Computational photonics
— scattering problems in guided wave optics

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Photonics

For already several decades a trend towards miniaturization of optical systems can be observed. Quite analogous to electronics, optical components with diverse functionalities are to be combined into single monolithic chips, denoted by the shorthands PIC or OIC for Photonic or Optical Integrated Circuits. Consequently, the field is called *integrated optics*, as a subdivision of *photonics*. The technology finds its most prominent applications in the rapid growth of global communications. For a number of reasons, ranging from a higher bandwidth to the inexpensiveness of optical fiber materials, components based on electric currents are more and more complemented or replaced by a technology on the basis of light. Besides telecommunications, optical sensing is another promising and growing field of application for integrated optical chips. Relatively cheap, compact, and highly sensitive devices are realizable for a variety of areas, including in particular the measurement of chemical concentrations for biological, medical, or environmental purposes.

Dielectric waveguides constitute the optical analogon to the conductor paths of microelectronics. Frequently these are small ribs or strips with cross section dimensions in the order of micrometers, fabricated by specific etching techniques from stacks of transparent dielectric films. Similar to optical fibers, the structures are able to confine, to "guide" light via the mechanism of total internal reflection. In the past years, research in integrated optics has seen a shift of emphasis towards concepts that can more effectively guide and trap the light, i.e. that offer possibilities for substantially higher integration densities. Examples are the many proposals for devices based on defects (channels, cavities) in photonic crystals, on photonic "wires" (conventional, high contrast dielectric waveguides), or on microring or -disk resonators.

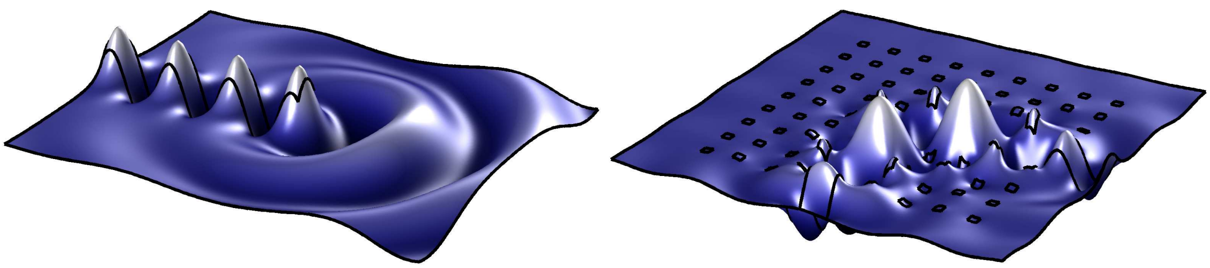

Fig. 1. Time snapshots of the optical electric field in two 2-D structures. Left: facet of a dielectric slab waveguide. Part of the incoming light is being reflected back into the waveguide, another part crosses the facet. There the formerly extremely focussed light spreads in the form of almost circular waves. Right: defect-waveguide in a photonic crystal. With hardly any radiation losses the light travels along a 90°-bend.

Concrete design efforts as well as fundamental investigations in the field rely heavily on computer simulations. All models are based on the Maxwell equations from classical electrodynamics. Analytical solutions, even for linear problems, exist only for few, highly symmetric, execptional cases. Hence one usually resorts to numerical methods. It turns out that rigorous discretizations e.g. in terms of finite elements lead to schemes with large, very often with unacceptably large computational effort, what concerns time and memory consumption. Besides the development of advanced "general purpose" numerical schemes, there is therefore also substantial interest in — necessarily simplifying — semi-analytical models for certain classes of problems. One of these schemes (quadridirectional eigenmode propagation, QUEP) will be looked at in the following paragraphs.

QUEP solver for 2-D scattering / Helmholtz problems

The spatially two dimensional propagation of optical waves of a certain polarization with fixed, given frequency is described by a standard Helmholtz equation. For typical situations in integrated optics, complications arise due to the nonconstant refractive index, which corresponds to the different materials the optical device is made of, and due to the fact that one actually considers open problems, where the boundary conditions for a necessarily limited computational domain deserve special attention. Given some optical influx, a solver for these scattering / Helmholtz problems should answer with (an approximation to) a solution of the Helmholtz equation on the computational window that connects smoothly to outgoing waves on all pieces of the boundary.

