

Modeling of photon scanning tunneling microscopy by 2-D quadridirectional eigenmode expansion



Manfred Hammer*

MESA⁺ Research Institute
University of Twente, The Netherlands

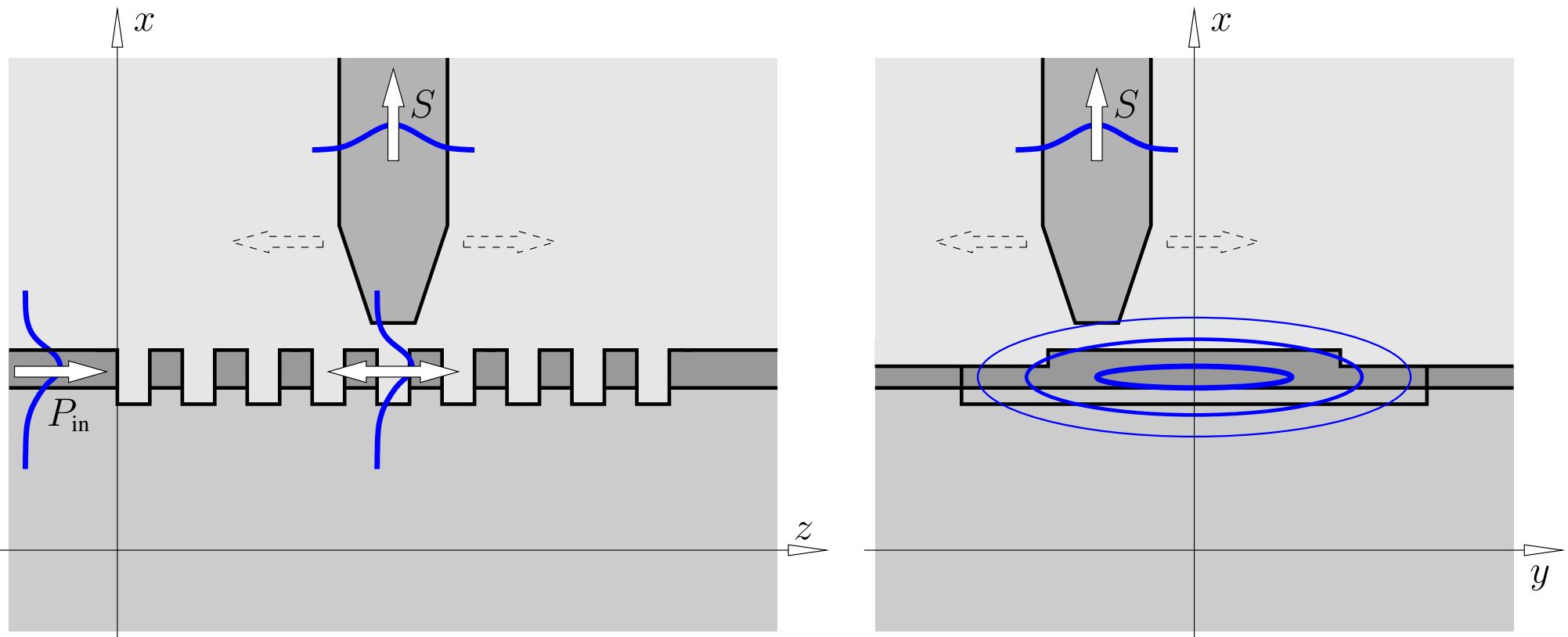
PIERS 2004, Progress in Electromagnetics Research Symposium, Pisa, Italy, 28. – 31.03.2004

* Department of Applied Mathematics, University of Twente
Phone: +31/53/489-3448

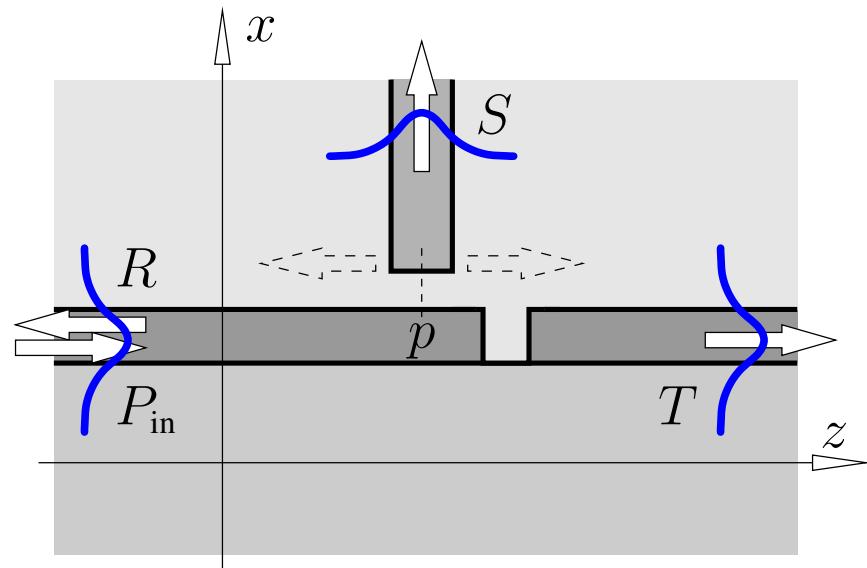
Fax: +31/53/489-4833

P.O. Box 217, 7500 AE Enschede, The Netherlands
E-mail: m.hammer@math.utwente.nl

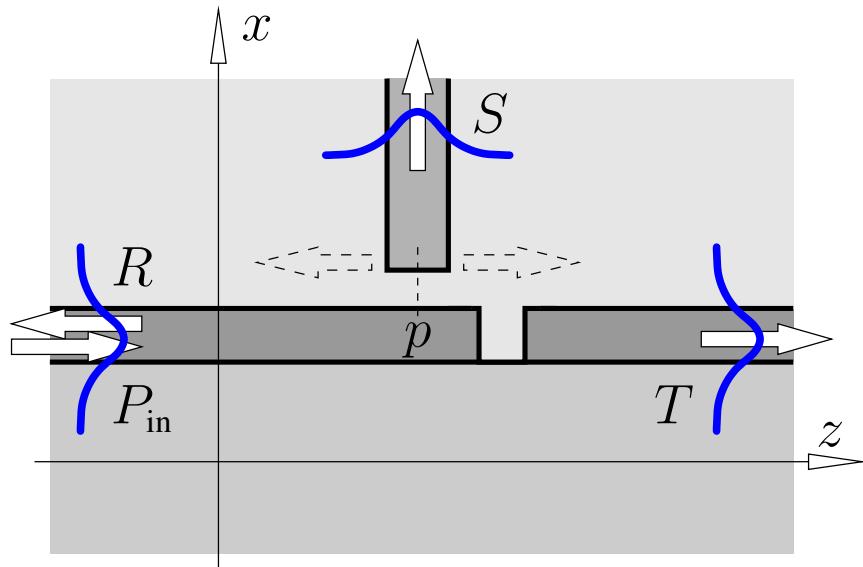
Photon scanning tunneling microscopy (PSTM) of photonic devices



Simplified 2-D model



Simplified 2-D model

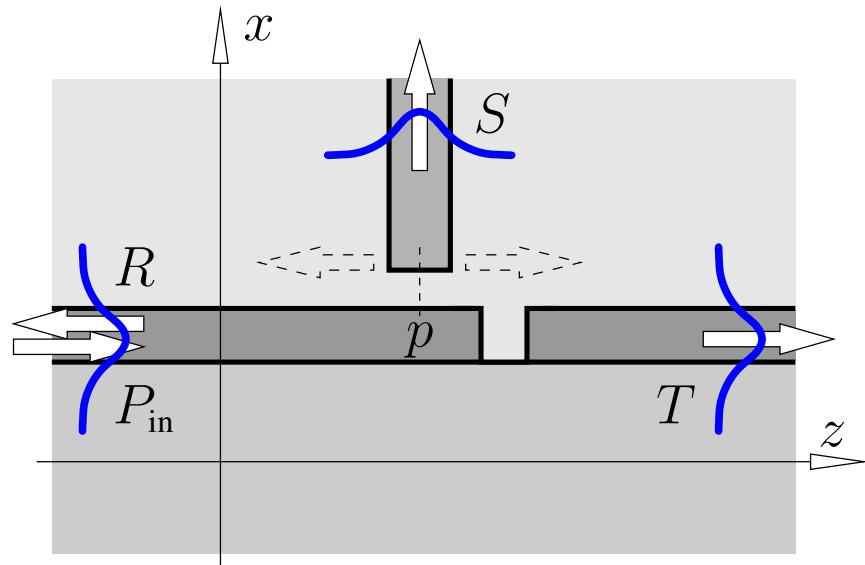


$$P_{\text{in}} = 1. \quad S(p) = ?$$

$$R(p), T(p) = ?$$

$$S(p) \xleftarrow{?} (\text{optical field})|_p$$

Simplified 2-D model



$$P_{\text{in}} = 1. \quad S(p) = ?$$

$$R(p), T(p) = ?$$

$$S(p) \xleftarrow{?} (\text{optical field})|_p$$

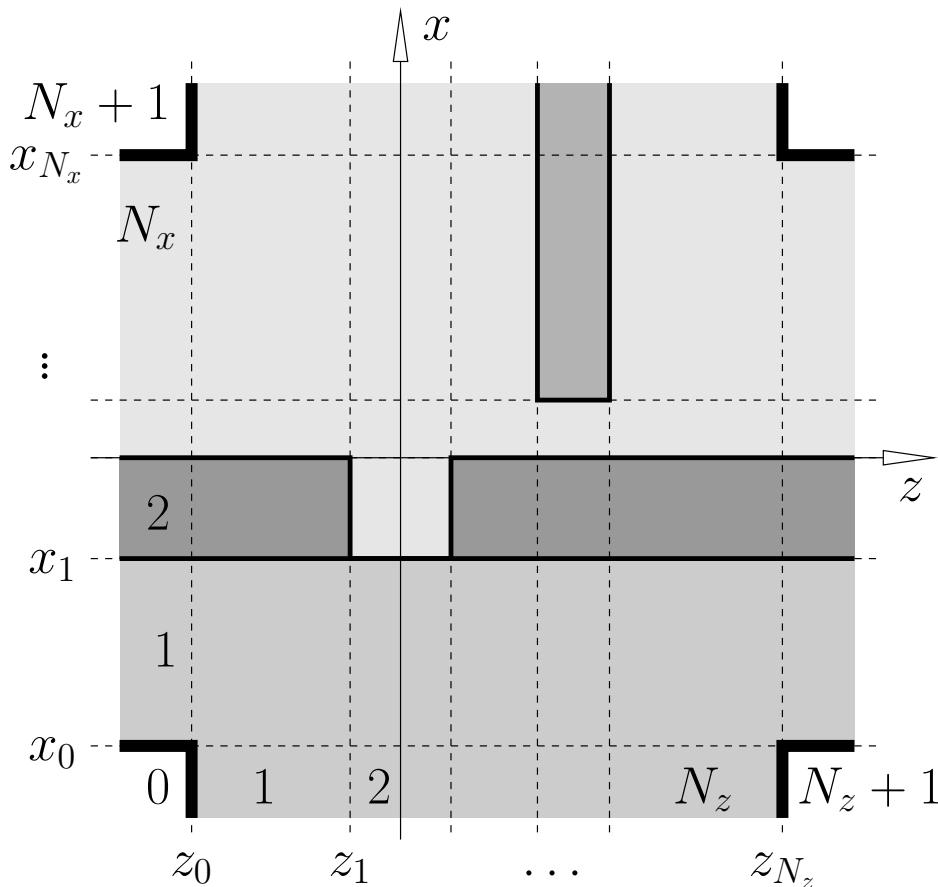
Fixed optical frequency, rectangular piecewise constant refractive index,
horizontal & vertical guided wave in- and outflux

→ *QUEP simulations*

Outline

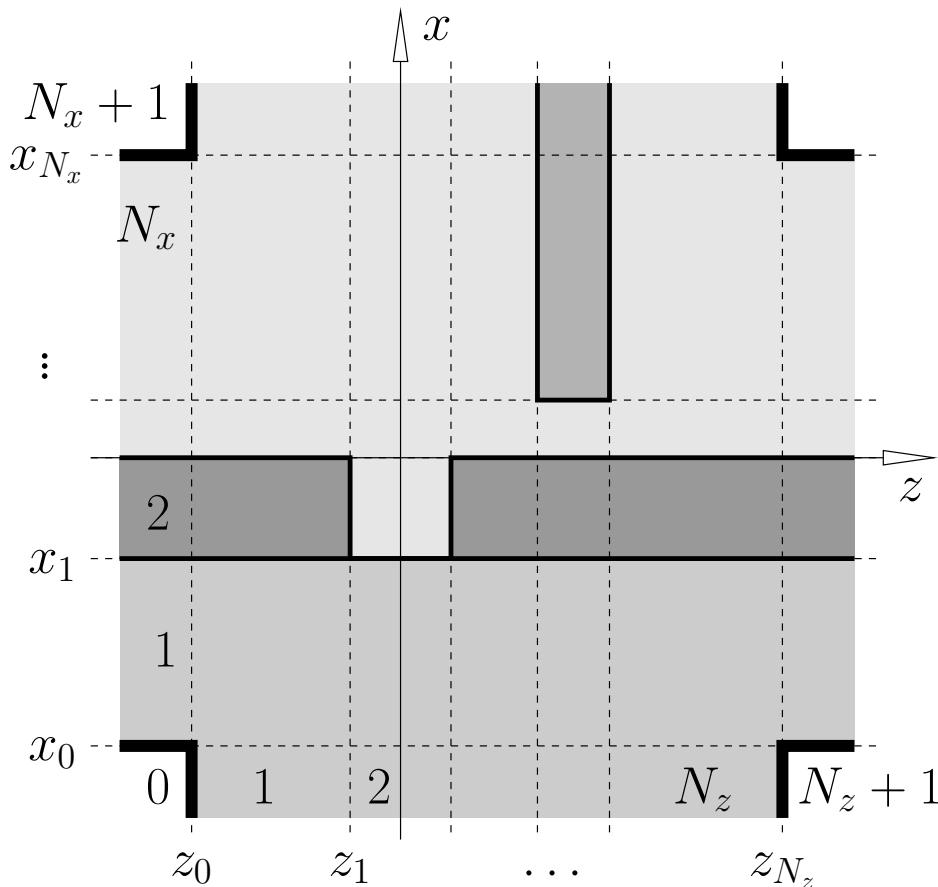
- Quadridirectional eigenmode propagation:
 - Problem setting
 - Eigenmode expansion
 - Algebraic procedure
- 2-D PSTM model, numerical results:
 - Probing evanescent fields
 - Hole defect in a slab waveguide
 - Short waveguide Bragg grating
 - Resonant defect cavity
 - Bragg grating: PSTM experiment & 2-D model

Simulations, problem setting



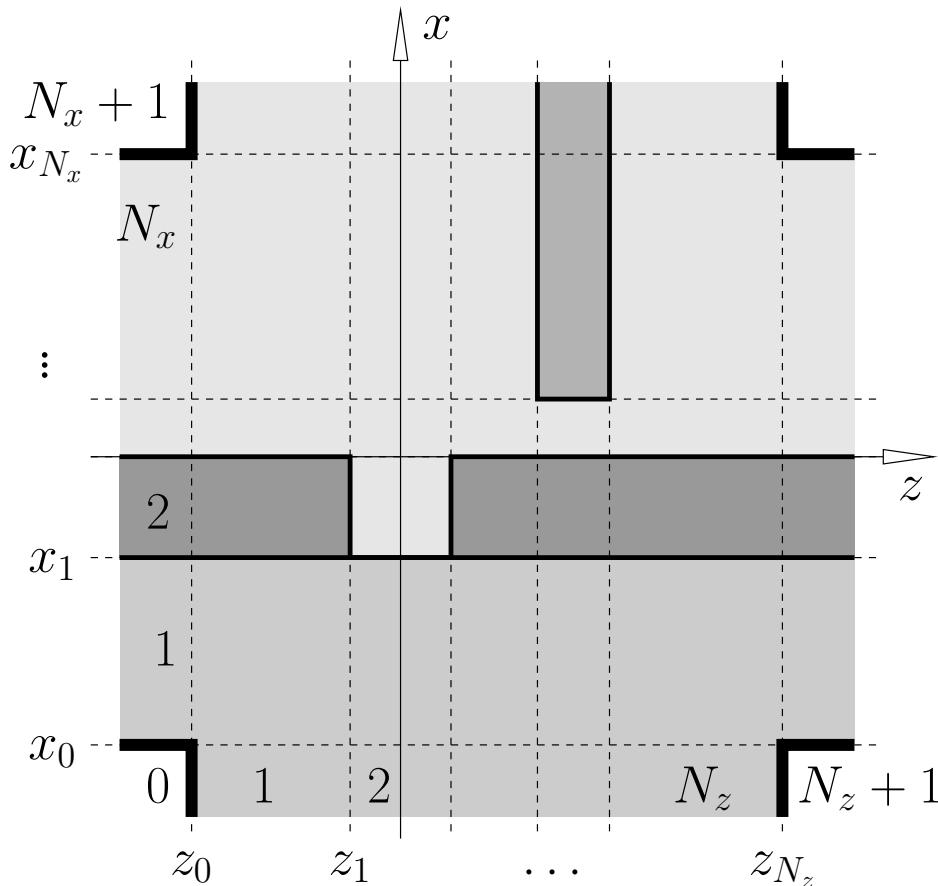
- 2-D TE/TM Helmholtz problem,
vacuum wavelength $\lambda = 2\pi/k$.

Simulations, problem setting



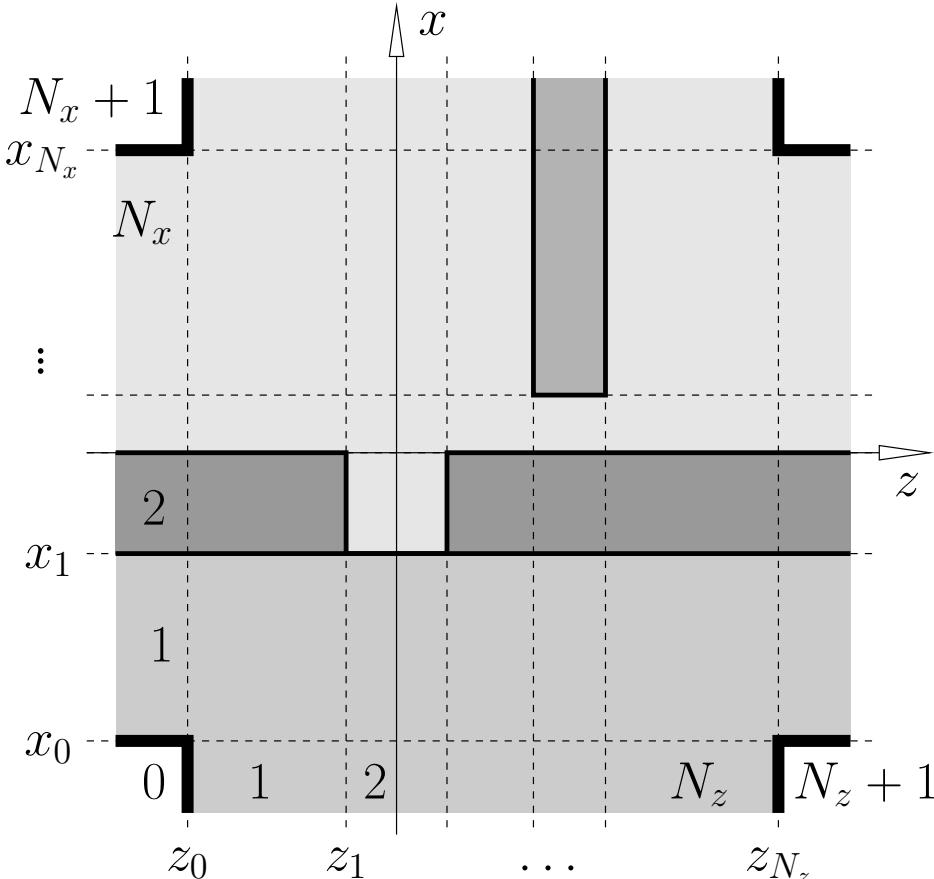
- 2-D TE/TM Helmholtz problem, vacuum wavelength $\lambda = 2\pi/k$.
- Piecewise constant, rectangular refractive index distribution; linear, lossless materials.

Simulations, problem setting



- 2-D TE/TM Helmholtz problem, vacuum wavelength $\lambda = 2\pi/k$.
- Piecewise constant, rectangular refractive index distribution; linear, lossless materials.
- Rectangular interior computational domain, influx & outflux across all four boundaries, outwards homogeneous external regions.

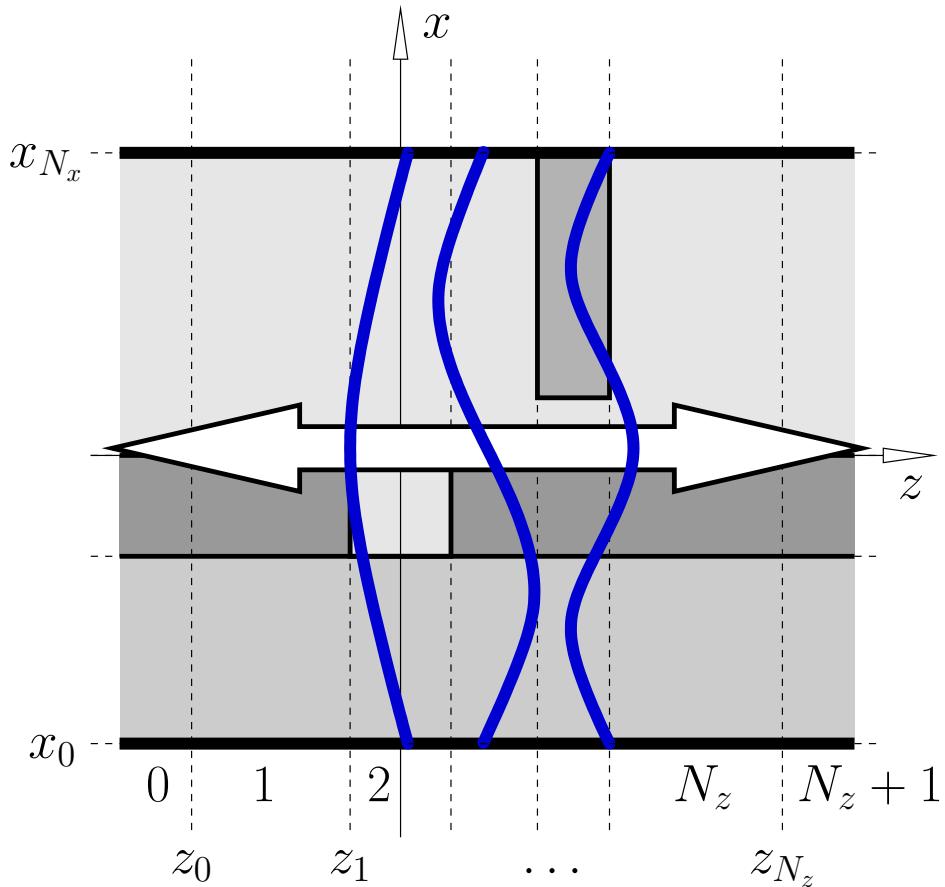
Simulations, problem setting



- 2-D TE/TM Helmholtz problem, vacuum wavelength $\lambda = 2\pi/k$.
- Piecewise constant, rectangular refractive index distribution; linear, lossless materials.
- Rectangular interior computational domain, influx & outflux across all four boundaries, outwards homogeneous external regions.
- Assumption $E_y = 0, H_y = 0$ on the corner points and on the external border lines is reasonable for the problems under investigation.

