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

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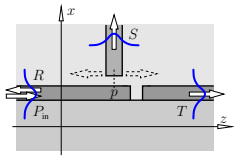
1 2-D PSTM modeling

Photon scanning tunneling microscopy (PSTM) becomes increasingly popular as a tool to study the local optical electromagnetic field close to the surface of devices from integrated optics / photonics. The microscope probes the optical field by detecting the optical power that is transferred via evanescent or radiative coupling to the tapered tip of an optical fiber near the surface of the sample. Scanning the tip across the surface is supposed to lead to a map of the evanescent optical field. For the present contribution we looked at a — highly simplifying — 2-D model of the microscope that includes the sample as well as the probe tip. Simple corrugated slab waveguides serve are samples. A half infinite piece of waveguide, oriented perpendicularly to the axis of the sample structures, represents the probe tip. The propagation of light with fixed frequency and definite polarization is considered.

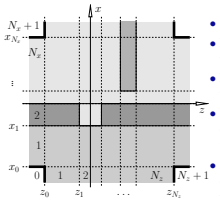


$P_{\text{in}} = 1.\quad S(p) = ?$
$R(p) = ?,\quad T(p) = ?$
$S(p) \overset{?}{\longleftrightarrow} (\text{Optical Field})|_p$

A recently proposed semianalytical simulation algorithm* constitutes a convenient tool for virtual experiments with this model. The simulations are based on bidirectional expansions of the electromagnetic field into eigenmodes associated with the piecewise constant refractive index structure, along each of the two relevant Cartesian coordinate axes. The examples below allow to estimate how the signal detected via the fiber is related to the field intensity at the probe tip, and how the presence of the probe influences the field distribution within the sample.

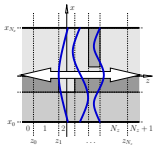
* M. Hammer, *Quadridirectional eigenmode expansion scheme for 2-D modeling of wave propagation in integrated optics*, Optics Communications (to appear in 2004); http://www.math.utwente.nl/~hammerm/Metric/

2 Quadridirectional eigenmode expansion

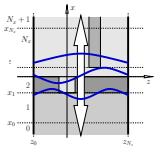


- 2-D Helmholtz problems, TE/TM.
- Piecewise constant, rectangular refractive index; linear, lossless materials.
- Fixed frequency $\omega = k\,\mathrm{c}$, vacuum wavelength $\lambda = 2\pi/k$.
- Rectangular interior domain, influx & outflux across all four boundaries, outwards homogeneous external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

Modal basis fields:



Slice s: $\psi^{\mathrm{d}}_{s,m}(x)$, $\pm\beta_{s,m}$, $d = \mathrm{f}, \mathrm{b}$.



Layer l: $\hat{\psi}^{\mathrm{d}}_{l,m}(z)$, $\pm\hat{\beta}_{l,m}$, $d = \mathrm{u}, \mathrm{d}$.

Discretization: $E_y = 0$ (TE) or $H_y = 0$ (TM) at $x = x_0, x_{N_x}$ or $z = z_0, z_{N_z}$.

Ansatz for the optical electromagnetic field:

$$\begin{pmatrix}\mathcal{E}\\ \mathcal{H}\end{pmatrix}(x,z,t) = \mathrm{e}^{\mathrm{i}\omega t}\times \qquad z_{s-1}\le z\le z_s,\ s=1,\dots,N_z,\quad x_{l-1}\le x\le x_l,\ l=1,\dots,N_x.$$

$$\mathrm{Re}\left\{\sum_{m=0}^{M_s-1} F_{s,m}\psi^{\mathrm{f}}_{s,m}(x)\,\mathrm{e}^{-\mathrm{i}\beta_{s,m}(z-z_{s-1})} + \sum_{m=0}^{M_s-1} B_{s,m}\psi^{\mathrm{b}}_{s,m}(x)\,\mathrm{e}^{+\mathrm{i}\beta_{s,m}(z-z_s)}\right.$$
$$\left.+\sum_{m=0}^{M_l-1} U_{l,m}\hat{\psi}^{\mathrm{u}}_{l,m}(z)\,\mathrm{e}^{-\mathrm{i}\hat{\beta}_{l,m}(x-x_{l-1})} + \sum_{m=0}^{M_l-1} D_{l,m}\hat{\psi}^{\mathrm{d}}_{l,m}(z)\,\mathrm{e}^{+\mathrm{i}\hat{\beta}_{l,m}(x-x_l)}\right\}.$$

