission intensity distribution. Using spectroscopic po-346 larimetry we demonstrate that the emission of this mode is fully linearly polarized along the 347 direction of the waveguide. This is supported by calculations of the electric field intensities 348 which show good qualitative agreement with both the measured intensity distributions and 349 polarization. Surprisingly, the vertically oriented electron beam can couple to this in-plane 350 mode, as a result of nonzero contributions from the out-of-plane field component at different 351

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. Spectroscopic cathodoluminescence imaging polarimetry is a powerful, noninvasive tool to measure light confinement, polarization and propagation at the nanoscale in photonic crystal waveguides and other complex nanophotonic structures.

358 Methods

³⁵⁹ Cathodoluminescence measurements

The measurements were performed in a FEI XL-30 SFEG (10–30 keV electron beam, \sim 30– 360 46 nA current) equipped with a home-built CL system.^{34,37,54} An aluminium parabolic mirror 361 collects the emitted light and directs it outside of the microscope to an optical setup. We 362 can measure the spectrum in the $\lambda_0=350-1000$ nm spectral range with a liquid-nitrogen-363 cooled back-illuminated silicon CCD array (Princeton Instruments Spec-10 100B) and in 364 the $\lambda_0=900-1600$ nm spectral range with a liquid-nitrogen-cooled InGaAs photodiode ar-365 ray (Princeton Instruments OMA V). Due to the readout noise of the individual pixels, we 366 smooth the spectra with a moving filter over a 2 nm bandwidth. We correct for the sys-367 tem response of the setup by using transition radiation from single crystal aluminium as a 368 reference.⁵⁸ A Faraday cup integrated in the sample holder measures the current of the elec-369 tron beam, which in combination with the system response allows us to determine the CL 370 emission probability. A quarter-wave plate (QWP, Thorlabs AQWP10M-1600) and linear 371 polarizer (Pol., Moxtek PUBB01A50M) are used together to measure the full polarization 372 state of the emitted radiation.³⁷ To measure the polarization we place a 3 mm wide slit in the 373 beam path followed by the QWP and Pol., which offers a good balance between signal inten-374 sity and polarization contrast.^{55,56} Because we focus all of the light passing through the slit 375 onto the spectrometer, the measured polarization is averaged over the zenithal angles that 376

are collected. A series of six measurements for different combinations of the QWP and Pol. 377 (horizontal/90°, vertical/0°, 45°, 135°, right- and left-handed circular) determine the Stokes 378 parameters, which fully describe the polarization state of the light. Measurement errors can 379 occur due to drift of the electron beam across the sample, bleaching or contamination leading 380 to a reduction in the measured intensity, as well as fluctuations in the current and optical 381 alignment of the mirror. For all spectral measurements we collect a dark reference spectrum 382 where we blank the electron beam, subtracting this from the data in the post-processing 383 stage. 384

385 Calculations

To calculate the modal fields of the photonic crystal waveguide, we calculated the eigenfre-386 quencies and complex field amplitudes E(r) using the MIT Photonics Band (MPB) code,⁵¹ 387 which is a plane-wave method that uses periodic boundary conditions to calculate the eigen-388 frequencies and eigenmodes of our PCWGs. The band structure diagrams were calculated 389 with the full 3D version. In order to conserve computational resources, we implemented a 390 2D version of the calculation using an effective index approximation to determine the field 391 profiles. The effective index of the slab was chosen to be that of a 220 nm thick slab of silicon 392 with the refractive index appropriate for each frequency range considered (for example for 393 wavelengths around $\lambda_0 = 1450$ nm, we used 3.484). This procedure yields an effective index 394 of 2.873 for TE modes and 1.831 for TM modes at $\lambda_0 = 1450$ nm. We determine the eigen-395 values between 99 % and 101 % of the desired frequency. The E_x , E_y , and E_z field profiles 396 (or eigenmodes) are calculated on a rectangular grid of points separated by a/16, ensuring 397 that the eigenfrequencies are converged to better than 0.1 %. The modes are normalized 398 such that $\int_{\text{unit cell}} \epsilon(r) * |E(r)|^2 dr = 1$. The calculations are performed for wavevectors in 399 the first irreducible Brillouin zone, after which we use symmetry arguments to add the fields 400 for different wavevectors with the correct weighting factor, over the full first Brillouin zone. 401 Essentially, we sum the field intensities over all wavevectors \mathbf{k} of the modes that occur within 402