Modal basis fields

Basis fields,
defined by Dirichlet boundary conditions $E_y = 0$ (TE) or $H_y = 0$ (TM):



Horizontally traveling eigenmodes:

M_x profiles

and propagation constants

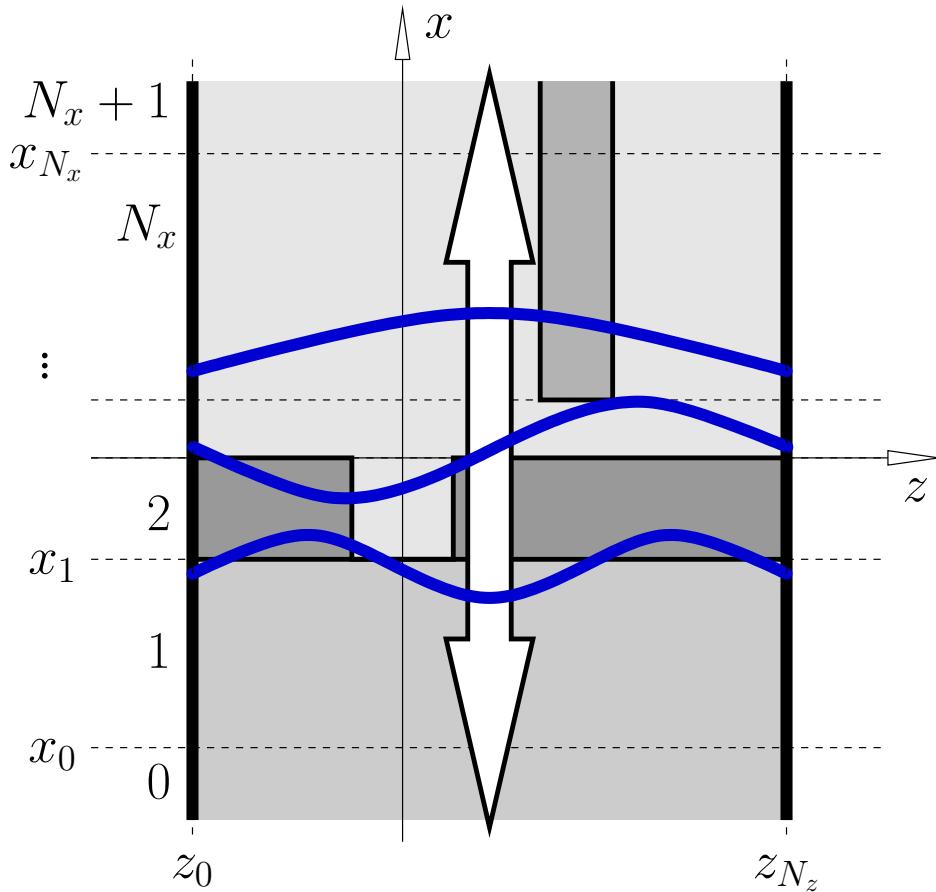
$$\psi_{s,m}^d(x)$$

$$\pm\beta_{s,m}$$

of order m , on slice s ,
for propagation directions $d = f, b$,

Modal basis fields

Basis fields,
defined by Dirichlet boundary conditions $E_y = 0$ (TE) or $H_y = 0$ (TM):



... and vertically traveling fields:

M_z profiles

and propagation constants

$$\begin{array}{c|c} \hat{\psi}_{l,m}^d(z) & \\ \hline & \pm \hat{\beta}_{l,m} \end{array}$$

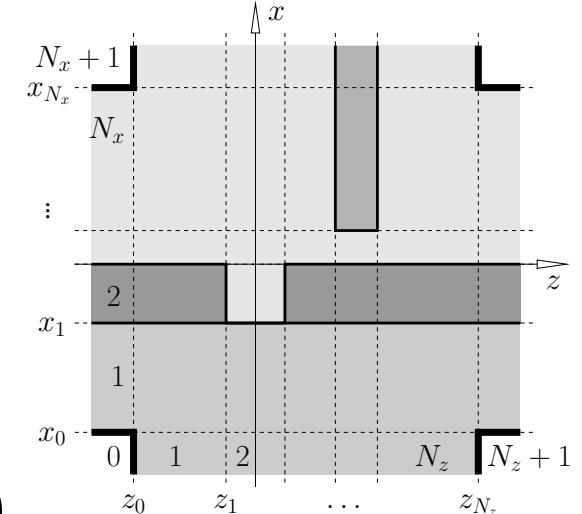
of order m , on layer l ,
for propagation directions $d = u, d$.

Eigenmode expansion

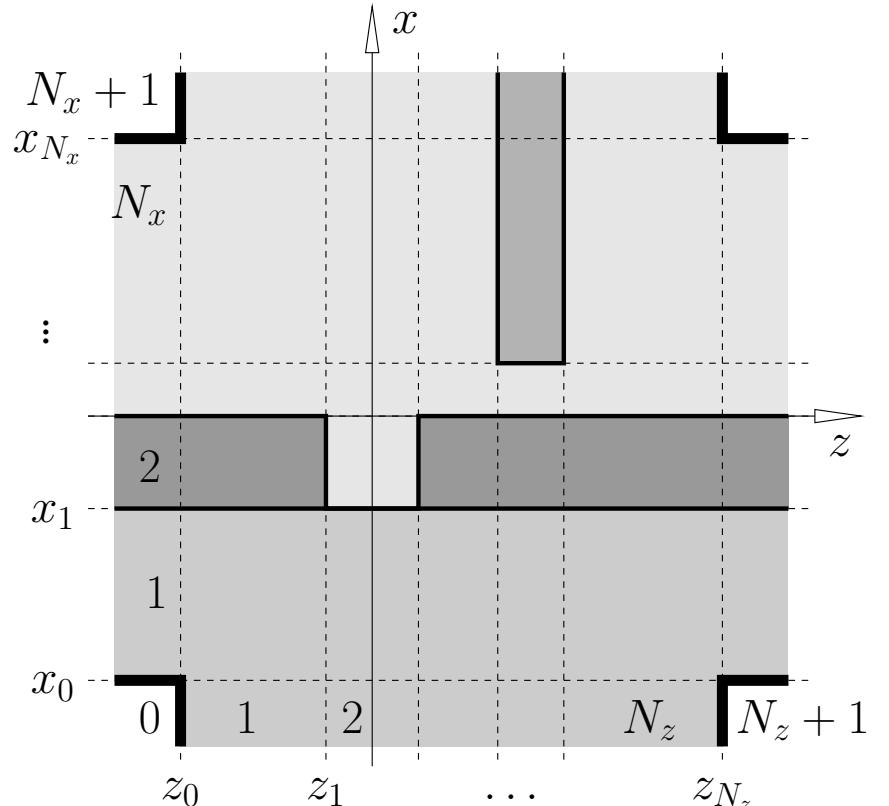
Ansatz for the optical field,

for $z_{s-1} \leq z \leq z_s$, $s = 1, \dots, N_z$,
and $x_{l-1} \leq x \leq x_l$, $l = 1, \dots, N_x$:

$$\begin{pmatrix} \boldsymbol{\varepsilon} \\ \boldsymbol{\mathcal{H}} \end{pmatrix}(x, z, t) = \operatorname{Re} \left\{ \sum_{m=0}^{M_x-1} F_{s,m} \psi_{s,m}^f(x) e^{-i\beta_{s,m}(z - z_{s-1})} \right. \\ + \sum_{m=0}^{M_x-1} B_{s,m} \psi_{s,m}^b(x) e^{+i\beta_{s,m}(z - z_s)} \\ + \sum_{m=0}^{M_z-1} U_{l,m} \hat{\psi}_{l,m}^u(z) e^{-i\hat{\beta}_{l,m}(x - x_{l-1})} \\ \left. + \sum_{m=0}^{M_z-1} D_{l,m} \hat{\psi}_{l,m}^d(z) e^{+i\hat{\beta}_{l,m}(x - x_l)} \right\} e^{i\omega t}.$$



Eigenmode expansion

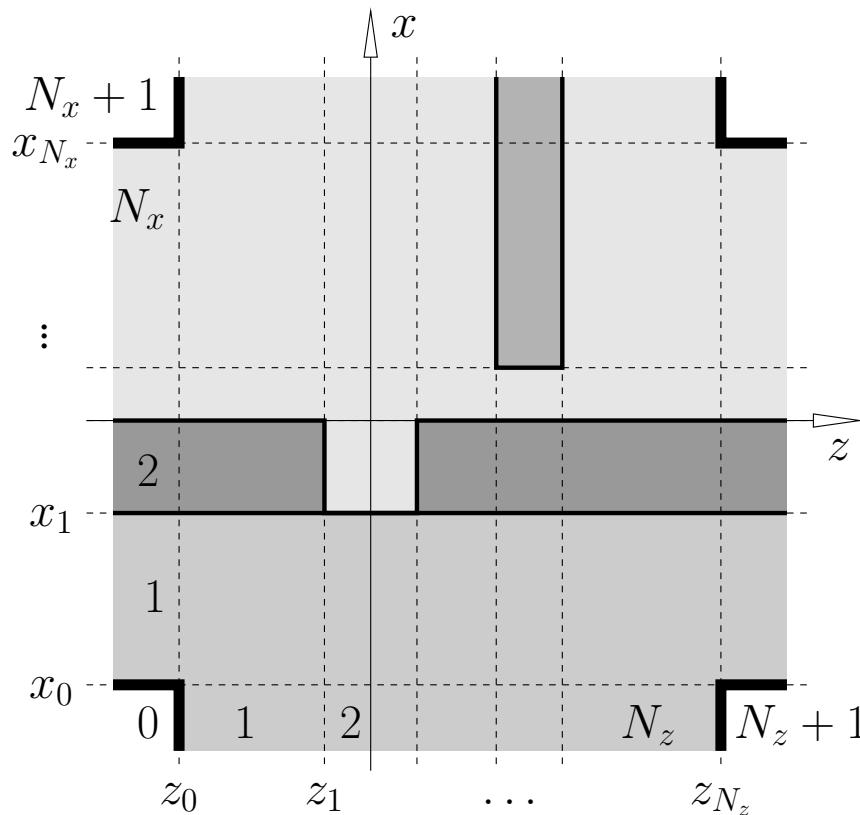


Mode products \leftrightarrow normalization, projection:

$$(\mathbf{E}_1, \mathbf{H}_1; \mathbf{E}_2, \mathbf{H}_2) = \frac{1}{4} \int (E_{1,x}^* H_{2,y} - E_{1,y}^* H_{2,x} + H_{1,y}^* E_{2,x} - H_{1,x}^* E_{2,y}) \, dx ,$$

$$\langle \mathbf{E}_1, \mathbf{H}_1; \mathbf{E}_2, \mathbf{H}_2 \rangle = \frac{1}{4} \int (E_{1,y}^* H_{2,z} - E_{1,z}^* H_{2,y} + H_{1,z}^* E_{2,y} - H_{1,y}^* E_{2,z}) \, dz .$$

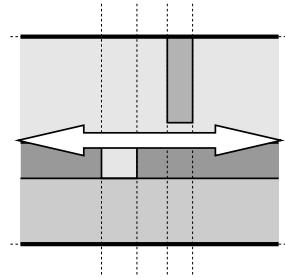
Algebraic procedure



- Consistent bidirectional projection at all interfaces
→ linear system of equations in $\{F_{s,m}, B_{s,m}, U_{l,m}, D_{l,m}\}$.
- Influx: $F_0, B_{N_x+1}, U_0, D_{N_z+1}$ → RHS, given.
- Outflux: $B_0, F_{N_x+1}, D_0, U_{N_z+1}$ → primary unknowns.

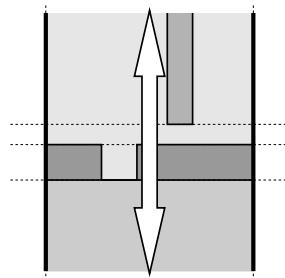
Algebraic procedure

- “Exact” mode profiles \longrightarrow interior problems decouple:



Solve for $\mathbf{F}_2, \dots, \mathbf{F}_{N_z}$ and $\mathbf{B}_1, \dots, \mathbf{B}_{N_z-1}$
in terms of \mathbf{F}_1 and \mathbf{B}_{N_z}

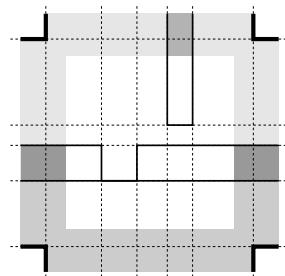
\longrightarrow BEP I.



Solve for $\mathbf{U}_2, \dots, \mathbf{U}_{N_x}$ and $\mathbf{D}_1, \dots, \mathbf{D}_{N_x-1}$
in terms of \mathbf{U}_1 and \mathbf{D}_{N_x}

\longrightarrow BEP II.

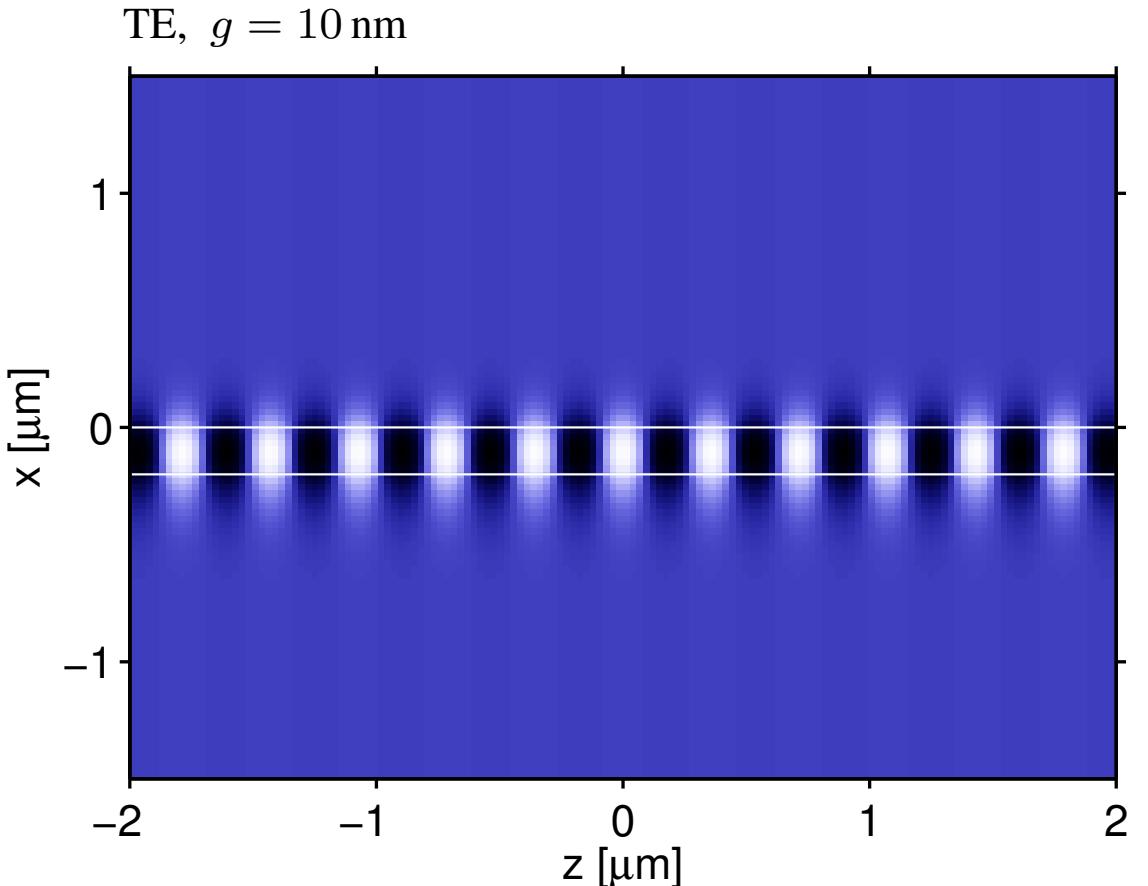
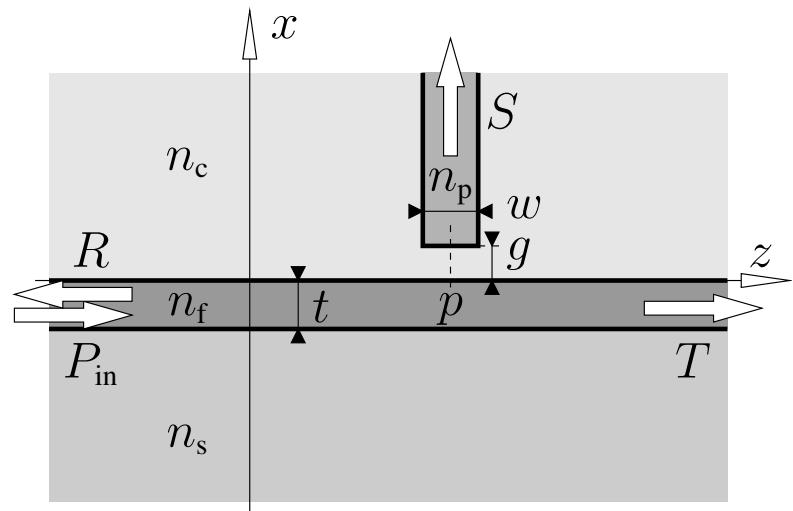
- Continuity of E and H on outer interfaces:



Interior BEP solutions
+ equations at $z = z_0, z_{N_z}, x = x_0, x_{N_x}$
 $\longrightarrow \mathbf{B}_0, \mathbf{F}_{N_x+1}, \mathbf{D}_0, \mathbf{U}_{N_z+1}$.

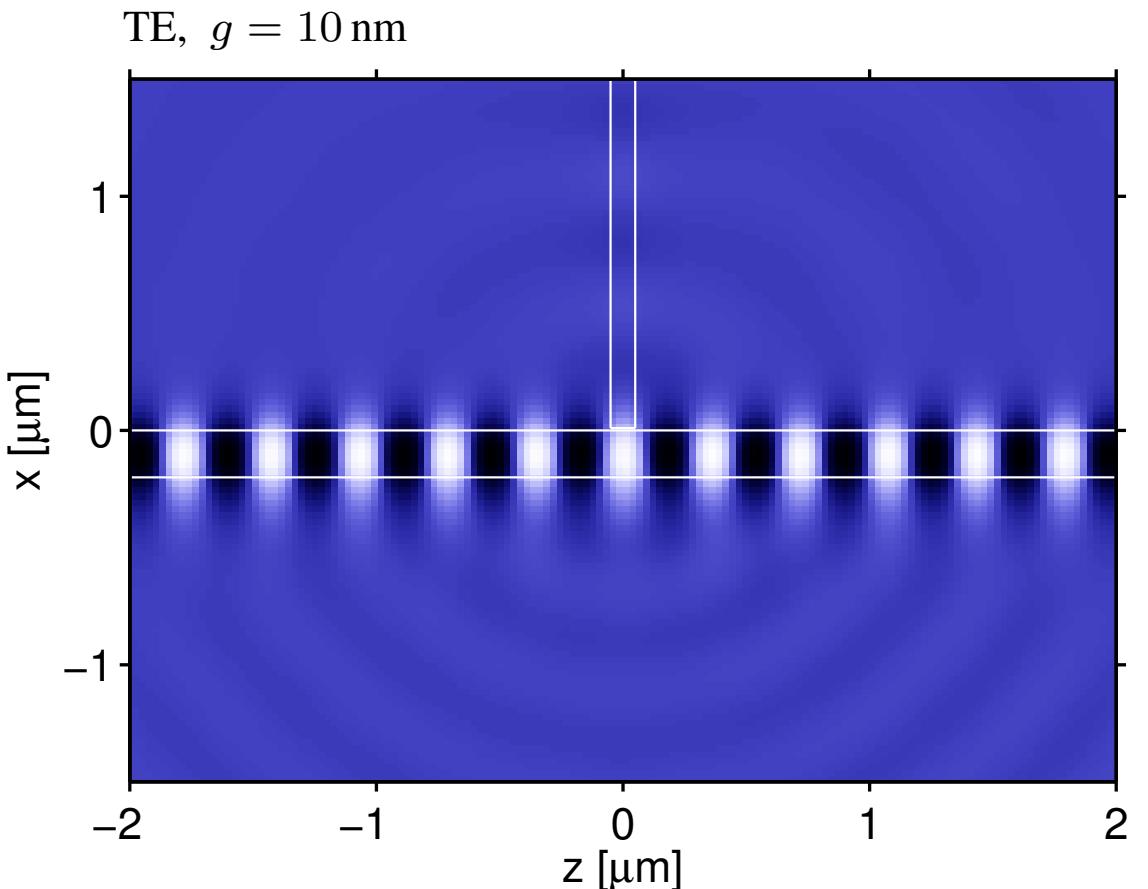
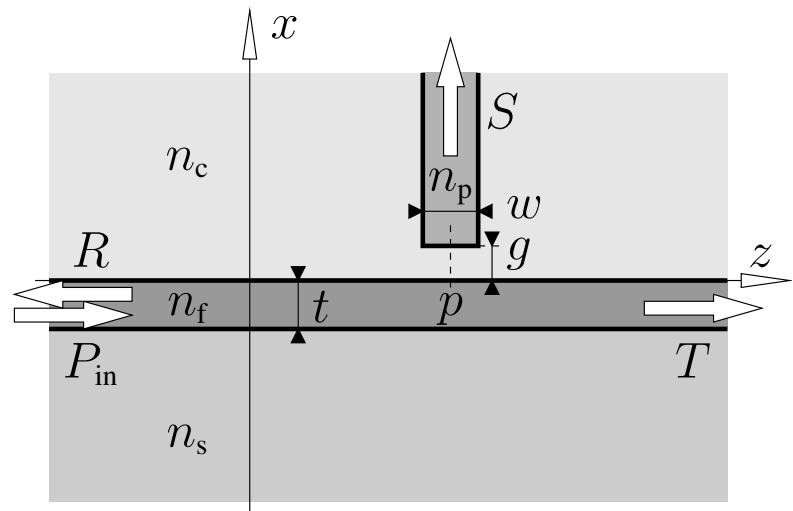
“QUadridirectional Eigenmode Propagation method” (QUEP).