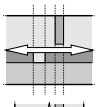
3 QUEP solution

Mode products: $\leftrightarrow$ normalization, projection

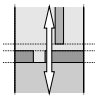
$$\langle\psi_1;\psi_2\rangle = \frac{1}{4}\int (E^*_{1,x}H_{2,y} - E^*_{1,y}H_{2,x} + H^*_{1,y}E_{2,x} - H^*_{1,x}E_{2,y})\mathrm{d}x\,,$$
$$\langle\hat{\psi}_1;\hat{\psi}_2\rangle = \frac{1}{4}\int (E^*_{1,y}H_{2,z} - E^*_{1,z}H_{2,y} + H^*_{1,z}E_{2,y} - H^*_{1,y}E_{2,z})\mathrm{d}z\,.$$

Algebraic procedure:

- Consistent bidirectional projection at all interfaces $\longrightarrow$ linear system of equations in $\{F_{s,m}, B_{s,m}, U_{l,m}, D_{l,m}\}$.
- Influx: $\boldsymbol{F}_0$, $\boldsymbol{B}_{N_z+1}$, $\boldsymbol{U}_0$, $\boldsymbol{D}_{N_z+1}$ $\longrightarrow$ RHS, given.
- Outflux: $\boldsymbol{B}_0$, $\boldsymbol{F}_{N_z+1}$, $\boldsymbol{D}_0$, $\boldsymbol{U}_{N_z+1}$ $\longrightarrow$ primary unknowns.
- "Exact" mode profiles $\longrightarrow$ interior problems decouple:



Solve for $\boldsymbol{F}_2,\dots,\boldsymbol{F}_{N_z}$ and $\boldsymbol{B}_1,\dots,\boldsymbol{B}_{N_z-1}$ in terms of $\boldsymbol{F}_1$ and $\boldsymbol{B}_{N_z}$ $\longrightarrow$ BEP I.



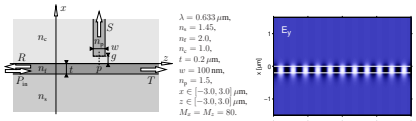
Solve for $\boldsymbol{U}_2,\dots,\boldsymbol{U}_{N_z}$ and $\boldsymbol{D}_1,\dots,\boldsymbol{D}_{N_z-1}$ in terms of $\boldsymbol{U}_1$ and $\boldsymbol{D}_{N_z}$ $\longrightarrow$ BEP II.

- Continuity of E and H on outer interfaces:

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

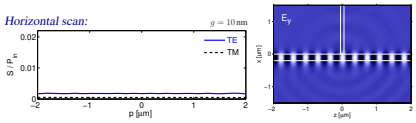
"QUadridirectional Eigenmode Propagation method" (QUEP).

4 Probing evanescent fields

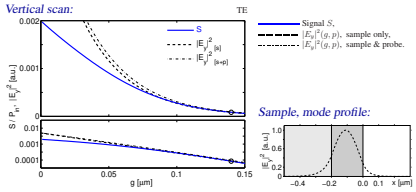


$\lambda = 0.633\,\mu\mathrm{m}$, $n_s = 1.45$, $n_t = 2.0$, $n_c = 1.0$, $t = 0.2\,\mu\mathrm{m}$, $w = 100\,\mathrm{nm}$, $n_p = 1.5$, $x \in [-3.0, 3.0]\,\mu\mathrm{m}$, $z \in [-3.0, 3.0]\,\mu\mathrm{m}$, $M_x = M_z = 80$.

Horizontal scan: $g = 10\,\mathrm{nm}$



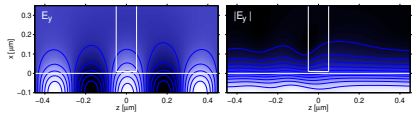
Vertical scan: TE



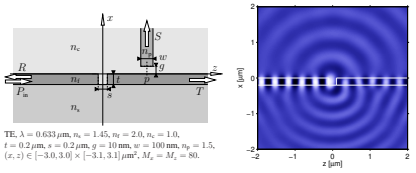
Signal S, $|E_y|^2(g,p)$, sample only, $|E_y|^2(g,p)$, sample & probe.

Sample, mode profile:

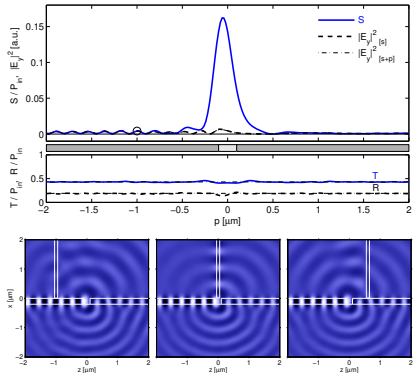
Probe tip neighborhood:



