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Spectral Signatures of Transverse Optical Modes in Semiconductor Nanowires: supplementary material

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1. MODAL SIGNATURES FOR DIFFERENT EMITTER POLARIZATIONS

In this study, a broadband dipole emitter is used to simulate fluorescence emission on the GaN NW using Lumerical finite difference time domain (FDTD) [1] simulations. The dipole can be orientated at different angles to simulate different emission polarizations. The results are shown in Fig. S1 where spectral leakage associated with different waveguide modes varies based on emitter orientation [2]. This is particularly obvious when comparing panels (d) and (e) where the dipole is polarized along the NW axis and polarized vertically respectively. The difference in relative intensity between spectral stripes associated with mode 3-4 and 5-6 (also between mode 5-6 and 7-8) in Fig. S1(d, e) suggests that the polarization of the emission modulates the modal composition.

2. IDENTIFYING WAVEGUIDE MODES FROM THEIR SPECTRAL SIGNATURES

This section describes the method used in section 5 of the main text to locate the cutoff limits of various waveguide modes and identify their respective mode numbers. As described in the main text, the spectral stripes in the hyperspectral image are the manifestation of leakage of waveguide modes above their cutoffs. Thus, the cutoff limits should lie below (shorter wavelengths) the spectral stripes. In the case shown in Fig. S2(b), two spectral stripes are visible which correspond to leakage of two neighboring non-degenerate modes. The red and blue lines approximate their respective cutoff limits. Specifically, at y ~ 6 µm, the red line is determined by locating the midpoint between the centers of the two stripes which are separated by ~ 60 nm. The centers of the stripes are determined by averaging 59 brightest

Fig. S1. FDTD simulations of a NW atop a glass substrate for different orientations of the simulated dipole emitter. (a) Adjusted height profile of the simulated NW from Fig. 6(d) in the main body of the manuscript. (b-e) Simulated hyperspectral data collected by an E-field monitor positioned 300 nm below GaN-glass interface. The broadband dipole emitter (positioned at y = 0) is polarized along x (c), y (d), and z (e) direction respectively. Panel (b) shows the average of results from Panels (c-e). The red solid lines indicates cutoff limits for waveguide mode 3-4, 5-6 and 7-8 respectively.
spectral points (span over 25 nm) on their respective leakage peaks. For regions where only one stripe is visible, the cutoff is found by adding (subtracting) 30 nm to the center of the lower (upper) stripe. The blue line is located 60 nm below the red line.

Modal analysis (Fig. 5 in main text) shows that cutoff wavelengths for various waveguide modes are distributed unevenly across the spectrum. Different neighboring non-degenerate modes are separated by different spectral distance. Therefore, for hyperspectral images where two or more spectral stripes are visible, their corresponding mode numbers can be identified. Specifically, \( \lambda_r = 2a/V_{\text{mode}} \) (Eq. 4 in main text) shows that edge length (and thus height) of the NW can be extracted from cutoff wavelengths of a mode and its V-number. Cutoff wavelengths for two different modes would yield the same NW heights only when the correct V-numbers are used. For example, in Fig. S2, if V-numbers for mode 3-4 (red) and mode 5-6 (blue) are used, the cutoff wavelengths (red and blue solid lines in panel (b)) predict the same heights (red and blue dashed-dotted lines in panel (c)), which differ by less than 5 nm. Thus, the red and blue lines are identified as cutoffs for mode 3-5 and 5-6 respectively. In contrast, if V-numbers for modes 1-2 and 3-4 or mode 5-6 and 7-8 are used, they would predict radically different heights (dotted and dashed lines). Hence, without the aid of topographical measurement such as AFM, we are able to identify the allowed waveguide modes within the NW across the hyperspectral space, Fig. S2(b): the region above the red line allows propagation of mode 1-2; the region between the red and blue lines allows mode 1-4; and the region below the blue line allows mode 1-6.

3. INTERPRETATION OF NW AFM IMAGES

Due to the limitations of atomic force microscopy (AFM), there is some uncertainty in nano-scale geometric characteristics of the scanned structure. The AFM topography is a convolution of the shapes of both the measured structure and the probe, which is specified as \( \sim 10 \text{ nm radius-of-curvature} \) for new probes used in our experiment, but which was not certain at the time the probe is used for NW measurements. This makes it difficult to resolve any potential curvature of NW apex. Note that nm-scale features such as the specific shape of the NW apex are generally less important for mode propagation in the waveguide since these modes do not concentrate light into sharp corners. However, our lack of knowledge about the probe curvature can lead to either overestimation or underestimation of the NW cross-sectional area (Fig. S3) which determines the modal cutoffs. In particular, if we assume that the NW cross section is an equilateral triangle with the measured height, then we would potentially underestimate the area, as indicated by dashed red curve in Fig. S3(c). On the other hand, if we assume that the NW in an equilateral triangle with sidewalls that match the measured AFM profile, then we would overestimate the area, as indicated by solid red curve in Fig. S3(c).