Probing evanescent fields



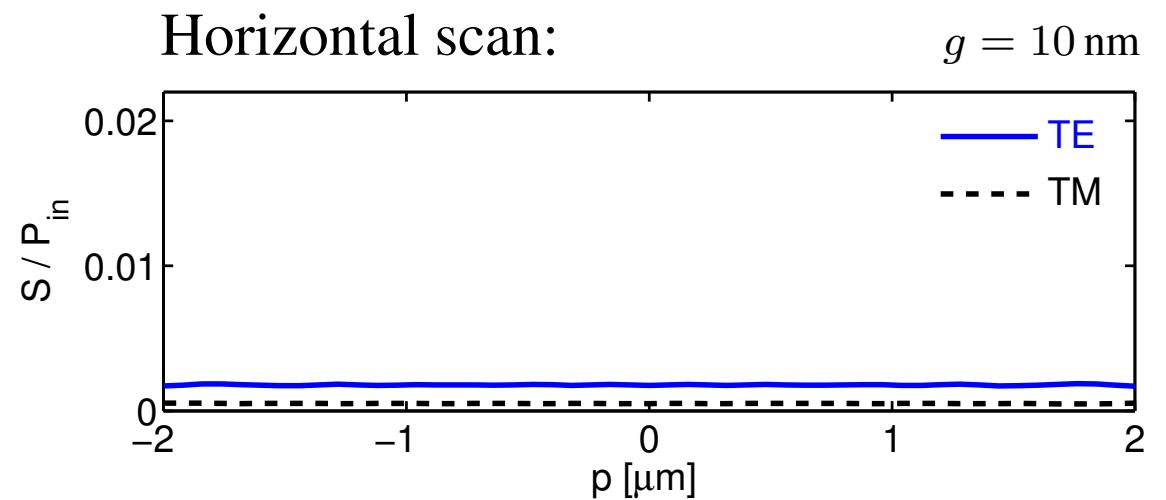
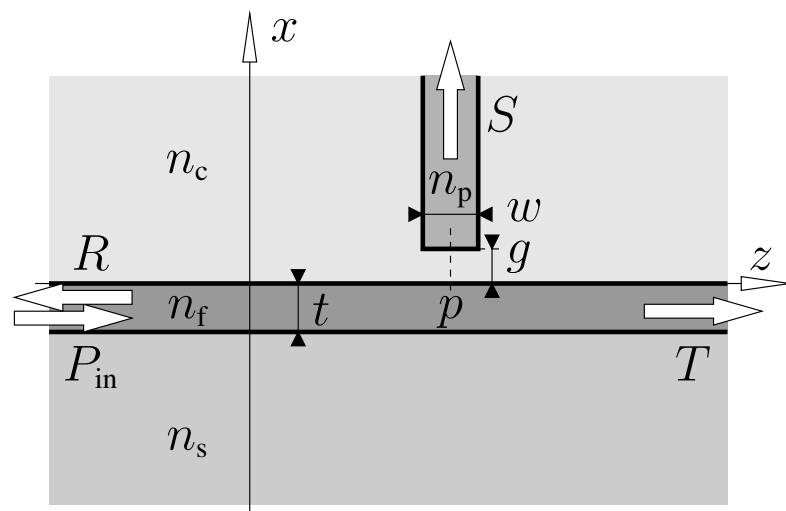
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
 $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 3.0] \mu\text{m}^2$, $M_x = M_z = 80$.

Probing evanescent fields



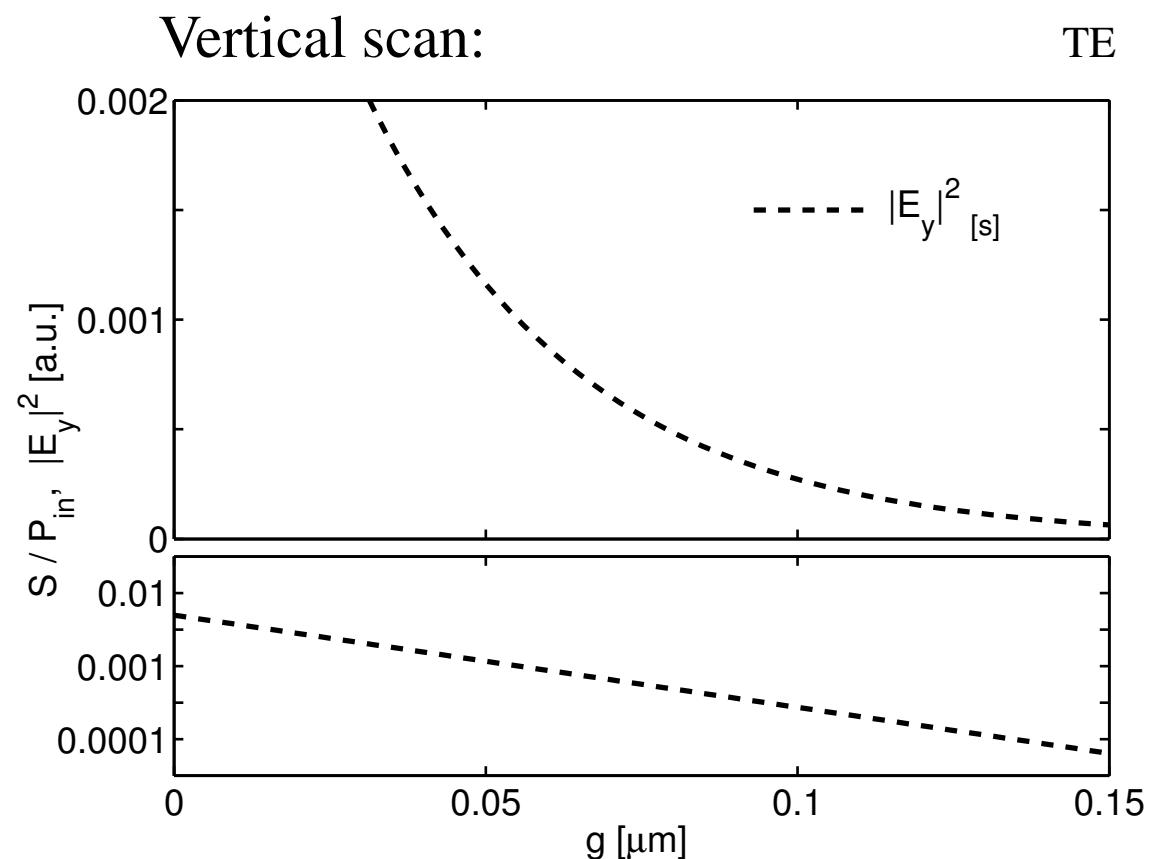
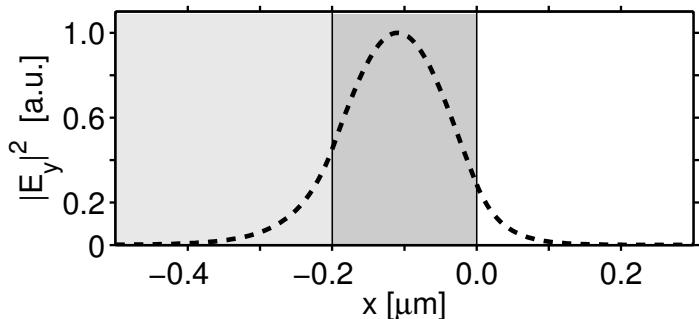
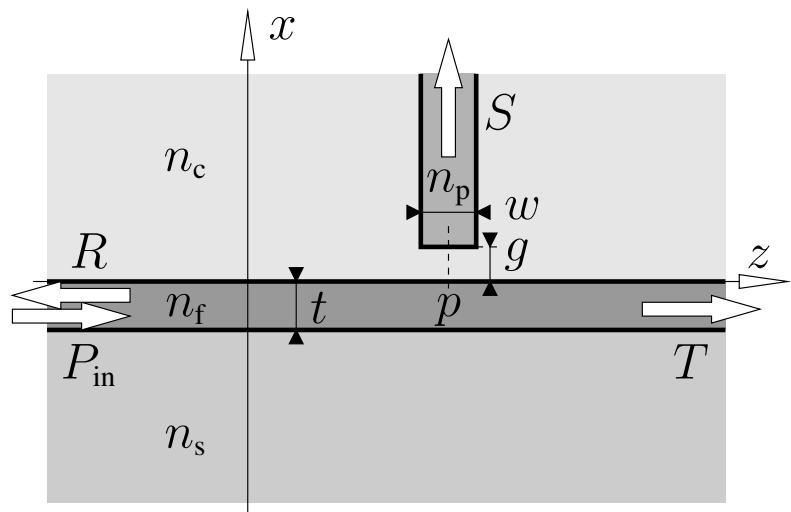
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
 $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 3.0] \mu\text{m}^2$, $M_x = M_z = 80$.

Probing evanescent fields

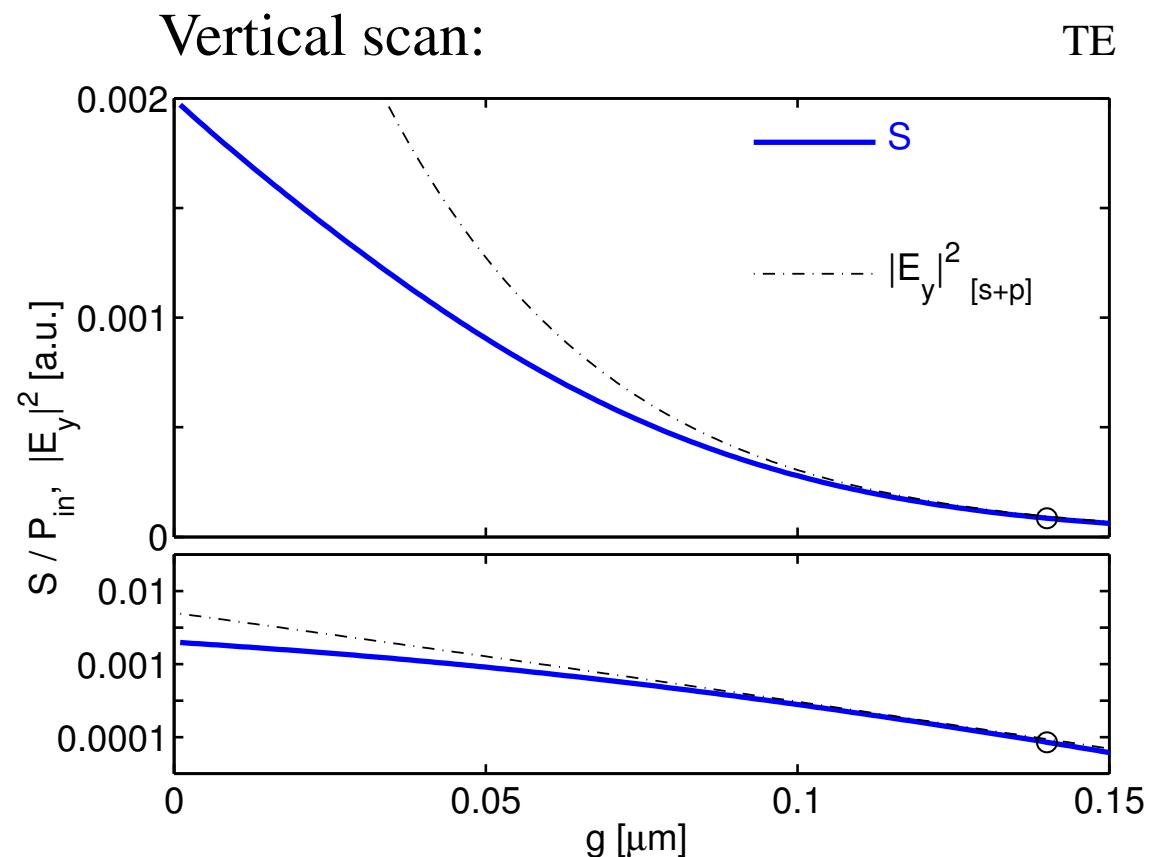
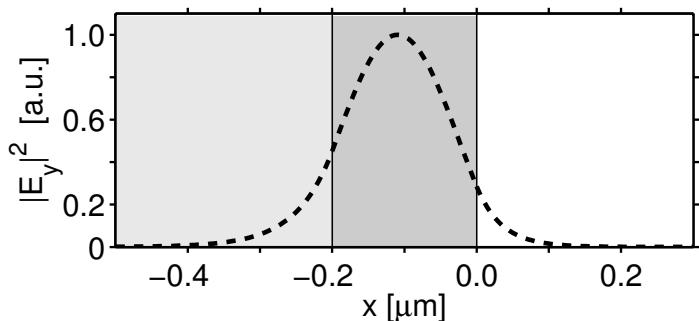
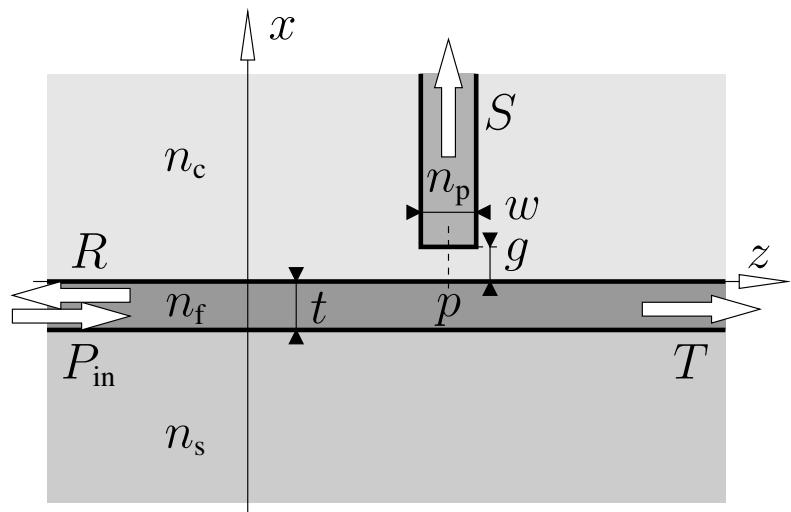


$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
 $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 3.0] \mu\text{m}^2$, $M_x = M_z = 80$.

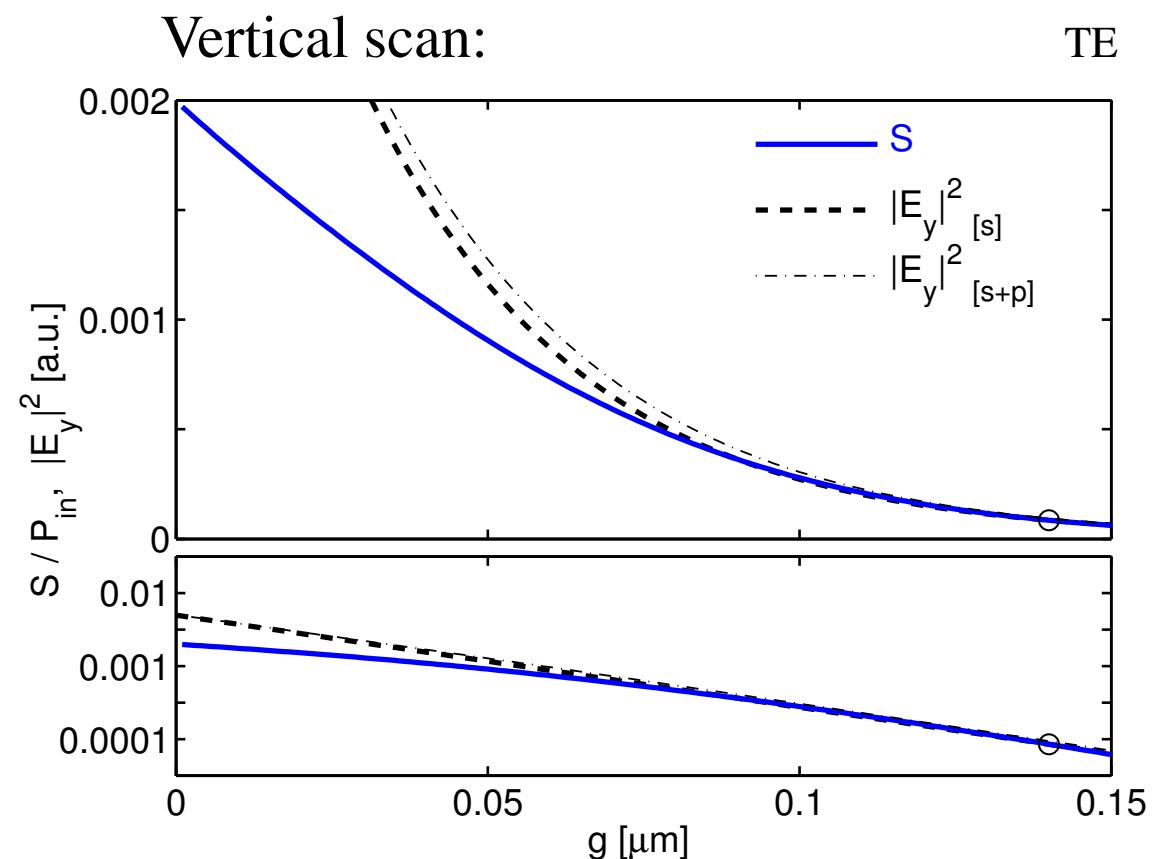
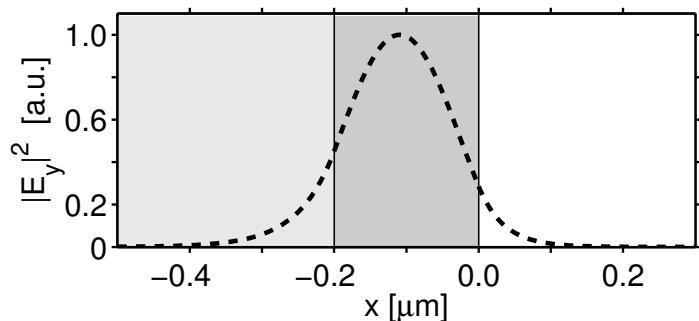
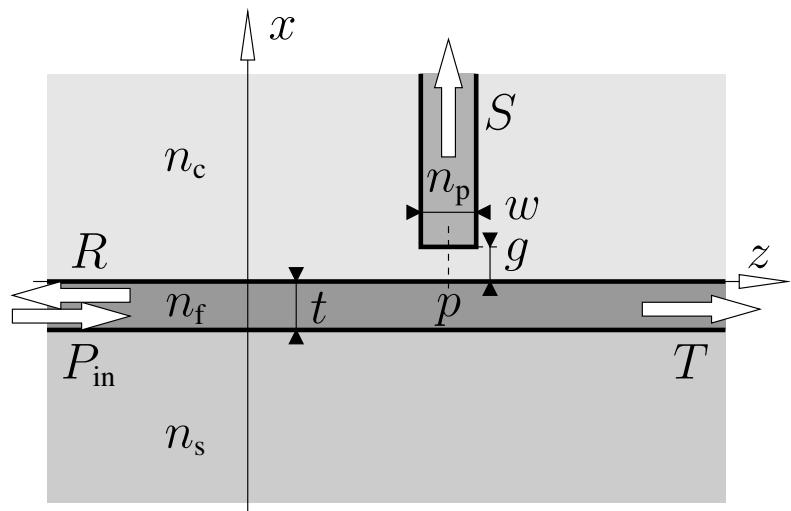
Probing evanescent fields