 $_{403}$ the frequency range of the calculation, at each position r:

$$\frac{1}{(2\pi)^3} \sum_{n=1}^N \int_k |E_{n\mathbf{k}}^{(i)}(\mathbf{r})|^2 \delta(\omega - \omega_{n\mathbf{k}}) d\mathbf{k}. \quad i = x, y, z.$$

For the leaky/guided mode results we only sum over the wavevectors above/below the light line. 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 $\lambda_0=1500$ nm). The intensity inside the holes is set to zero to better compare the results to the measurements, since there is no polarizable material in the empty holes the electron beam does not produce radiation even if there can be a high field intensity and/or LDOS in the holes.

411 Supporting Information Available

The Supporting Information contains measured data from an additional sample, an input section of the waveguide studied here and for shorter wavelengths. Additionally, 2D calculations for TM polarization, 3D calculations for TE polarization, and a comparison of the calculated field components of the even and odd waveguide modes are presented. We also explain the spectroscopic polarimetry method in more detail.

⁴¹⁷ This material is available free of charge via the Internet at http://pubs.acs.org/.

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$_{421}$ Notes

A.P. is co-founder and co-owner of Delmic BV, a startup company developing a commercial
product based on the cathodoluminescence system that was used in this work.

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592 Graphical TOC Entry





Figure 1: (a) Scanning electron micrograph of one of the silicon PCWGs 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. The gray regions denote the continuum of available modes above and below the photonic band gap, within which we distinguish an even (blue) and odd (red) waveguide mode. The black dashed line corresponds to the light line of air. (d,e) Calculation of the modal intensity distributions of the odd (e) and even (f) waveguide modes, for $\lambda_0 = 1450$ nm, normalized to the maximum intensity for all polarizations and wavelengths. The white circles show the positions of the holes. (f) 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. Here we can focus the light onto a NIR spectrometer or filter the emitted beam with a (vertically oriented) slit and measure the full polarization state using a quarter-wave plate and linear polarizer. The PCWGs for all measurements in the main text are oriented along the y-axis of the coordinate system.



Figure 2: Measured CL emission probability of WG2, as a function of wavelength and excitation position, for center wavelengths of $\lambda_0=1170$ nm (a), $\lambda_0=1185$ nm (b), $\lambda_0=1400$ nm (c), and $\lambda_0=1425$ nm (d) (20 nm bandwidth). Black crosses denote the two locations for which we show spectra in Figure 3.



Figure 3: (a) CL emission probability as a function of wavelength, measured on WG2, comparing the spectra obtained for two different excitations positions A (red) and B (blue) indicated in Figure 2. (b) CL spectra obtained for excitation position A on five different waveguides (WG1–WG5) with different hole size. The inset shows the wavelength of the dominant peak as a function of hole radius. (c) Polarization-filtered spectra measured on WG2 for excitation position A. We determine the Stokes parameters S0 (black), S1 (turquoise), S2 (blue) and S3 (green) and use them to separate the polarized contribution (red) from the unpolarized contribution that is due to the background luminescence from the substrate (gray). We note that S1 and the polarized contribution overlap at $\lambda_0 \sim 1425$ nm.



Figure 4: 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 field intensity $|E_y|^2$ for the odd waveguide mode at $\lambda_0=1450$ nm and the corresponding calculation for $|E_x|^2$ (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 $|E_y|^2$ (e) and $|E_x|^2$ (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 S7 of the Supporting Information.