Sampling artifacts can also contribute to uncertainty in the NW apex height, and thus deduced cross-sectional area. In particular, even with an infinitesimally sharp AFM probe and NW apex, the scanning window for each pixel can introduce systematic underestimation of the height when scanning across non-flat area such as a NW apex due to averaging. When scanning across the apex of an isosceles triangular cross section with side wall angle \( \alpha \) (relative to the base), this underestimation can

\[
\Delta z = y_1 - y_2 = 2 \alpha \sqrt{\frac{R^2 - (R - y_1)^2}{2R}} - \Delta
\]

Fig. S2. Using spectral signatures to deduce NW height assuming different mode numbers. (a) Integrated fluorescence intensity map when the laser is positioned near the middle of the NW. (b) One-dimensional hyperspectral data from (a). (c) Comparison of NW height deduced from mode cutoff assuming different mode numbers. The red and blue height profiles in panel (c) are deduced from red and blue cutoff lines in panel (b) respectively. The dotted lines indicate deduced heights that assume the red and blue cutoff lines represent cutoffs for mode 1-2 and 3-4 respectively, whereas dashed-dotted lines assume mode 3-4 and 5-6, and dashed lines assume mode 5-6 and 7-8.

Fig. S3. Interpreting the AFM image of a NW. (a) AFM image with \( \sim 49\text{-nm lateral pixel size and}\ \sim 14\text{-ms scan time per pixel.} \) (b) Histogram of data (\( \Delta z \)) from panel (d) (\( y = 1 \mu m \) to \( y = 12 \mu m \)). (c) Cross-sectional profile of the NW (black line) interpolated from the red line in panel (a). The upper (lower) bound of the actual cross-sectional shape is illustrated as red solid (dashed) line. The difference of apex height between the upper and lower bound is labeled as \( \Delta z \). (d) \( \Delta z \) along the length of the NW. (e) Apex height (lower bound) along the length of the NW.
be analytically calculated as

\[ \Delta(x) = \frac{x}{L} \tan \alpha x + \frac{L - x}{L} \tan \alpha (L - x) = \tan \alpha (L - 2x + \frac{2x^2}{L}) , \]

where \( L \) is the pixel width and \( x \) is window position relative to the apex. For Fig. S3 (\( L = 49 \) nm; same NW from Fig. 4 and 6 in the main text), since the scanning direction is angled at \( \sim 66 \) degrees relative to NW, the scanned side wall angle effectively satisfies \( \tan \alpha = (\tan 66^{\circ})(\sin 66^{\circ}) \). Thus, even with an ideal probe and NW apex, we can expect underestimation in the height of at least \( \sim 19 \) nm \( (x = L/2) \), at most \( \sim 39 \) nm \( (x = 0) \), and \( \sim 26 \) nm on average.

Taking these effects into account, we can establish the lower and upper bound of the NW geometry based on the AFM geometry, as shown in Fig. S3(c). The upper bound is an equilateral triangle (red solid line) that is traced from the midpoints of the side wall of the AFM geometry (black line). The lower bound is found by utilizing the same apex height as the measured value. The height difference between the upper and lower bound, \( \Delta z \), is plotted on Fig. S3(d) as a function of distance along the NW \( (y) \), and a histogram of these values is plotted in panel (b), showing an average value of \( \sim 53 \) nm with \( \sim 5 \) nm standard deviation and a 95% confidence interval of about \( \pm 10 \) nm. In the main text, a constant \( \Delta z \) (53 nm for this wire) along the NW length is used to avoid introducing nonphysical geometric features that arise from other measurement artifacts when scanning across the NW side walls.

4. POSITIONAL SENSITIVITY OF LASER COUPLING

This section experimentally demonstrates the positional sensitivity of laser coupling. As shown in Fig. S4(b), moving the laser focus from the left facet to the middle of the NW \( (y = 2.02 \mu m \) to \( y = 5.15 \mu m \)) decreases the fluorescence signal along the NW significantly, which suggests a decrease in the intensity of the excitation laser along the NW (i.e., waveguiding of the laser is suppressed). When the laser is focused about \( 500 \) nm from the end facet at \( y = 2.52 \mu m \) (red dashed line), the fluorescence signal along the NW is similar to the case where it is focused near the NW center (black solid line), indicating minimal coupling of the laser into guided modes. The positional sensitivity can be characterized qualitatively by observing the light signal near one end facet of the NW while moving the laser focus toward the other, as shown in Fig. S4(d). The idealized simulation (green) shows effective coupling when the end facet falls within the diffraction-limited laser spot, while the experimental results (red and blue) are about three times as broad. This is consistent with the comparison of laser spot size between simulation and experiment, as shown in Fig. S4(c). It is also worth noting that the fluorescence and laser light have similar positional sensitivity despite the fact that fluorescence can be further broadened by delocalization effects [3] such as carrier diffusion and secondary emission, which means that these effects have no significant impact on coupling.

REFERENCES

1. D. M. Sullivan, *Electromagnetic Simulation Using the FDTD Method* (Wiley-IEEE Press, 2013), 2nd ed.
2. Z. Li, K. Bao, Y. Fang, Y. Huang, P. Nordlander, and H. Xu, “Correlation between incident and emission polarization in nanowire surface plasmon waveguides,” Nano Lett. 10, 1831–1835 (2010).
3. W. Tian, C. Zhao, J. Leng, R. Cui, and S. Jin, “Visualizing carrier diffusion in individual single-crystal organolead halide perovskite nanowires and nanoplates,” J. Am. Chem. Soc. 137, 12458–12461 (2015).