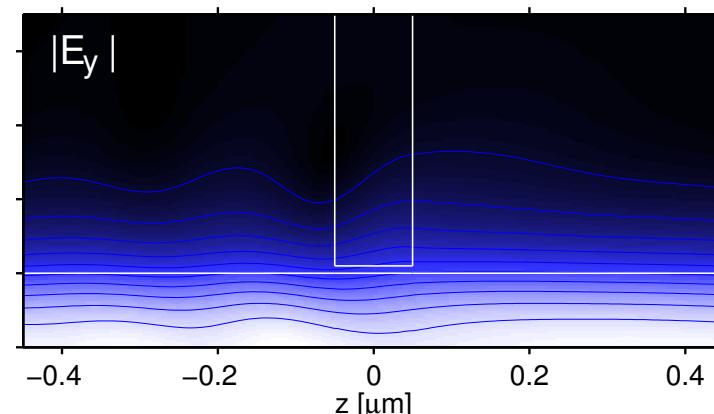
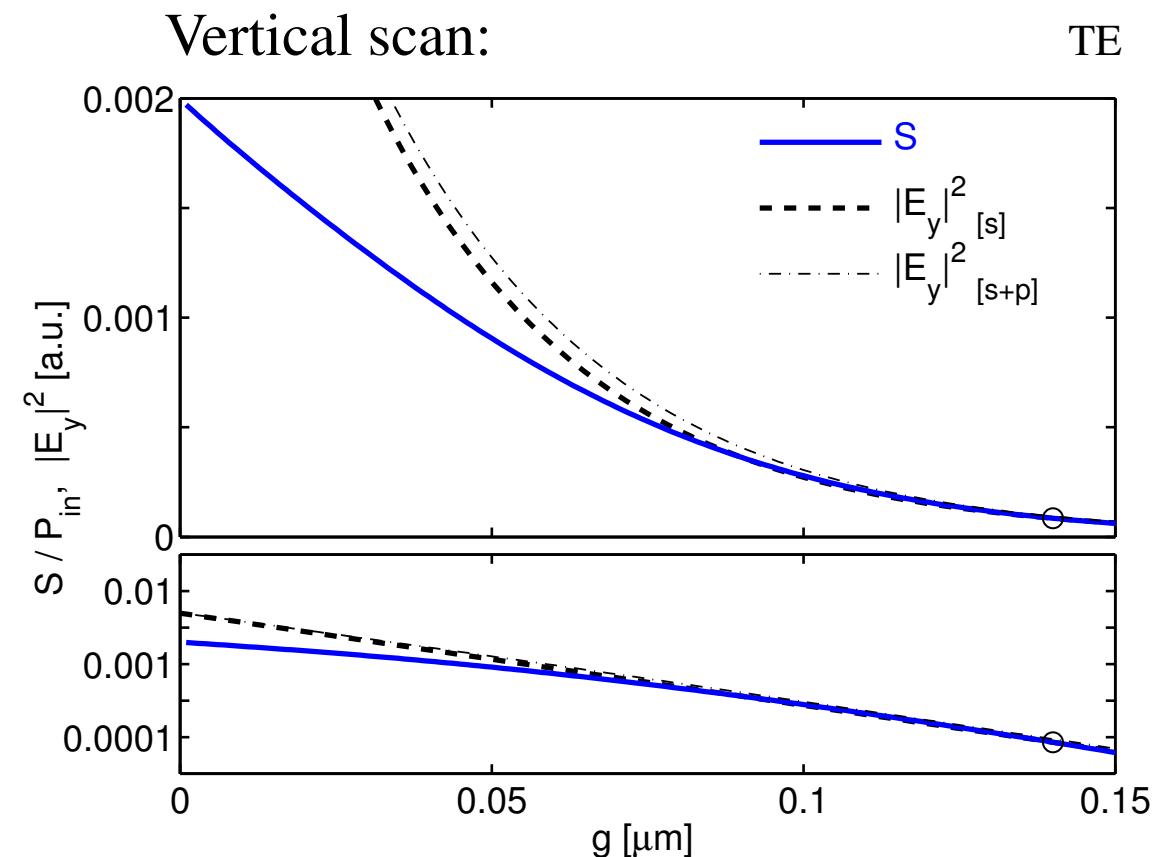
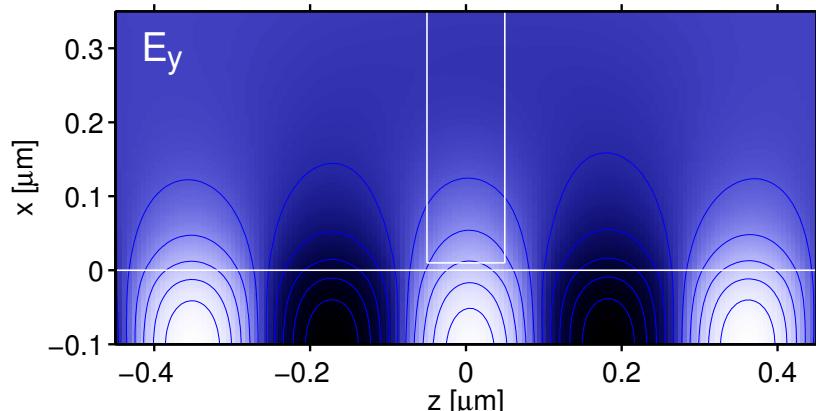
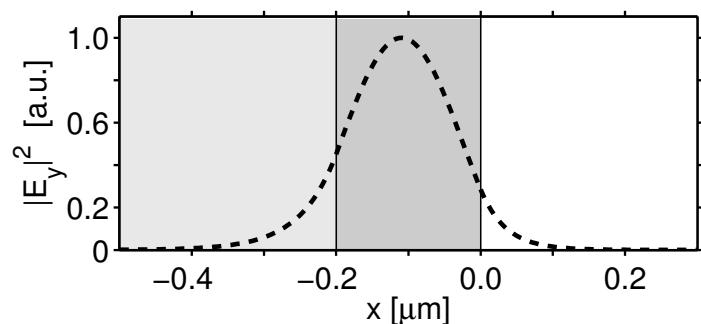
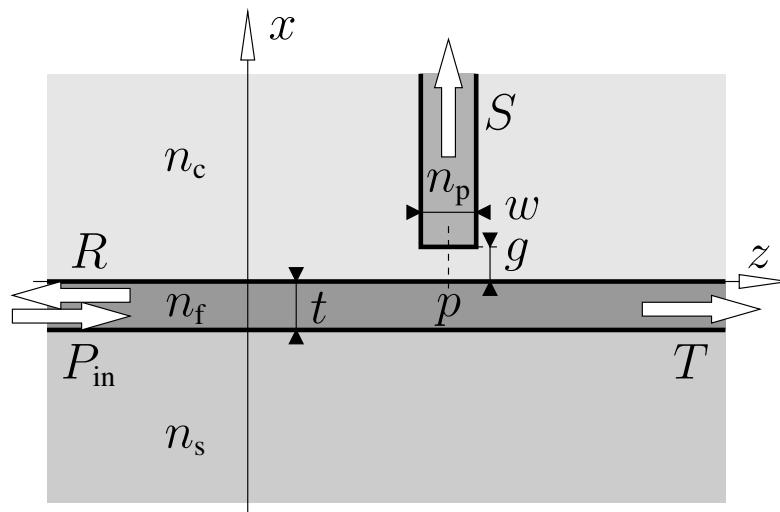
Probing evanescent fields



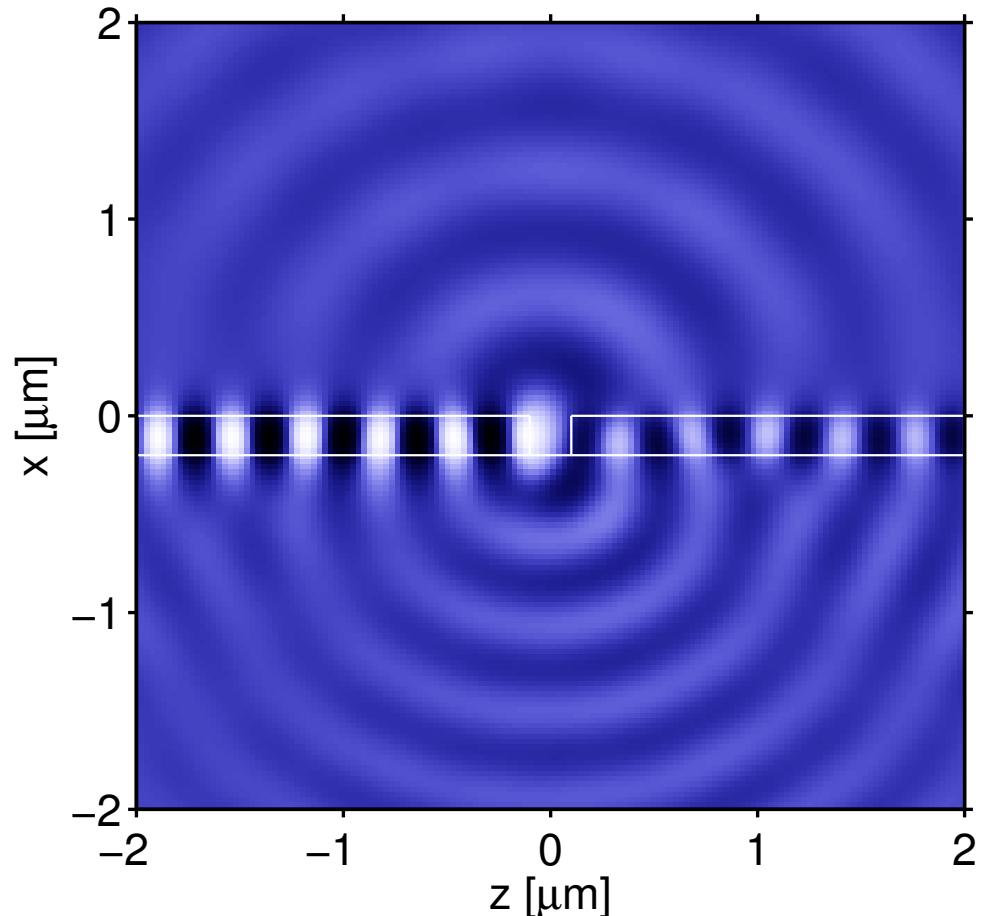
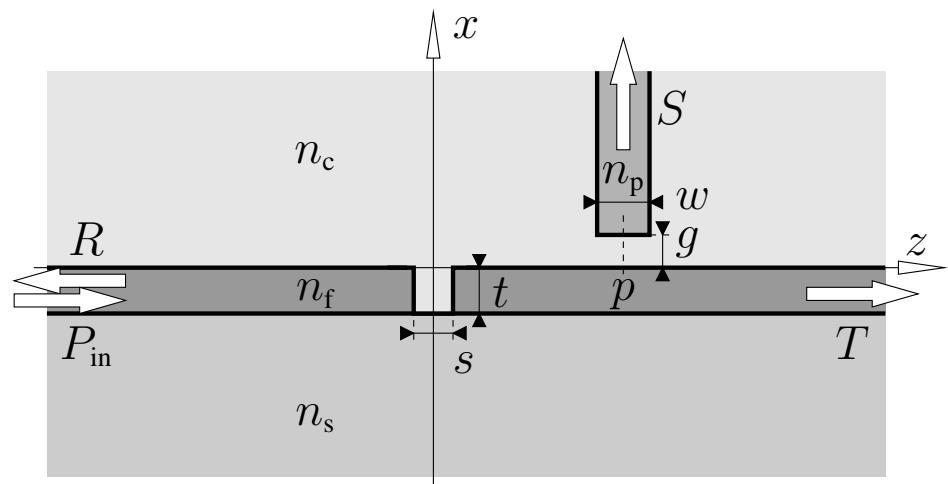
Probing evanescent fields



Probing evanescent fields

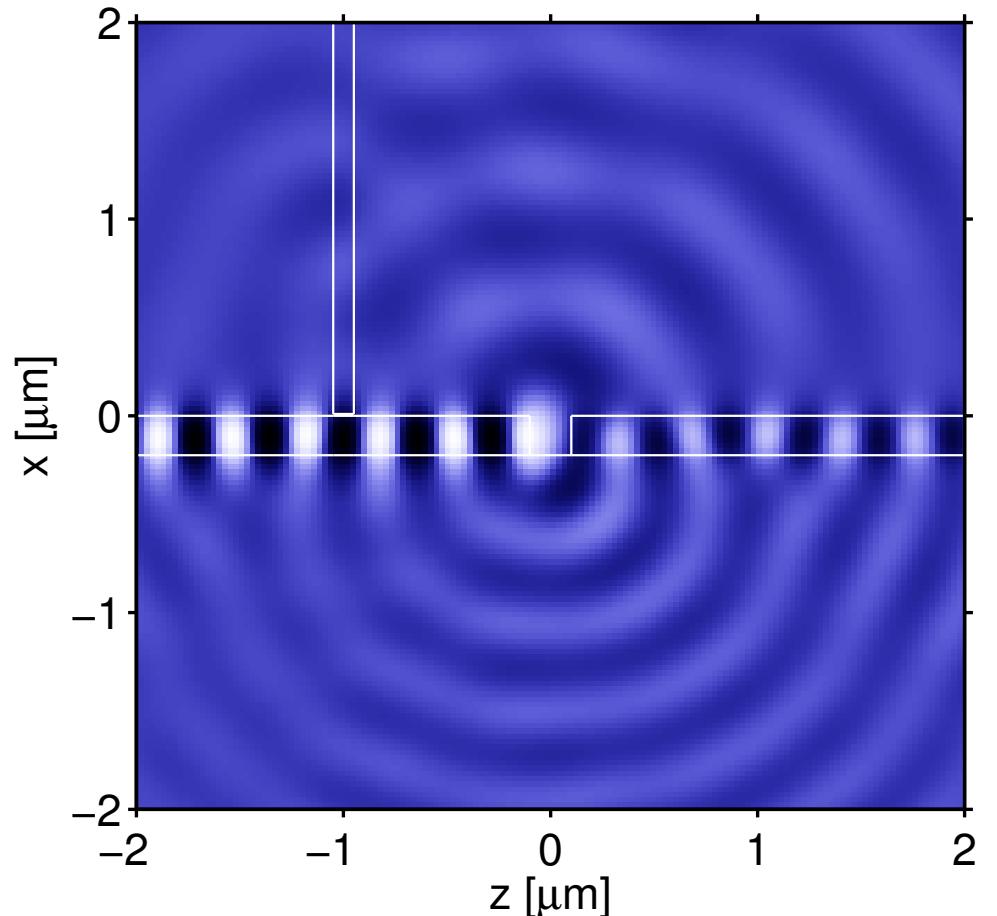
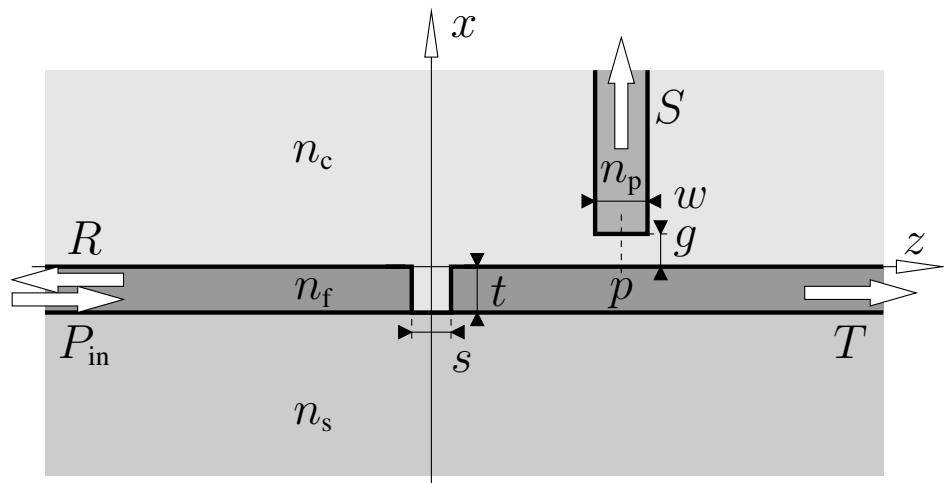


Hole defect in a slab waveguide



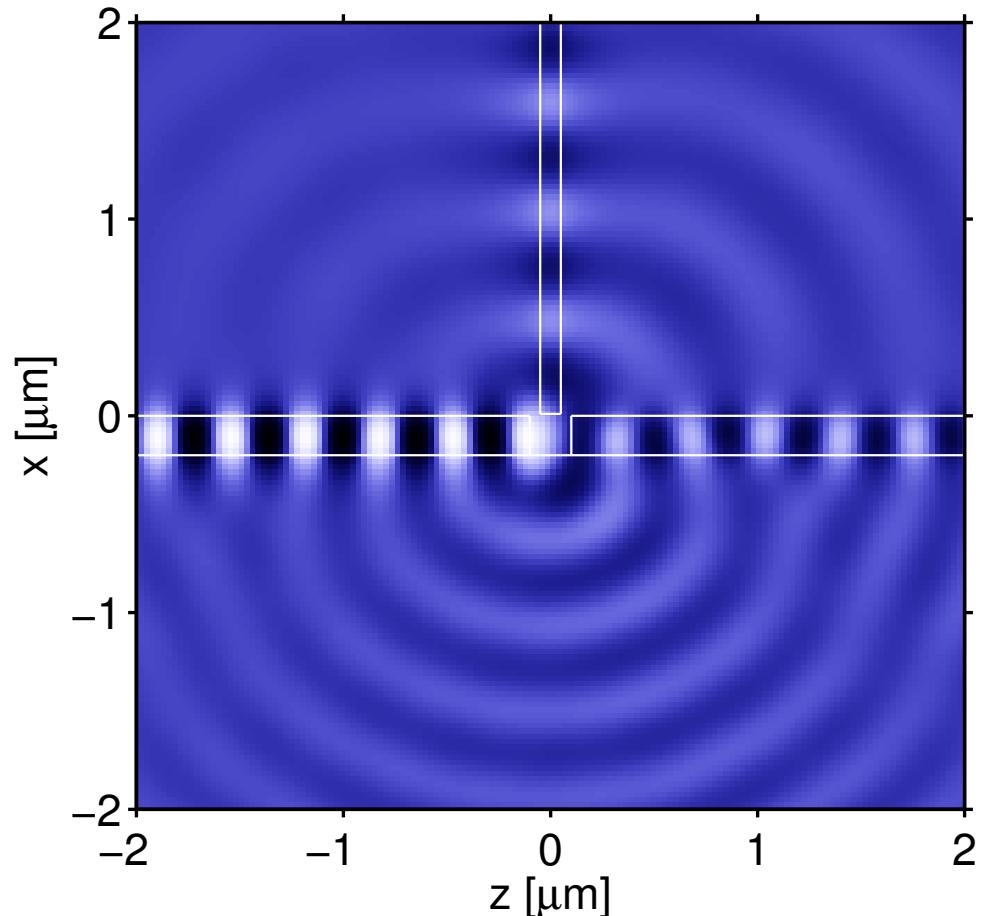
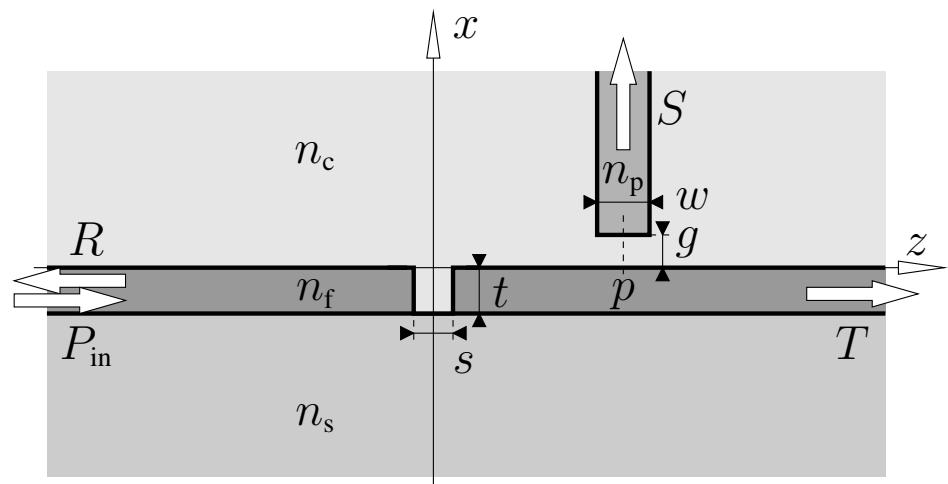
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $s = 0.2 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$, TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.1, 3.1] \mu\text{m}^2$, $M_x = M_z = 80$.

Hole defect in a slab waveguide



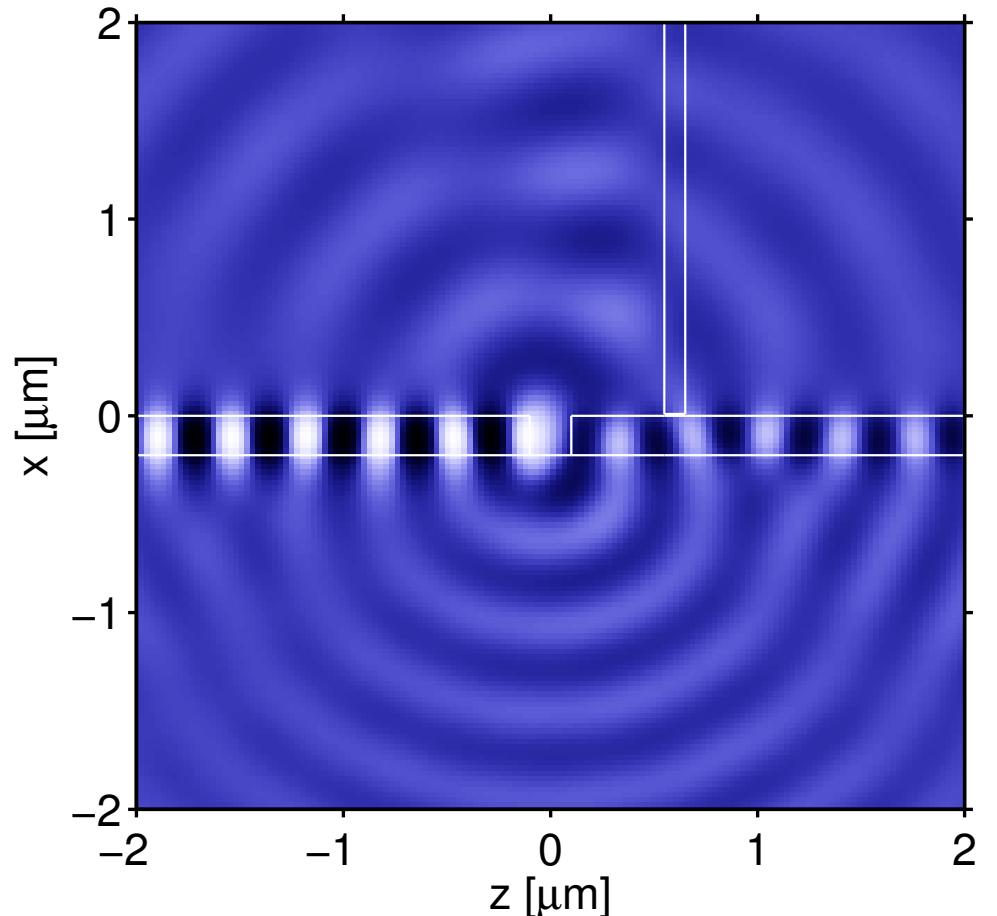
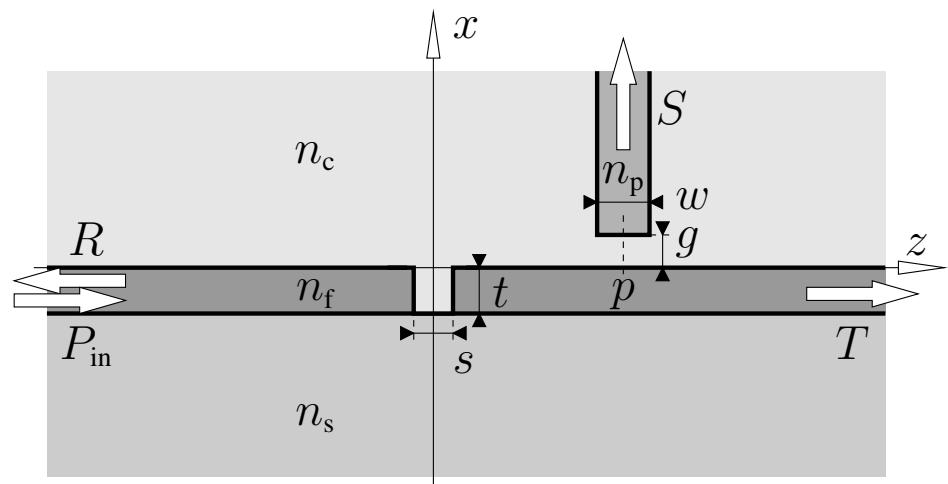
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $s = 0.2 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$, TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.1, 3.1] \mu\text{m}^2$, $M_x = M_z = 80$.