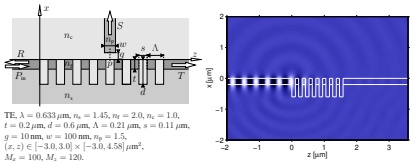
5 A hole defect



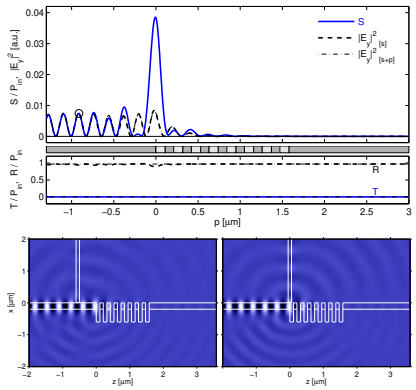
TE, $\lambda = 0.633\,\mu\mathrm{m}$, $n_s = 1.45$, $n_t = 2.0$, $n_c = 1.0$, $t = 0.2\,\mu\mathrm{m}$, $s = 0.2\,\mu\mathrm{m}$, $g = 10\,\mathrm{nm}$, $w = 100\,\mathrm{nm}$, $n_p = 1.5$, $(x,z) \in [-3.0, 3.0] \times [-3.1, 3.1]\,\mu\mathrm{m}^2$, $M_x = M_z = 80$.



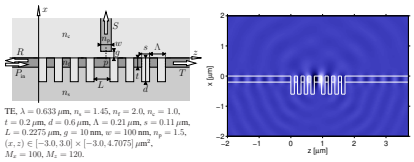
6 Short waveguide Bragg grating



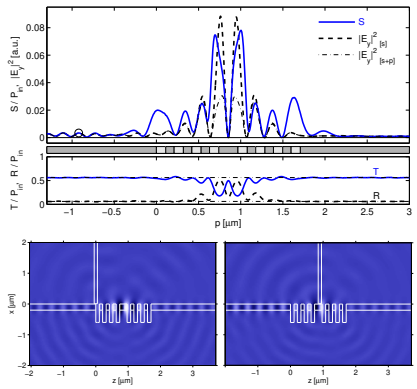
TE, $\lambda = 0.633\,\mu\mathrm{m}$, $n_s = 1.45$, $n_t = 2.0$, $n_c = 1.0$, $t = 0.2\,\mu\mathrm{m}$, $d = 0.6\,\mu\mathrm{m}$, $\Lambda = 0.21\,\mu\mathrm{m}$, $s = 0.11\,\mu\mathrm{m}$, $g = 10\,\mathrm{nm}$, $w = 100\,\mathrm{nm}$, $n_p = 1.5$, $(x,z) \in [-3.0, 3.0] \times [-3.0, 4.58]\,\mu\mathrm{m}^2$,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



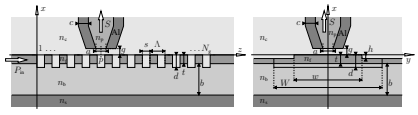
7 Resonant defect cavity



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

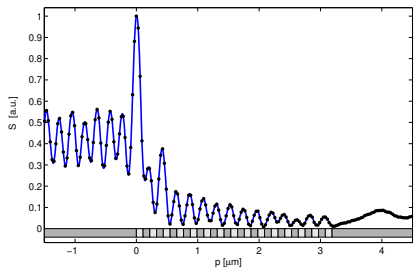


8 Bragg grating: PSTM experiment *



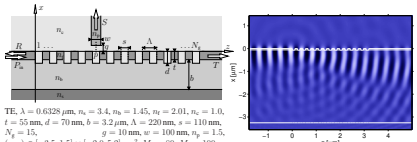
Sample: Rib waveguide with a series of deep, rectangular slits, $n_c = 3.4$, $n_b = 1.45$, $n_t = 2.01$, $n_c = 1.0$, $h = 11\,\mathrm{nm}$, $w = 1.5\,\mu\mathrm{m}$, $W = 2.5\,\mu\mathrm{m}$, $t = 55\,\mathrm{nm}$, $b = 3.2\,\mu\mathrm{m}$, $\Lambda = 220\,\mathrm{nm}$, $s = 110\,\mathrm{nm}$, $d =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

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

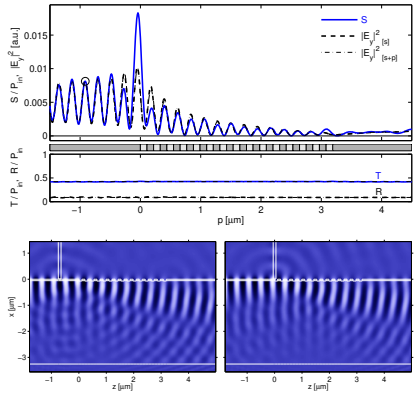


* E. Flück, M. Hammer, A. M. Otter, J. P. Korterijk, L. Kuipers, N. F. van Hulst, *Amplitude and phase evolution of optical fields inside periodic photonic structures*, Journal of Lightwave Technology **21**(5), 1384-1393 (2003)

9 Bragg grating: 2-D model



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



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