Hole defect in a slab waveguide



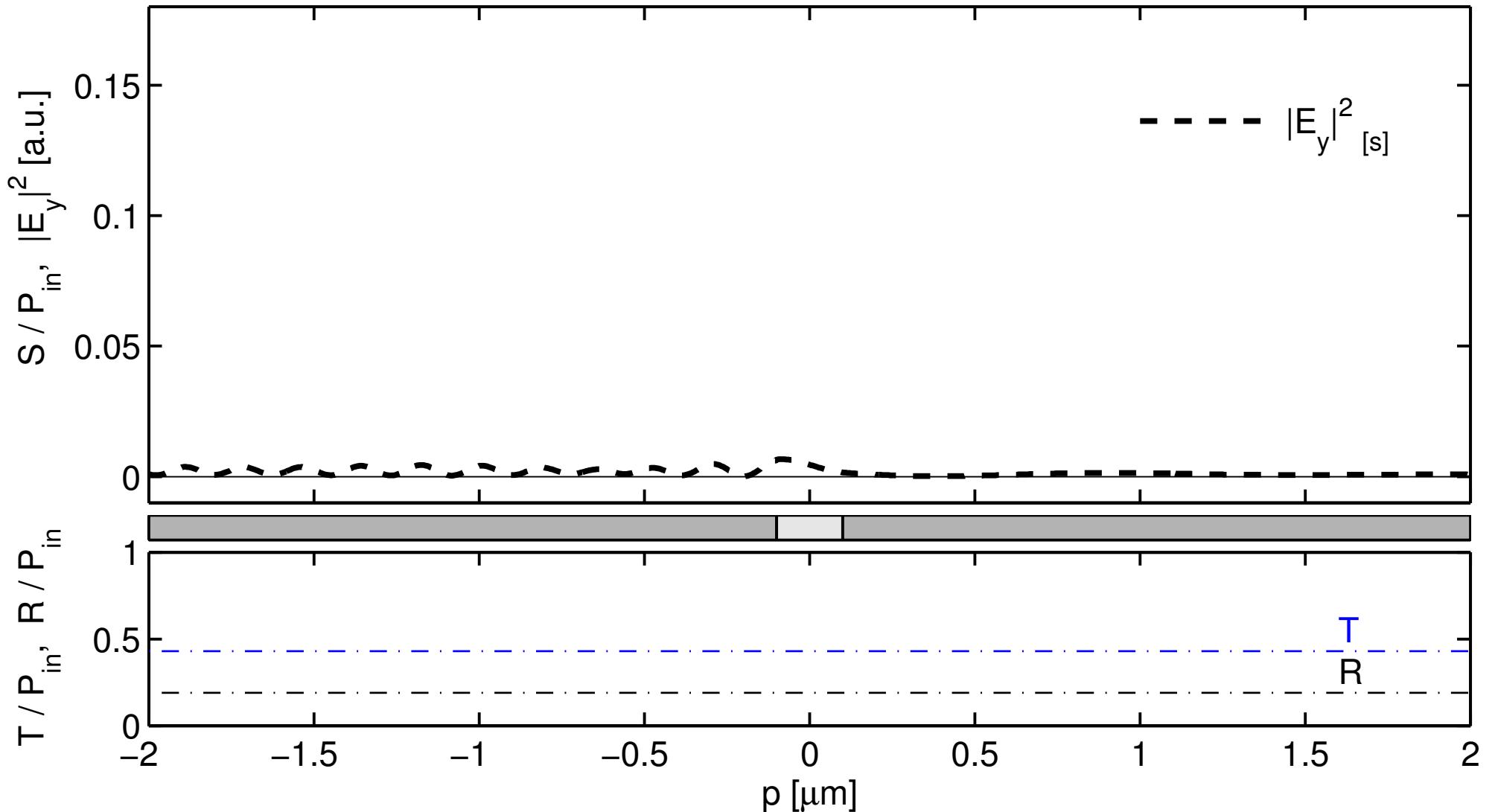
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $s = 0.2 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$, TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.1, 3.1] \mu\text{m}^2$, $M_x = M_z = 80$.

Hole defect in a slab waveguide

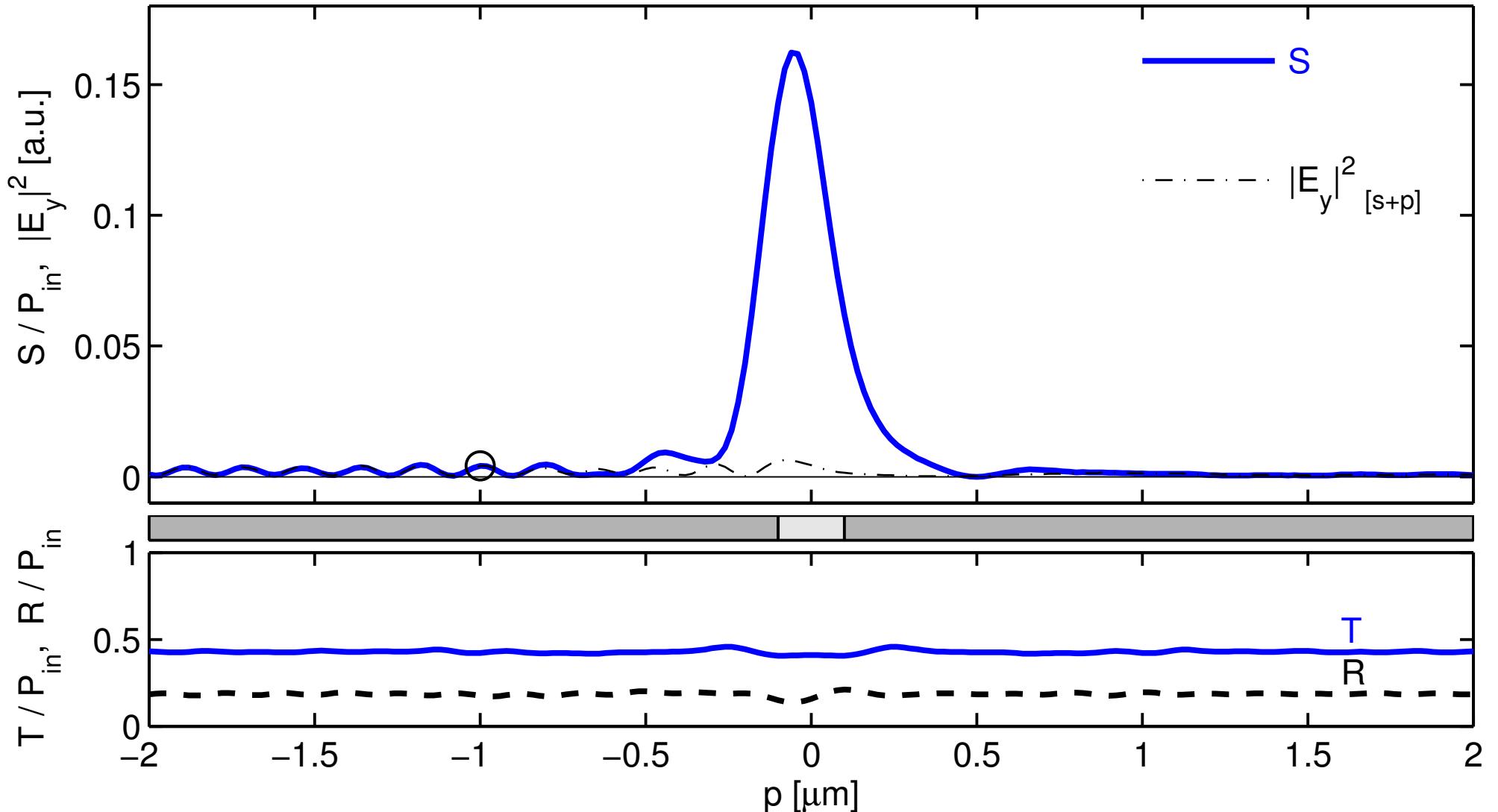


$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $s = 0.2 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$, TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.1, 3.1] \mu\text{m}^2$, $M_x = M_z = 80$.

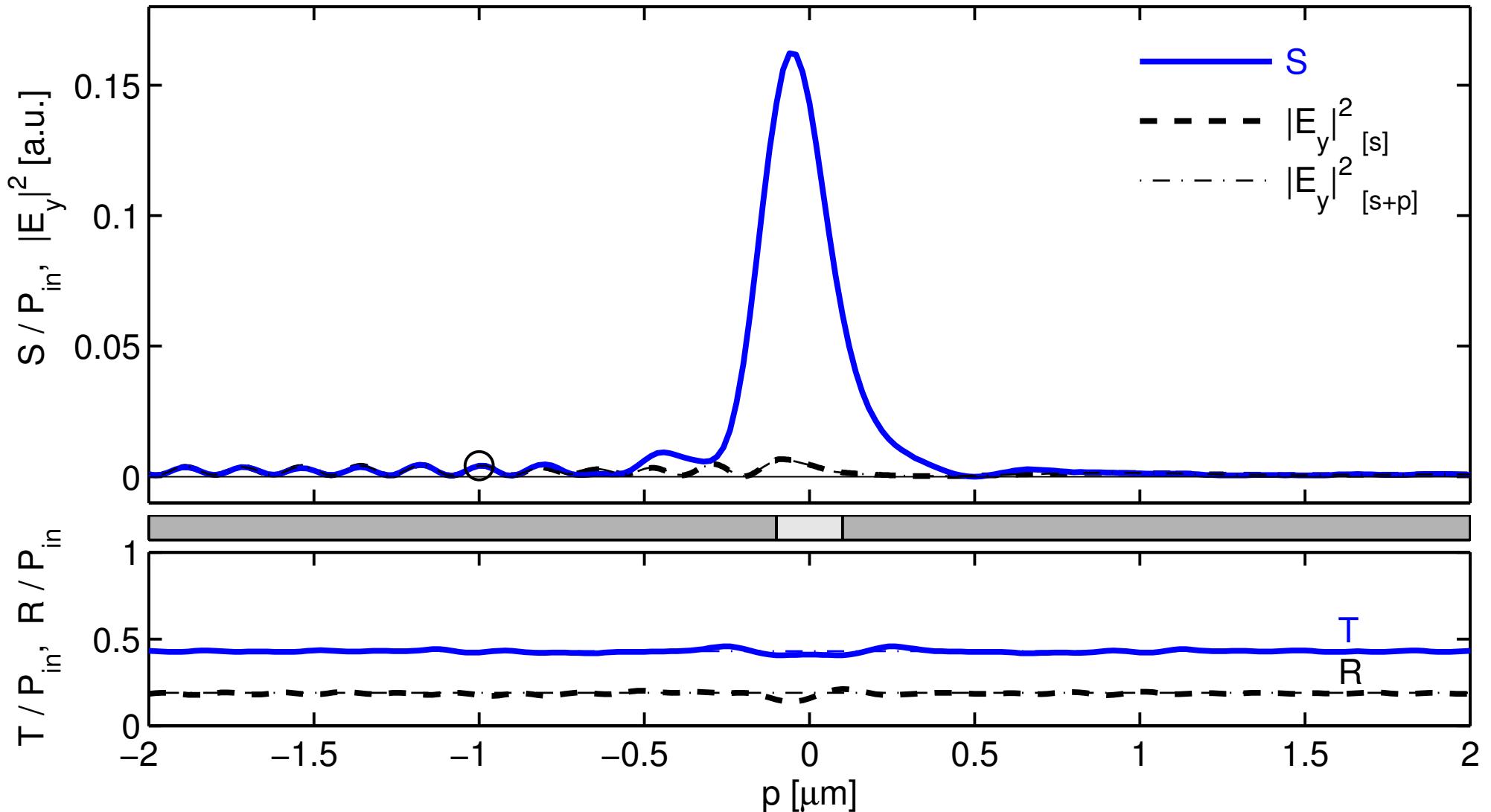
Hole defect in a slab waveguide



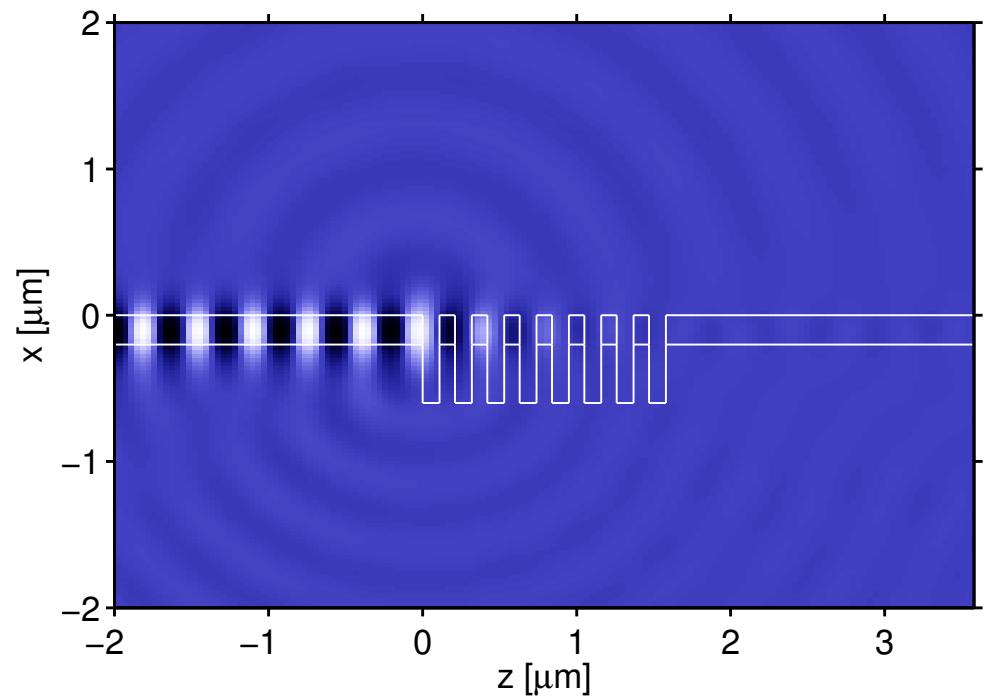
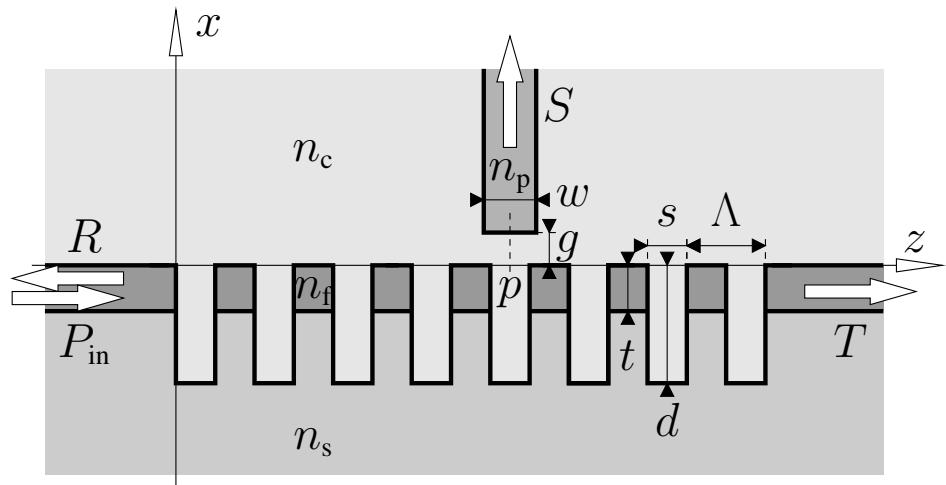
Hole defect in a slab waveguide



Hole defect in a slab waveguide

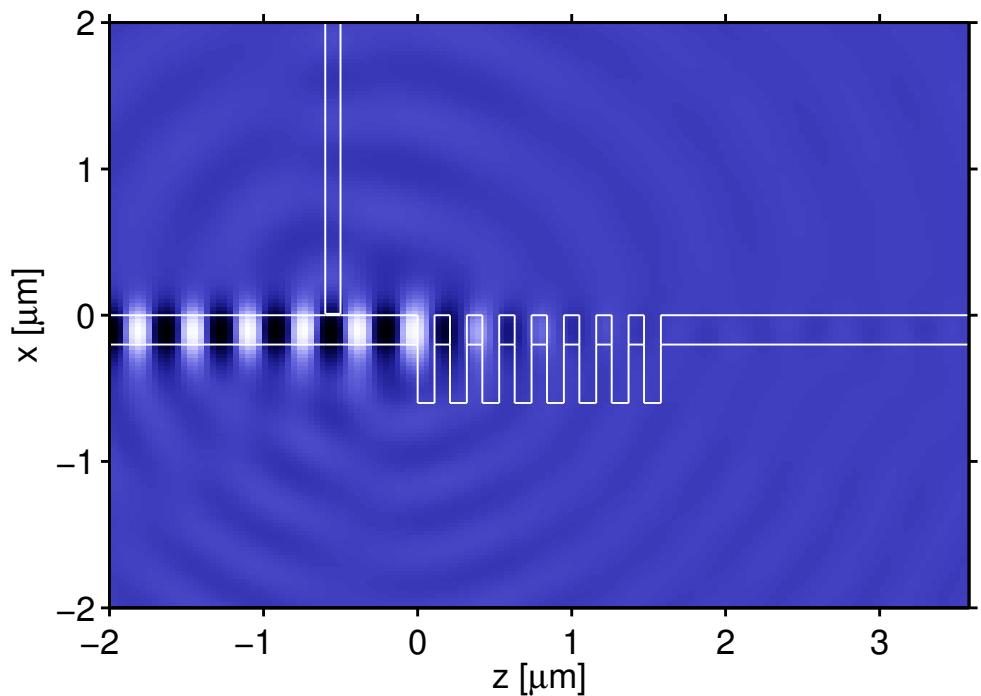
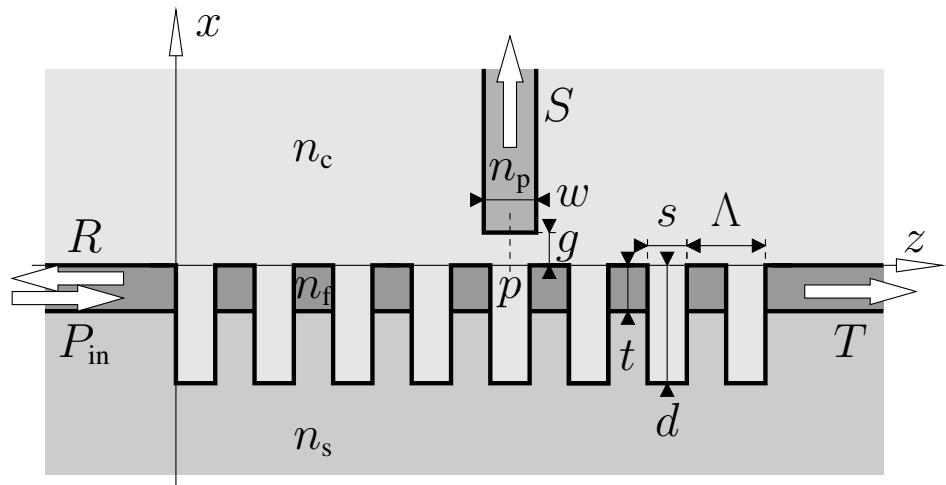


Short waveguide Bragg grating



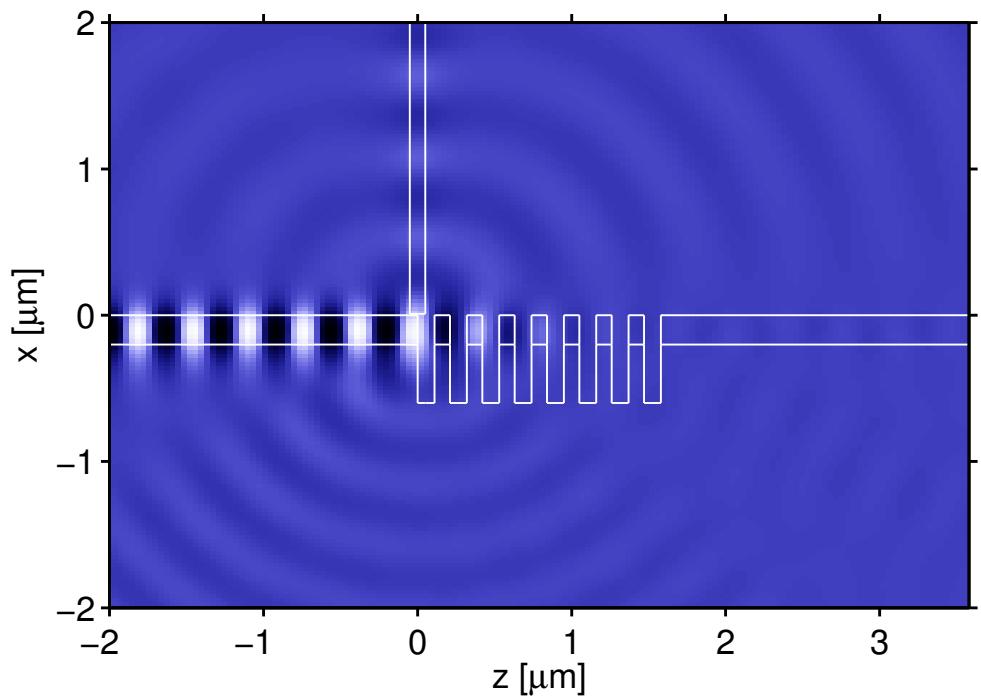
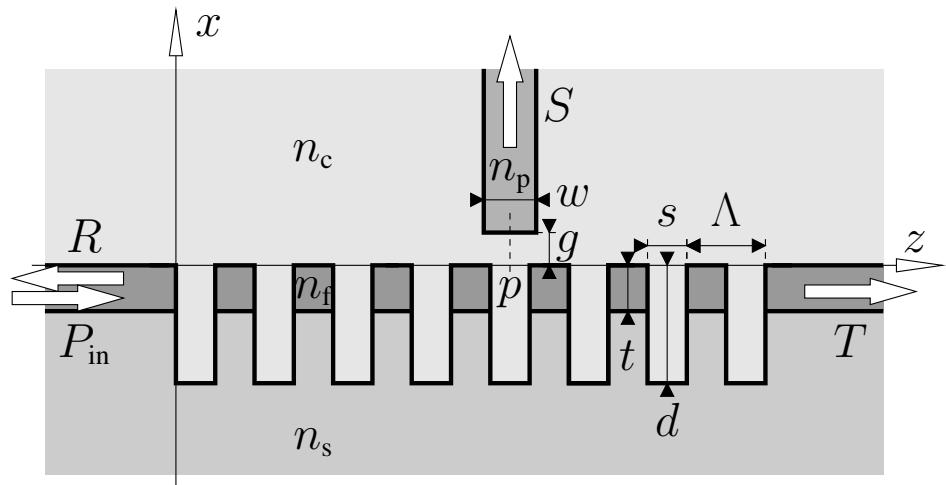
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $d = 0.6 \mu\text{m}$,
 $\Lambda = 0.21 \mu\text{m}$, $s = 0.11 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 4.58] \mu\text{m}^2$, $M_x = 100$, $M_z = 120$.

Short waveguide Bragg grating



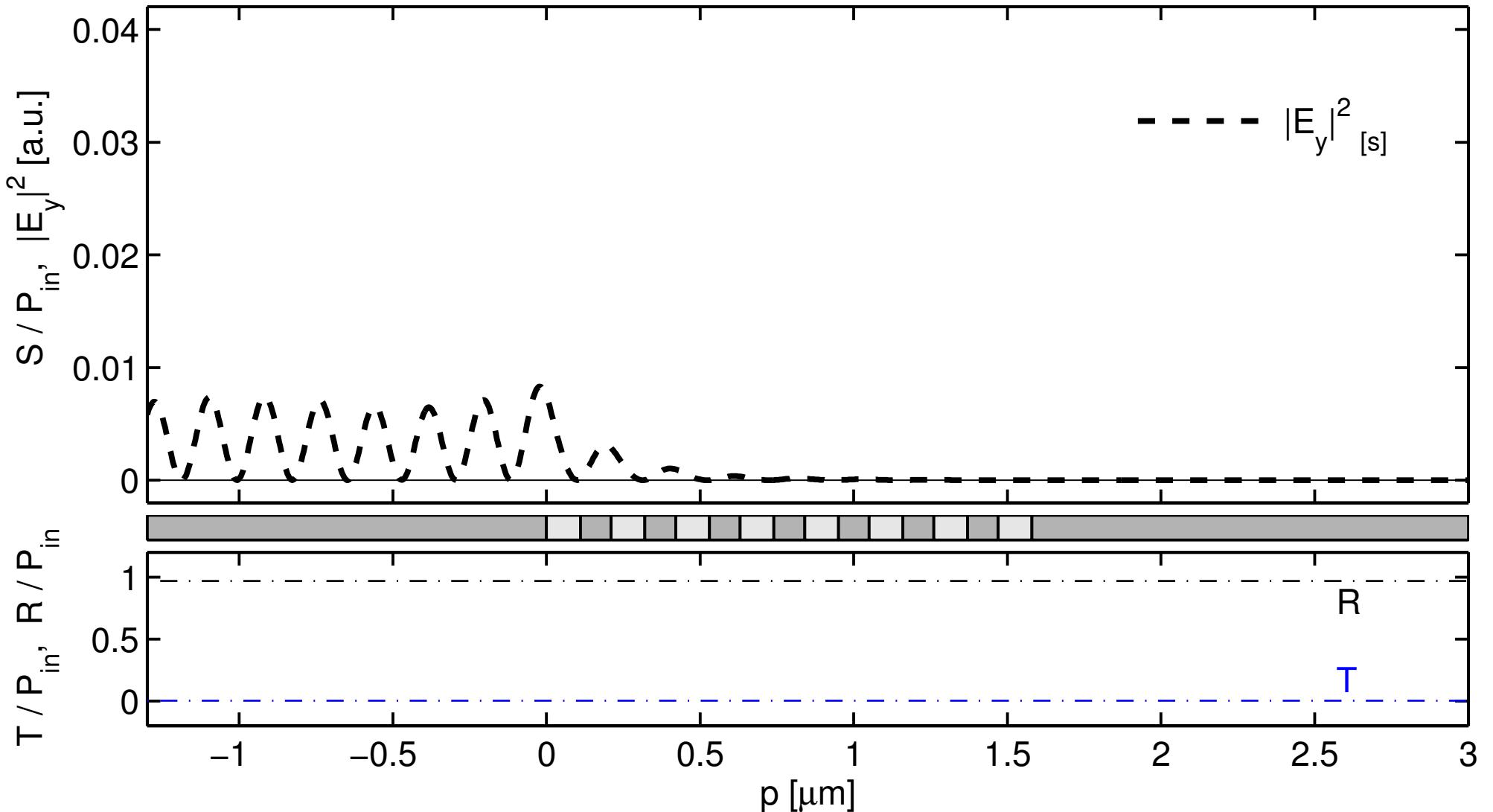
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $d = 0.6 \mu\text{m}$,
 $\Lambda = 0.21 \mu\text{m}$, $s = 0.11 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 4.58] \mu\text{m}^2$, $M_x = 100$, $M_z = 120$.

Short waveguide Bragg grating

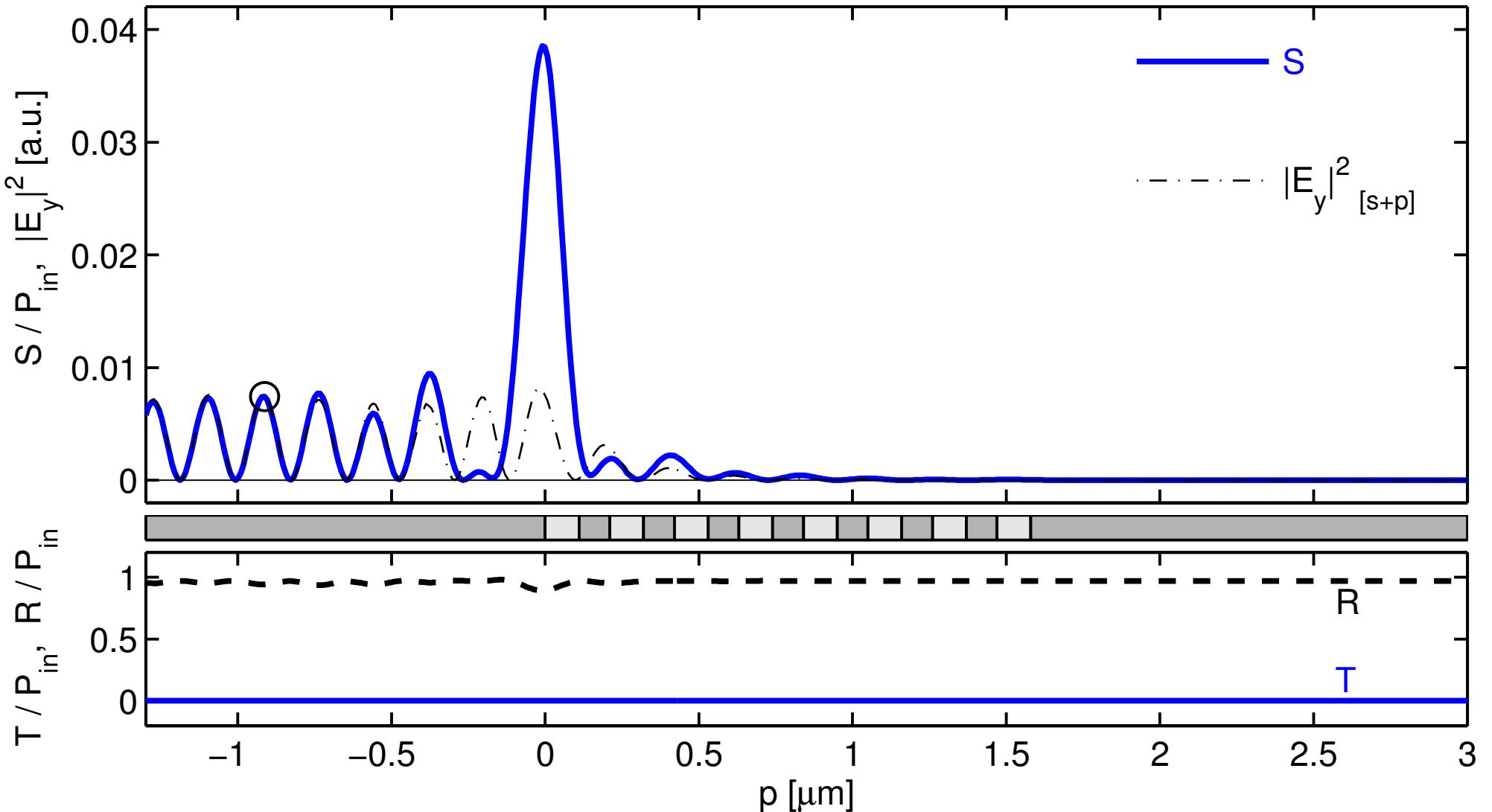


$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $d = 0.6 \mu\text{m}$,
 $\Lambda = 0.21 \mu\text{m}$, $s = 0.11 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 4.58] \mu\text{m}^2$, $M_x = 100$, $M_z = 120$.

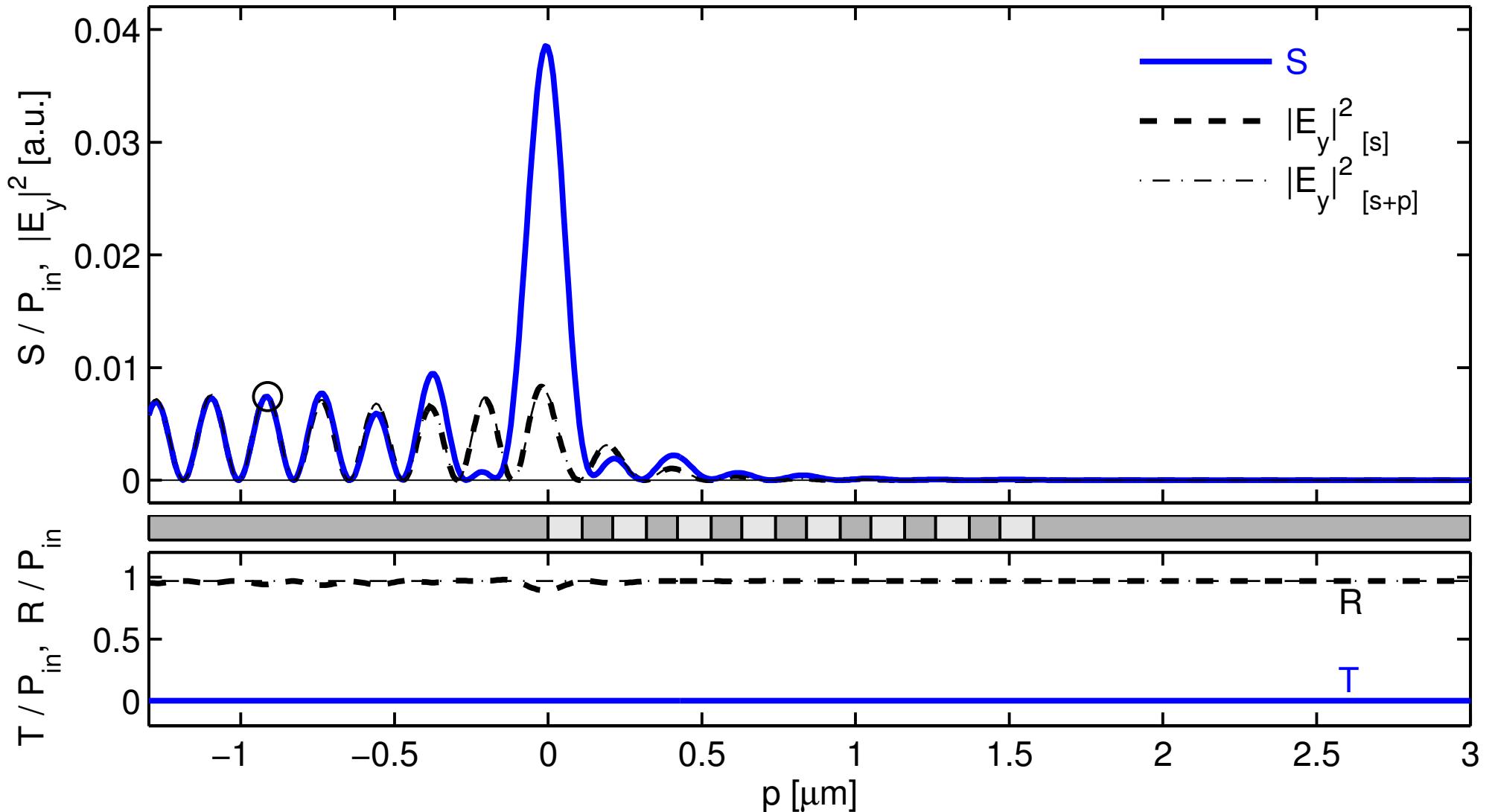
Short waveguide Bragg grating



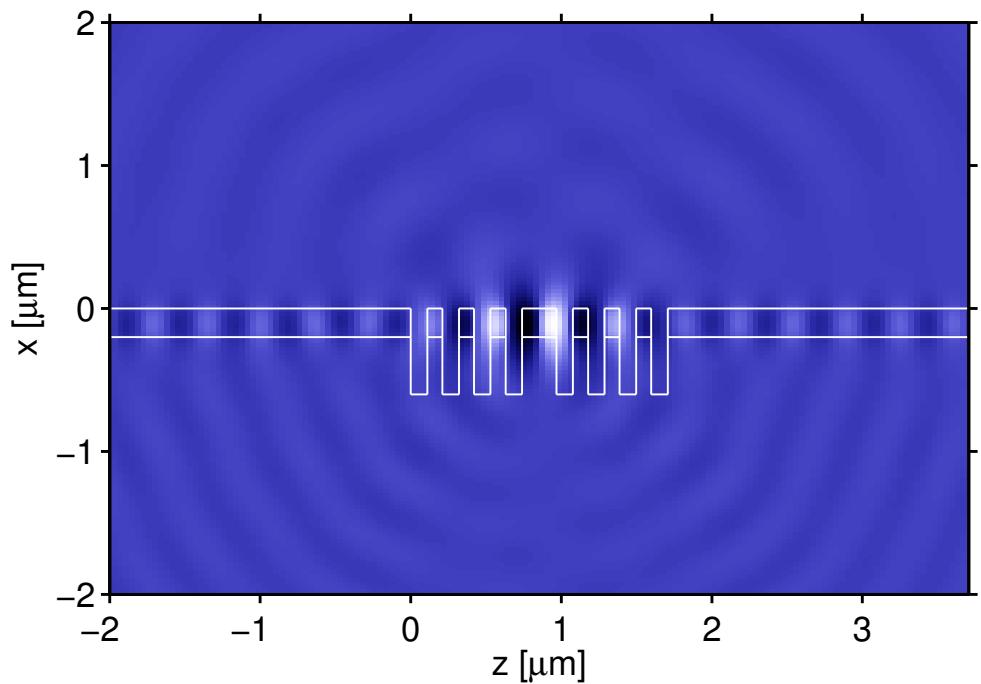
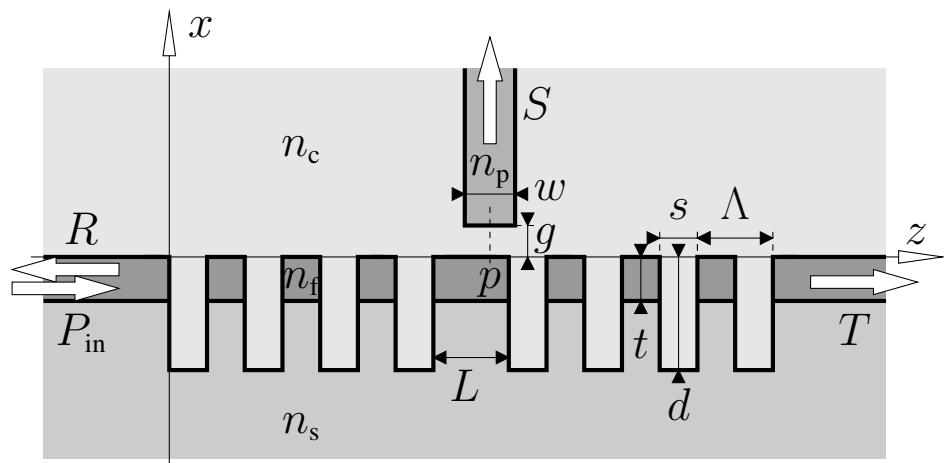
Short waveguide Bragg grating



Short waveguide Bragg grating

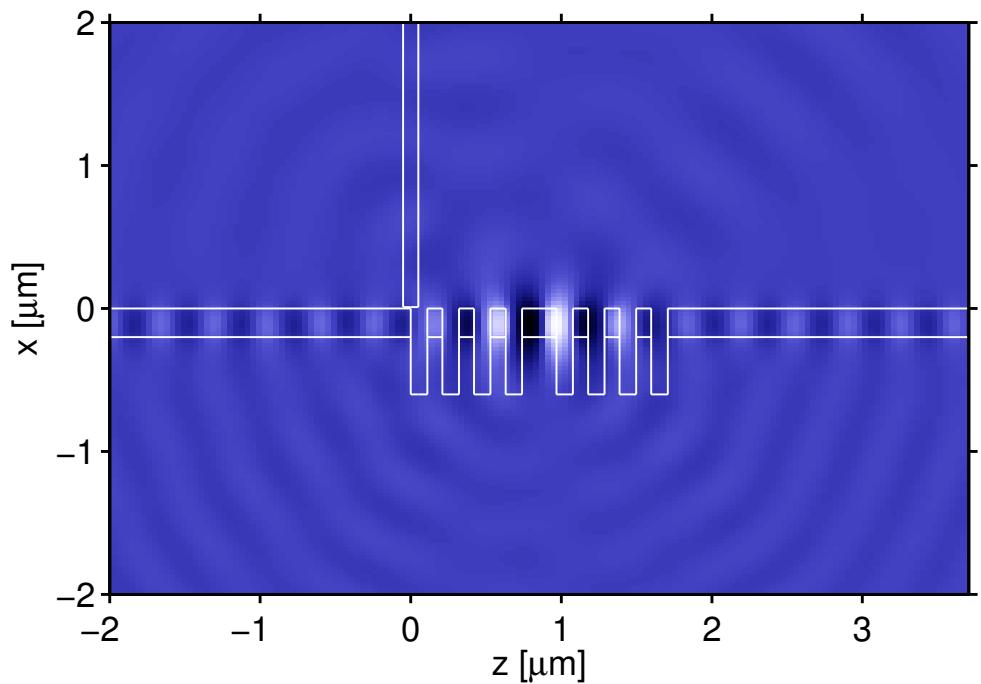
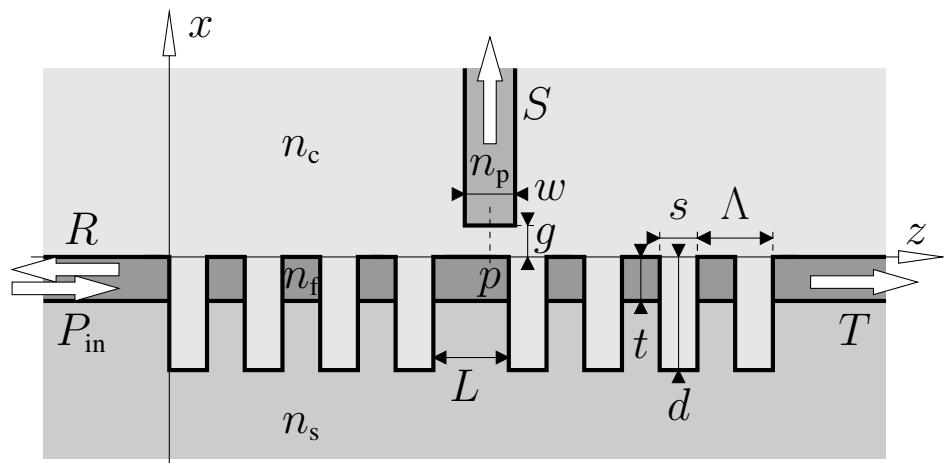


Resonant defect cavity



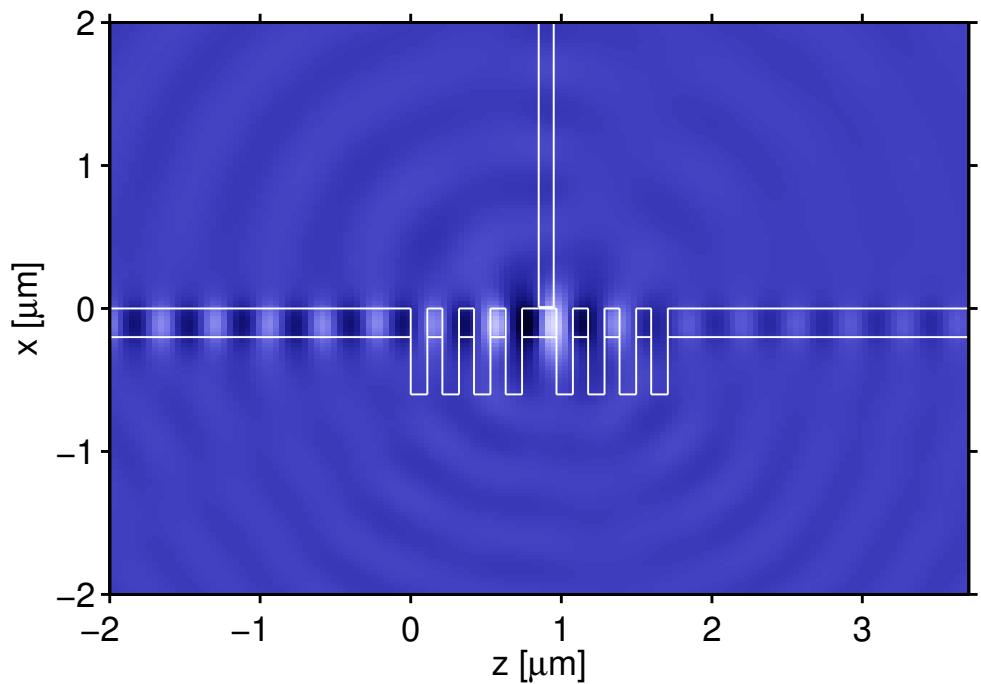
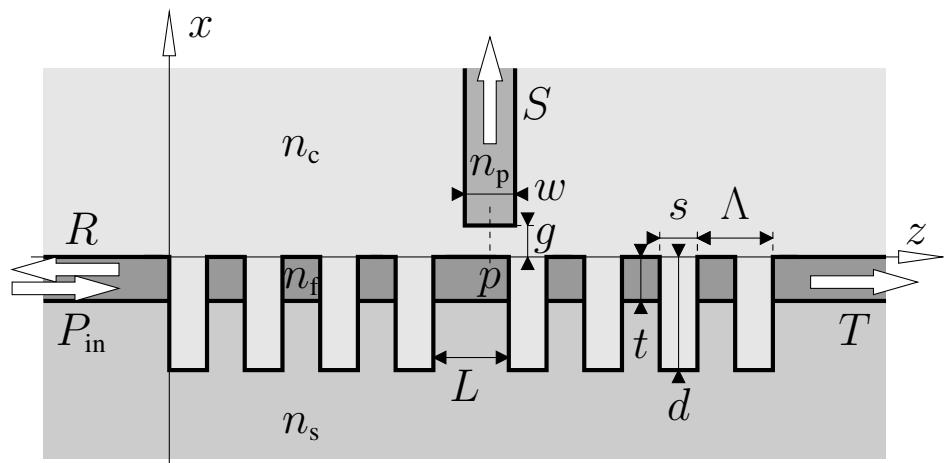
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $d = 0.6 \mu\text{m}$,
 $\Lambda = 0.21 \mu\text{m}$, $s = 0.11 \mu\text{m}$, $L = 0.2275 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 4.7075] \mu\text{m}^2$, $M_x = 100$, $M_z = 120$.

Resonant defect cavity



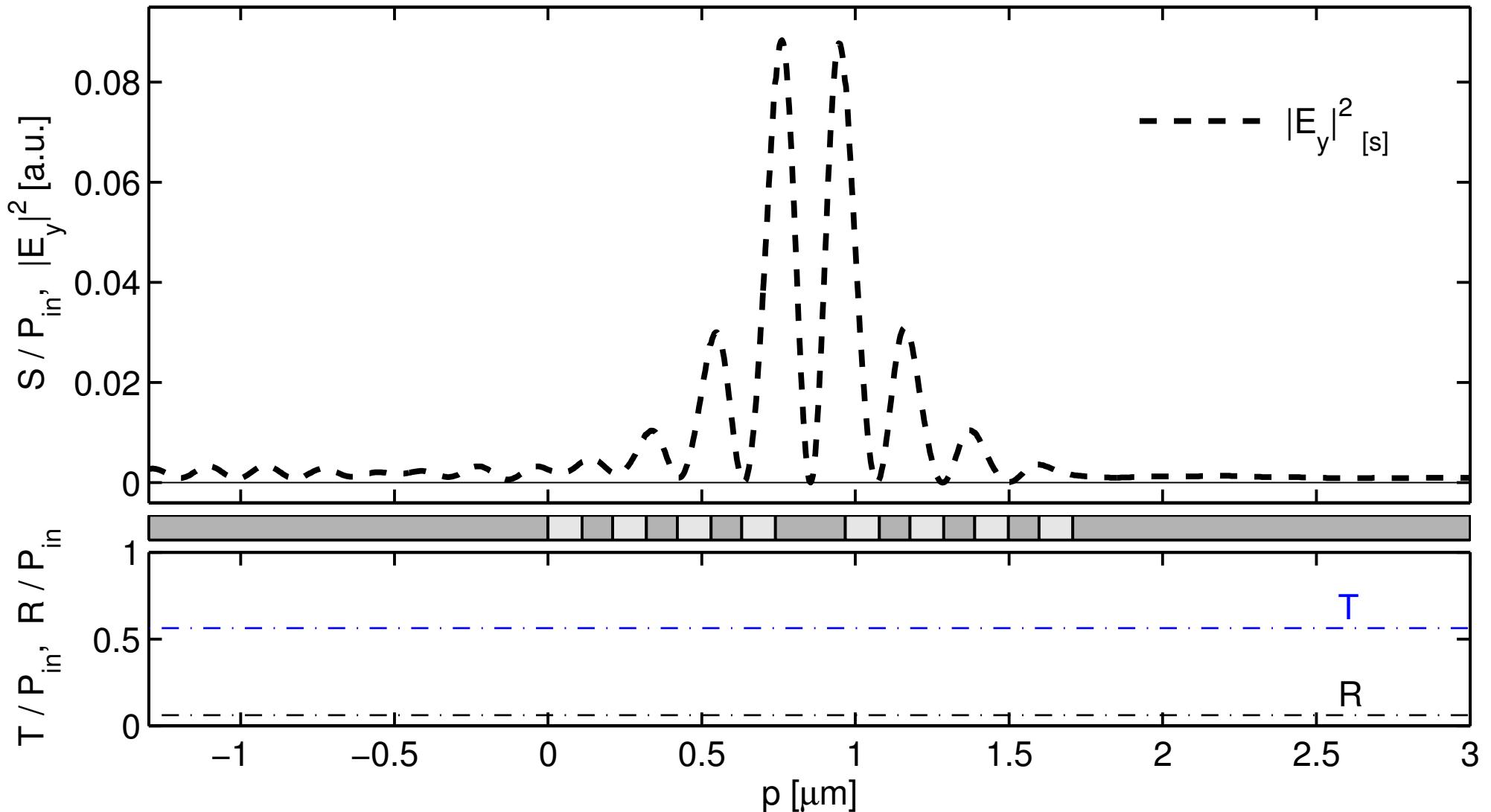
$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $d = 0.6 \mu\text{m}$,
 $\Lambda = 0.21 \mu\text{m}$, $s = 0.11 \mu\text{m}$, $L = 0.2275 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 4.7075] \mu\text{m}^2$, $M_x = 100$, $M_z = 120$.

Resonant defect cavity

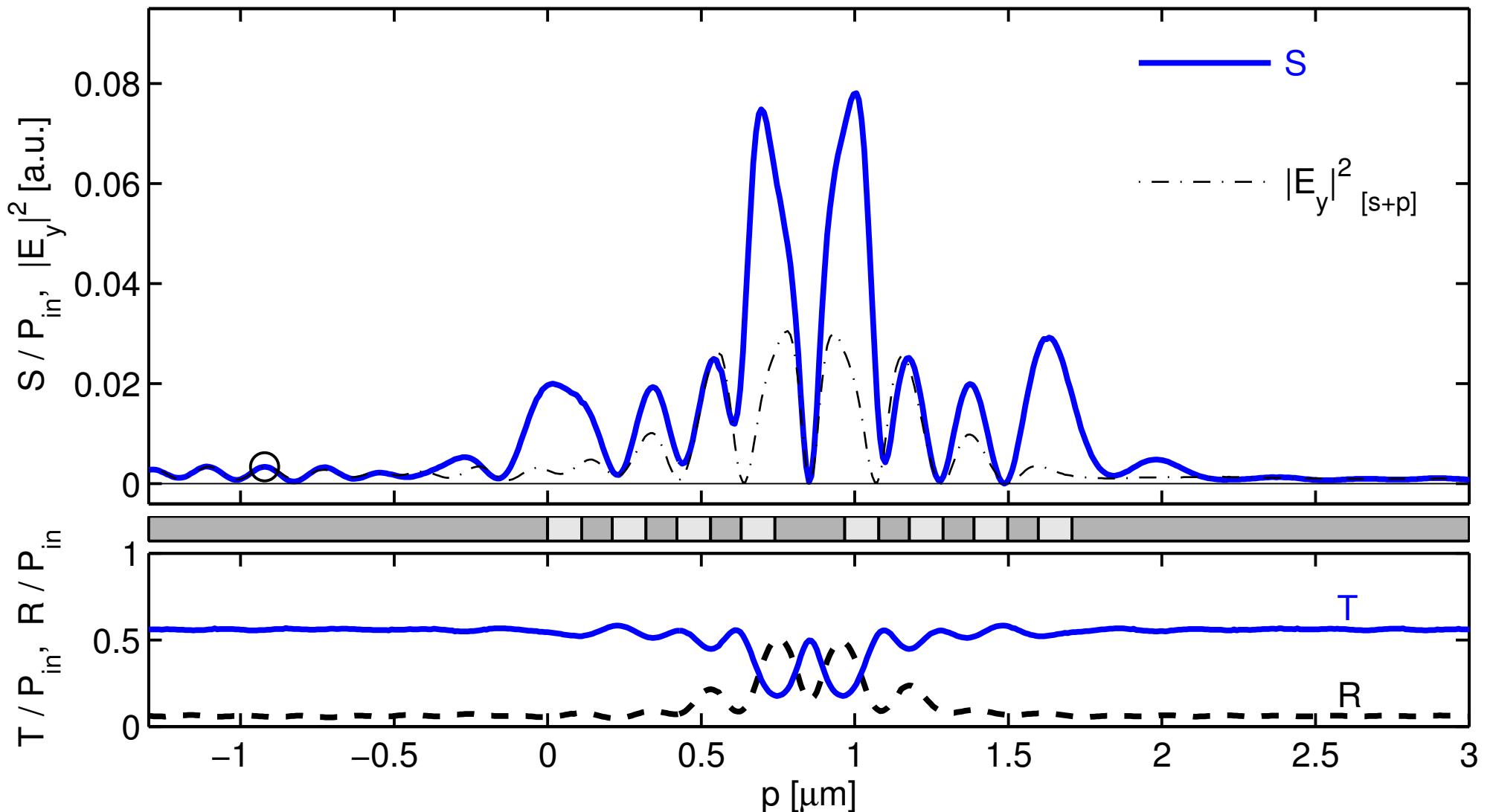


$n_s = 1.45$, $n_f = 2.0$, $n_c = 1.0$, $t = 0.2 \mu\text{m}$, $d = 0.6 \mu\text{m}$,
 $\Lambda = 0.21 \mu\text{m}$, $s = 0.11 \mu\text{m}$, $L = 0.2275 \mu\text{m}$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.633 \mu\text{m}$, $(x, z) \in [-3.0, 3.0] \times [-3.0, 4.7075] \mu\text{m}^2$, $M_x = 100$, $M_z = 120$.

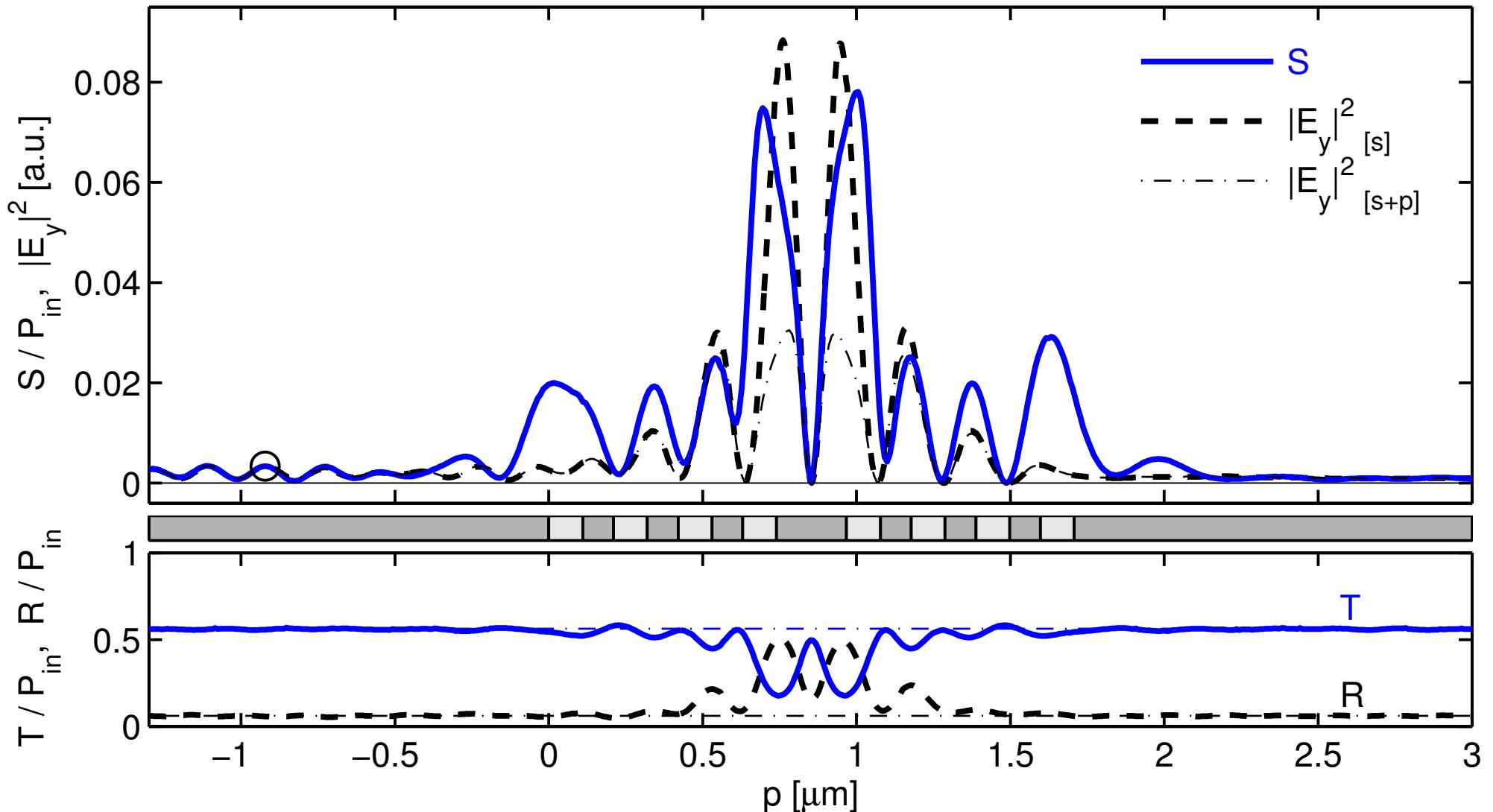
Resonant defect cavity



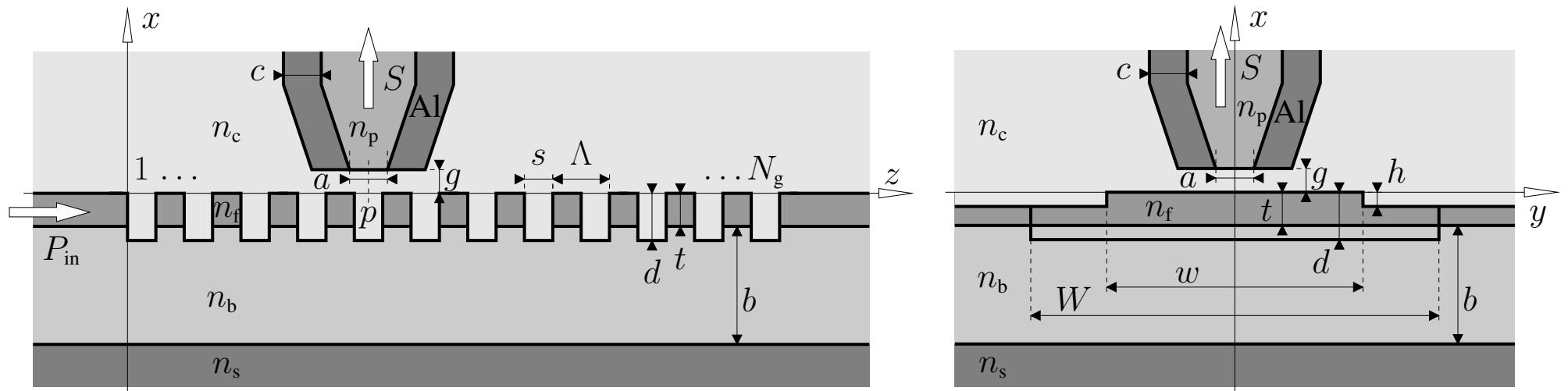
Resonant defect cavity



Resonant defect cavity



Bragg grating: PSTM experiment *

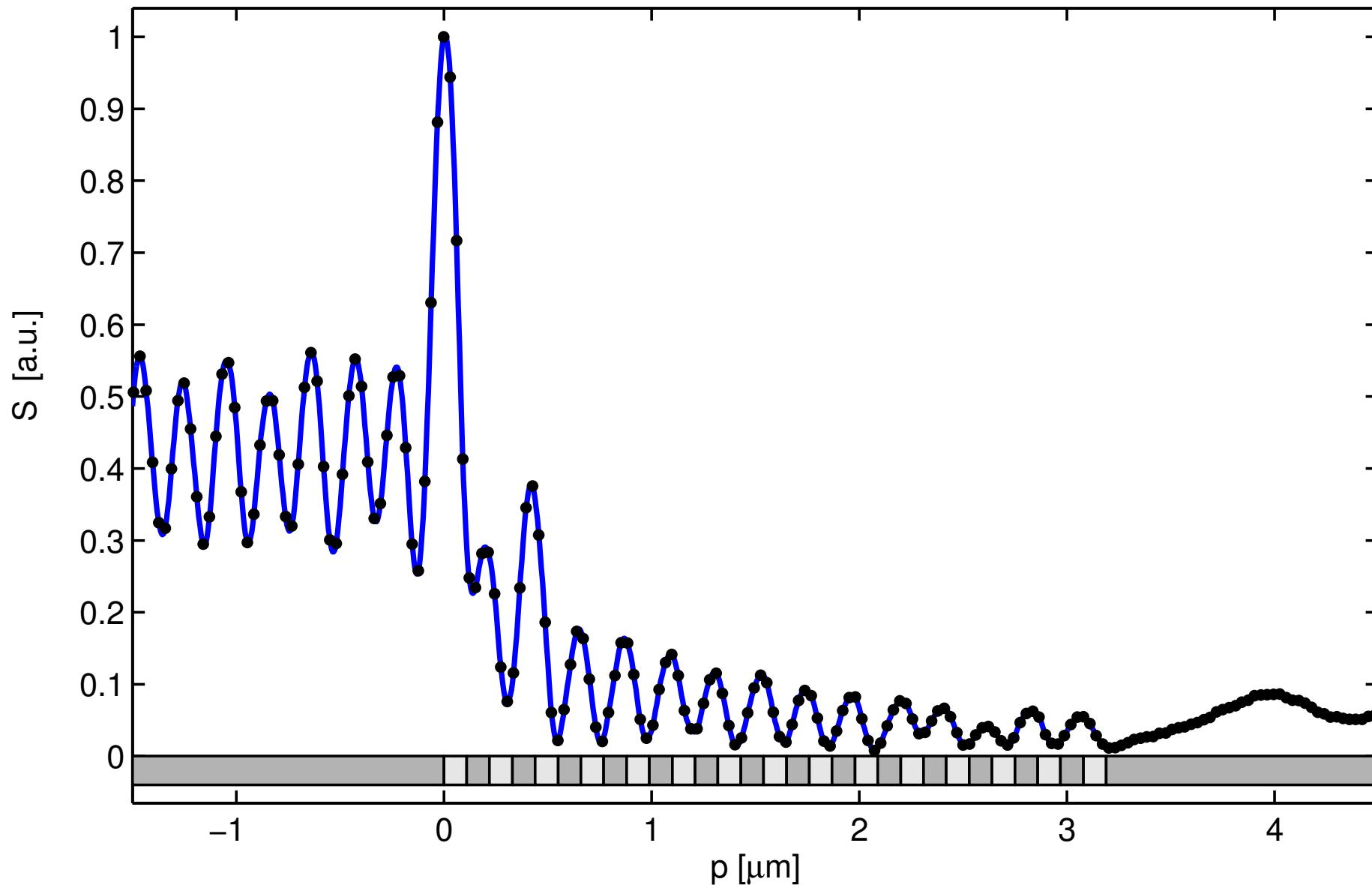


Sample: Rib waveguide with a series of deep, rectangular slits,
 $n_s = 3.4$, $n_b = 1.45$, $n_f = 2.01$, $n_c = 1.0$, $t = 55 \text{ nm}$, $h = 11 \text{ nm}$, $w = 1.5 \mu\text{m}$,
 $W = 2.5 \mu\text{m}$, $b = 3.2 \mu\text{m}$, $\Lambda = 220 \text{ nm}$, $s = 110 \text{ nm}$, $d = 70 \text{ nm}$, $N_g = 15$.

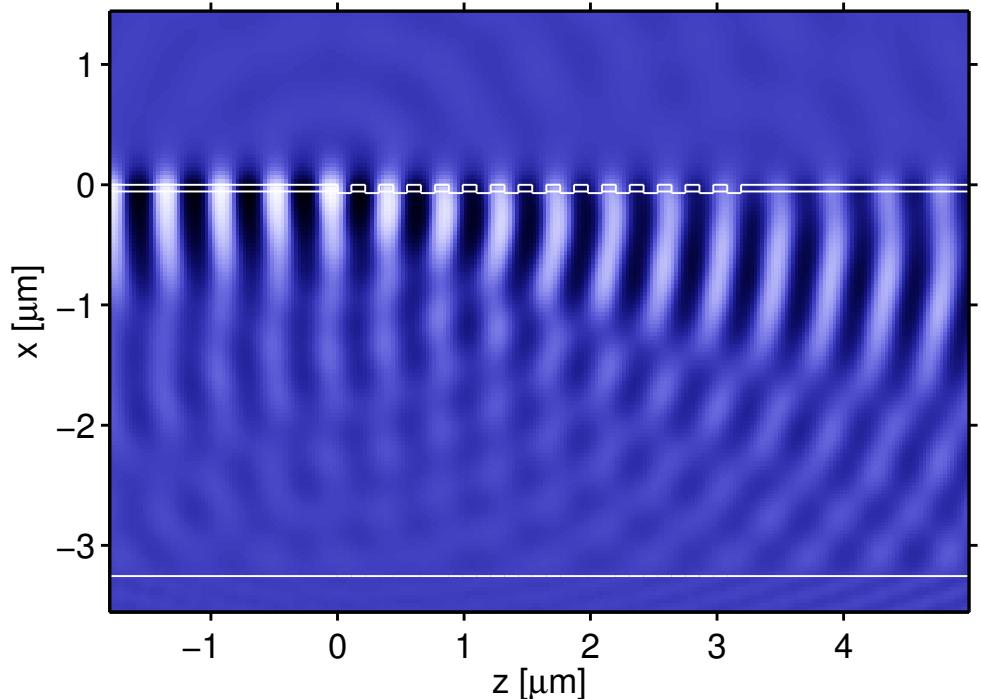
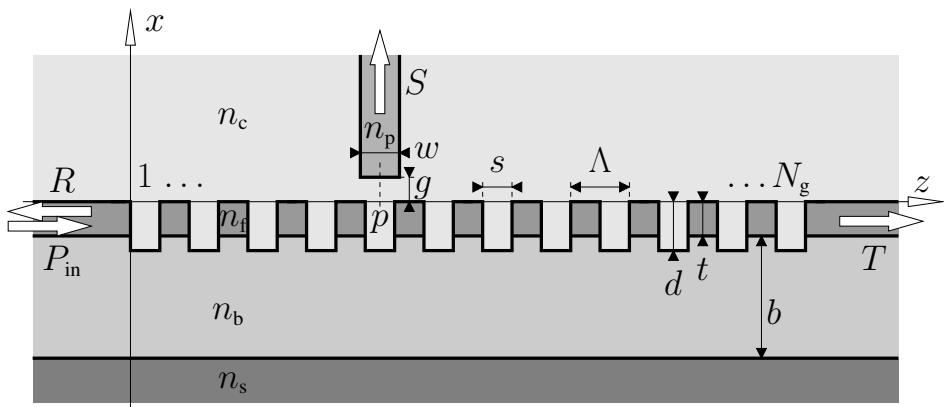
Probe: Tapered cylindrical fiber tip with aluminium coating,
 $a \approx 80 \text{ nm}$, $c \approx 100 \text{ nm}$, $g = 10 \text{ nm}$, $n_p = 1.5$;
TE polarized light, vacuum wavelength $\lambda = 0.6328 \mu\text{m}$.

* E. Flück, M. Hammer, A. M. Otter, J. P. Korterijk, L. Kuipers, N. F. van Hulst,
Amplitude and phase evolution of optical fields inside periodic photonic structures,
Journal of Lightwave Technology **21**(5), 1384-1393 (2003)

Bragg grating: PSTM experiment

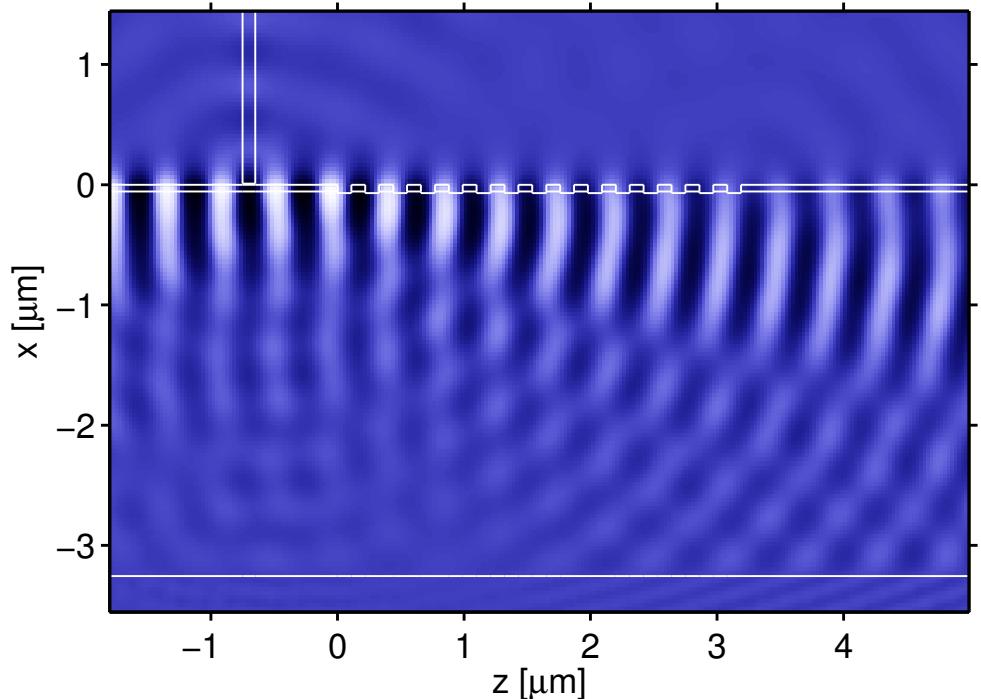
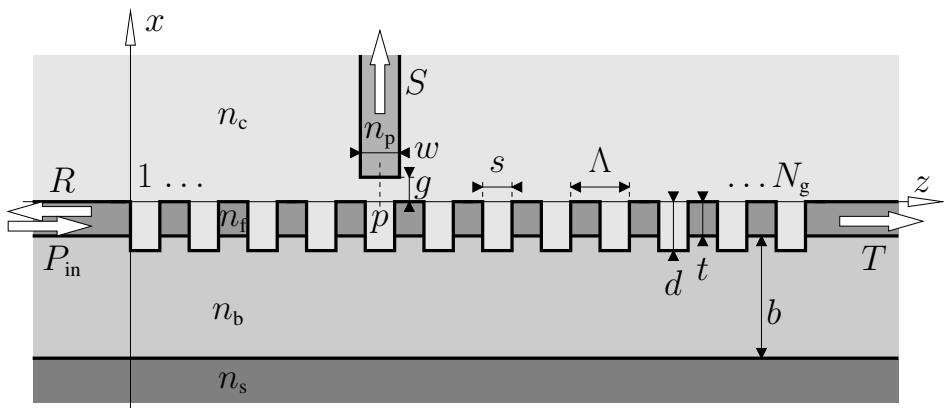


Bragg grating: QUEP model



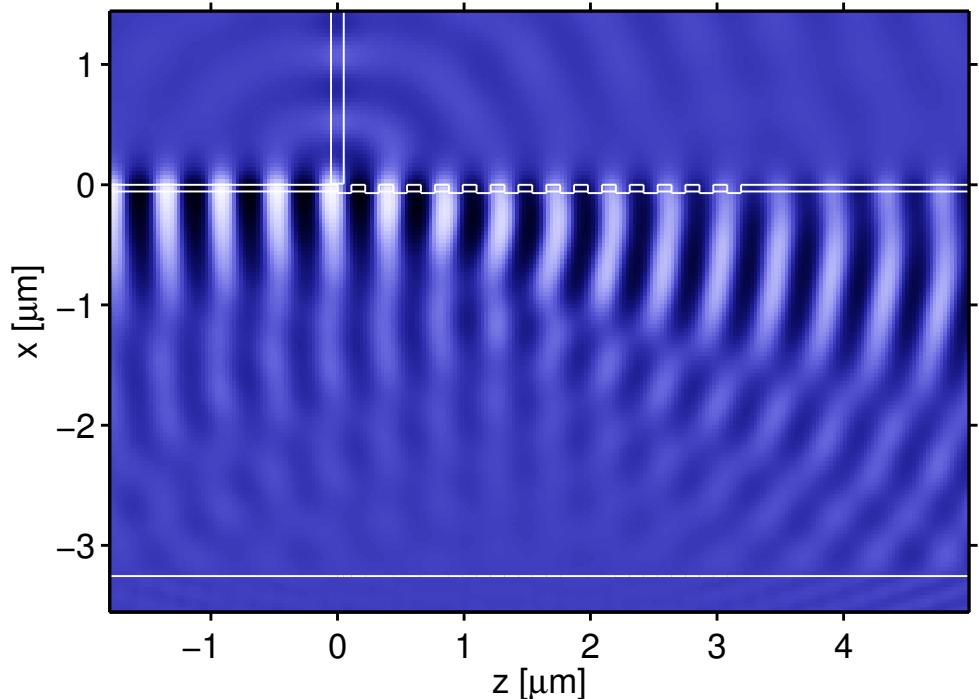
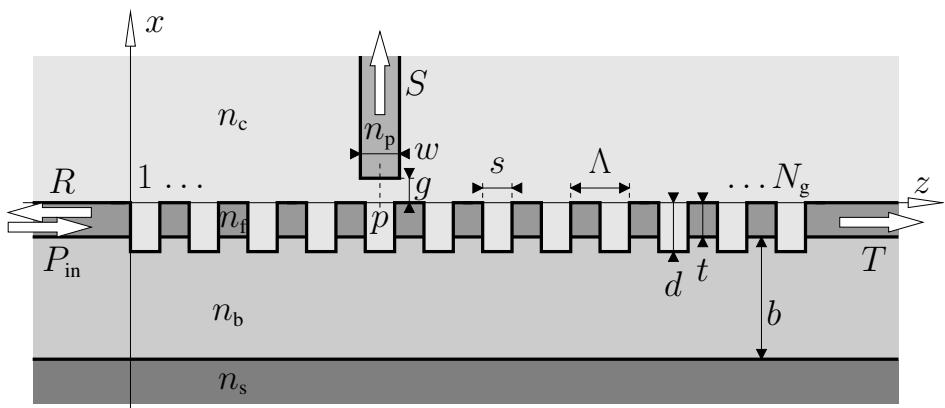
$n_s = 3.4$, $n_b = 1.45$, $n_f = 2.01$, $n_c = 1.0$, $t = 55 \text{ nm}$, $b = 3.2 \mu\text{m}$, $d = 70 \text{ nm}$,
 $\Lambda = 220 \text{ nm}$, $s = 110 \text{ nm}$, $N_g = 15$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.6328 \mu\text{m}$, $(x, z) \in [-3.5, 1.5] \times [-2.0, 5.2] \mu\text{m}^2$, $M_x = 80$, $M_z = 100$.

Bragg grating: QUEP model



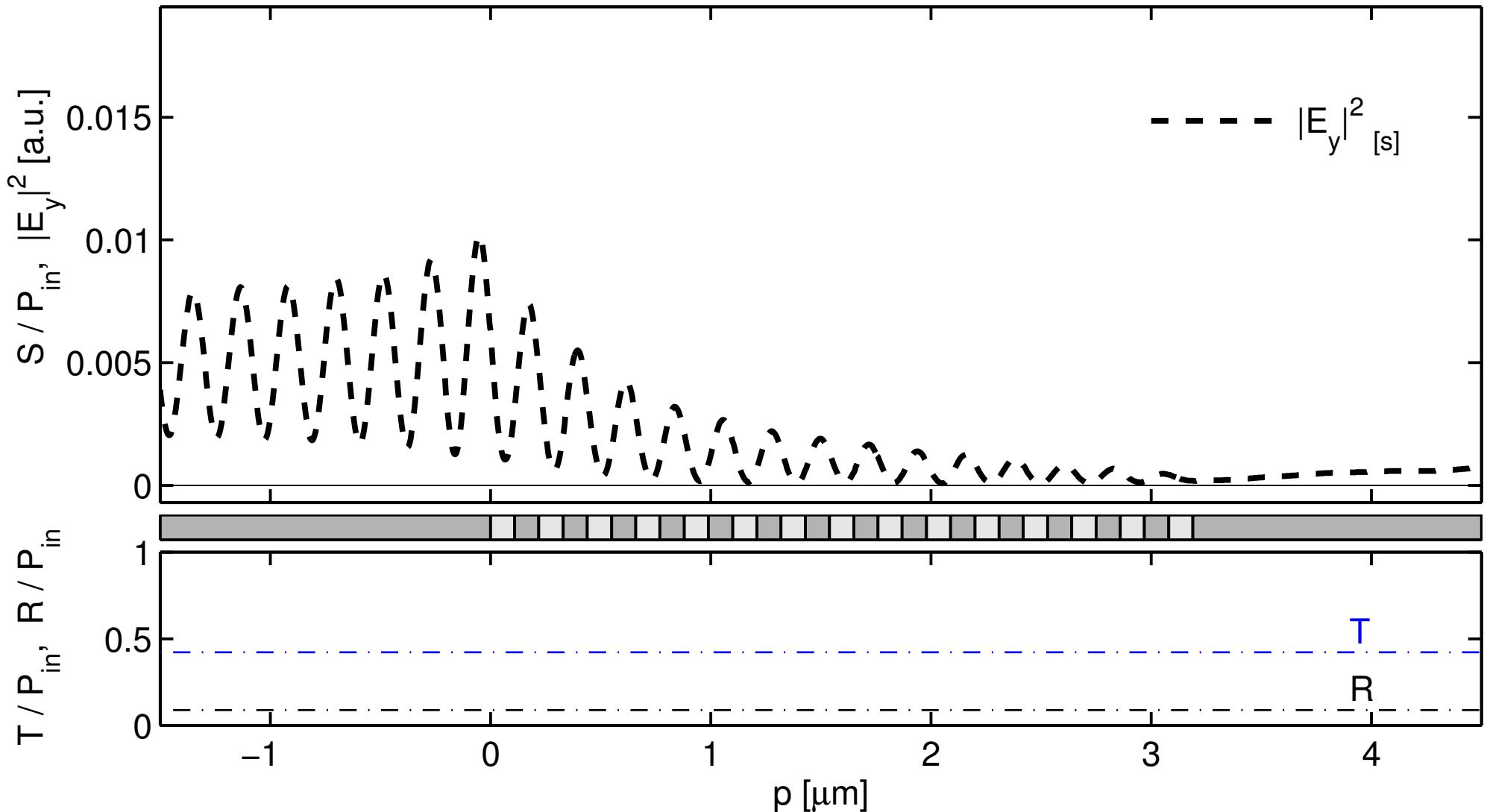
$n_s = 3.4$, $n_b = 1.45$, $n_f = 2.01$, $n_c = 1.0$, $t = 55 \text{ nm}$, $b = 3.2 \mu\text{m}$, $d = 70 \text{ nm}$,
 $\Lambda = 220 \text{ nm}$, $s = 110 \text{ nm}$, $N_g = 15$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.6328 \mu\text{m}$, $(x, z) \in [-3.5, 1.5] \times [-2.0, 5.2] \mu\text{m}^2$, $M_x = 80$, $M_z = 100$.

Bragg grating: QUEP model

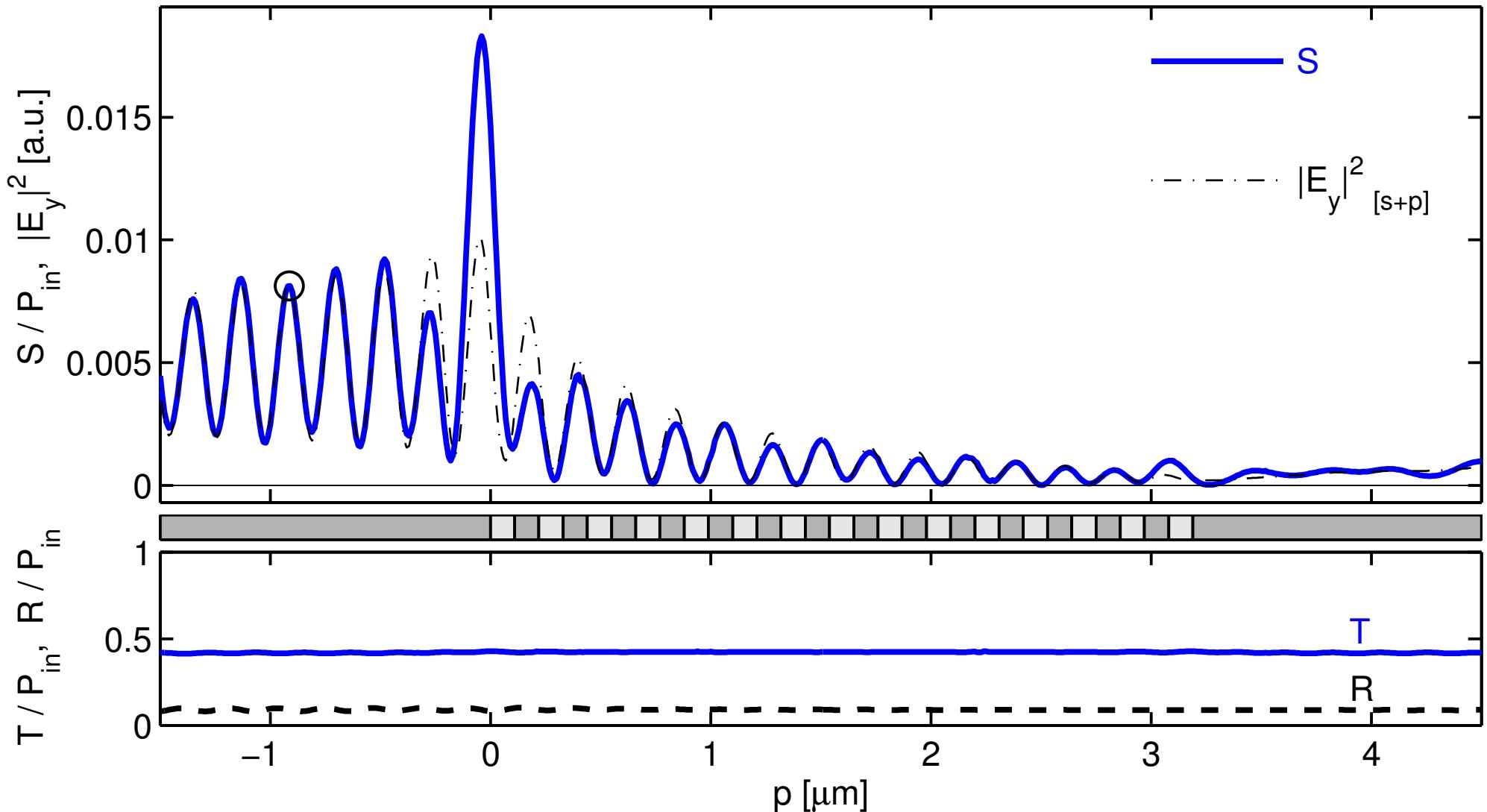


$n_s = 3.4$, $n_b = 1.45$, $n_f = 2.01$, $n_c = 1.0$, $t = 55 \text{ nm}$, $b = 3.2 \mu\text{m}$, $d = 70 \text{ nm}$,
 $\Lambda = 220 \text{ nm}$, $s = 110 \text{ nm}$, $N_g = 15$, $g = 10 \text{ nm}$, $w = 100 \text{ nm}$, $n_p = 1.5$,
TE, $\lambda = 0.6328 \mu\text{m}$, $(x, z) \in [-3.5, 1.5] \times [-2.0, 5.2] \mu\text{m}^2$, $M_x = 80$, $M_z = 100$.

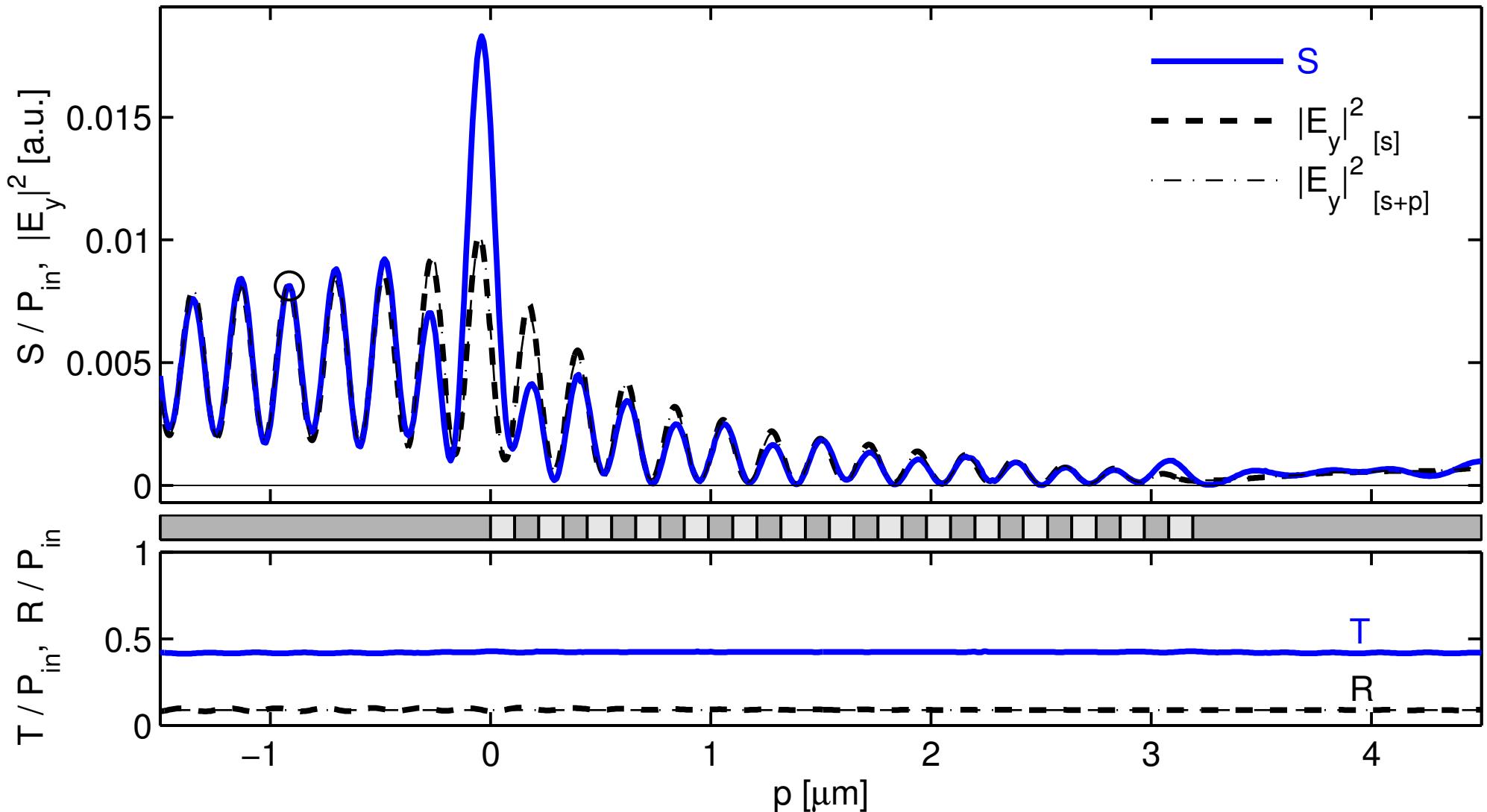
Bragg grating: QUEP model



Bragg grating: QUEP model



Bragg grating: QUEP model



2-D PSTM modeling

QUEP scheme:

a semianalytical quadridirectional eigenmode expansion technique,
here applied as convenient tool for “virtual” PSTM experiments:

- Evanescent field probing, signal $\propto |E|^2$.
- Direct scattering into the probe tip.
- Resonance breakdown caused by the presence of the probe.
- Reasonable mapping of evanescent fields for specific configurations.
- Ample qualitative agreement with real PSTM experiments
on a waveguide Bragg grating.