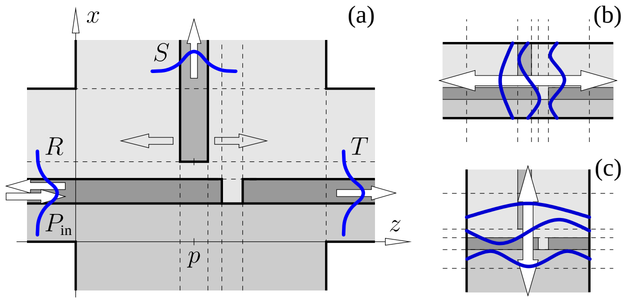

Fig. 2. (a): An example for a 2-D integrated optical scattering problem (a schematic of the PSTM model, see last section), here consisting of a slab waveguide with a hole in the core (the sample), and a half-infinite vertical waveguide segment (the probe). Dashed lines indicate the division of the structure into layers and slices, as required for the QUEP simulations. (b, c): QUEP basis fields; the solution of the scattering problem is expanded into eigenmodes of local 1-D multilayer slab profiles that travel along the horizontal (b) and vertical axes (c).

We now restrict to configurations with purely real, isotropic, and piecewise constant refractive index profile, where all dielectric interfaces are parallel to one of the coordinate axes. The interesting region is enclosed by a rectangular frame. A solution of the Helmholtz problem is then sought on a cross-shaped computational domain that consists of this interior window, together with the outwards unbounded external stripes that are connected to the four edges. On the four corner points of the inner rectangle and on the boundaries of the external regions, the basic field components are assumed to vanish. The bold corners in Figure 2(a) indicate the restriction of the computational domain.

To define basis fields for an eigenmode expansion, two types of divisions of this domain are considered. On the one hand, one views the structure as a sequence of vertical slices (b), such that within each slice the refractive index profile is constant along the z-axis. With each slice one can now associate a complete set of *modes*: solutions of a standard Sturm-Liouville eigenvalue problem that emerges if one views the (x-dependent) refractive index profile of that slice as being extended towards $z = \pm\infty$, introduces Dirichlet boundary conditions, and looks for fields that vary harmonically with z. For the present case of piecewise constant refractive index profiles one can compute analytical representations of these modes in a reliable and highly efficient way. The modes associated with the individual slices (x-dependent profiles, propagation along the z-axis) constitute one set of basis fields. On the other hand, the structure is decomposed into a stack of horizontal layers (c), where the permittivity is constant along the x-axis within each layer. The modes associated with the separate layers (z-dependent profiles, propagation along the x-axis) form a second set of basis fields. In conclusion, modes traveling in the positive and negative x- and z-directions contribute, hence one could call this a "quadridirectional" eigenmode expansion.

Superpositions of all basis modes establish the ansatz for the optical field, defined piecewise for the individual slices respectively layers. This ansatz satisfies the relevant wave equation everywhere in the computational domain, with the exception of the horizontal and vertical segment boundaries, where the Maxwell equations require certain continuity conditions to be satisfied. Consistent projection of these equalities onto the basis elements ("overlap" computations) with respect to suitable mode products allows to extract a linear system of equations in the so far unknown coefficients of the eigenmode expansion.

It turns out that the emerging system of equations permits a stepwise solution. As far as only the segments inside the inner rectangle are concerned, the contributions of the horizontally and vertically propagating modes are decoupled. Conventional bidirectional eigenmode propagation (BEP) schemes can be applied. The partial solutions (viewpoints Figure 2(b, c)) are subsequently connected by the equations that belong to the continuity conditions at the four outer edges of the computational rectangle. Only this last (essential) combination step establishes a solution of the wave equation on the entire cross-shaped computational domain. The optical influx is specified by prescribing the amplitudes of all inwards traveling basis fields on the exterior regions. This forms a right hand side to the linear system, which is then solved for all remaining expansion coefficients, with the amplitudes of the outgoing basis fields on the exterior stripes as primary unknowns.

The QUEP simulations treat the light propagation along both coordinate axes precisely alike. As an alternative to the viewpoint of the cross-shaped computational domain, the perpendicular, dependent superposition of BEP expansions may be viewed as a way to establish *fully transparent boundary conditions* (exception: the corner points) for the inner rectangular computational window, with a straightforward possibility of modeling guided wave influx and outflux. Though somewhat restrictive what concerns the geometrical variability, the technique offers an accurate and quite efficient platform for computational experiments with the PSTM model below.

A model of a photon scanning tunneling microscopy experiment

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 close to the surface of the sample. Scanning the tip across the surface leads to a map of the evanescent optical field, i.e. gives clues about the local light propagation through the device.

As a step beyond the mere analysis of the sample device, one can consider simulations that include the sample as well as the probe tip. We looked at a — highly simplifying — 2D model of the microscope; Figure 2(a) shows a schematic. 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.

As an example for a most simple sample for a localized corrugation, we look at a square hole defect in a slab waveguide. Figure 3 summarizes the results of a PSTM scan across the hole distortion; Figure 4 shows three examples for the resulting optical field.

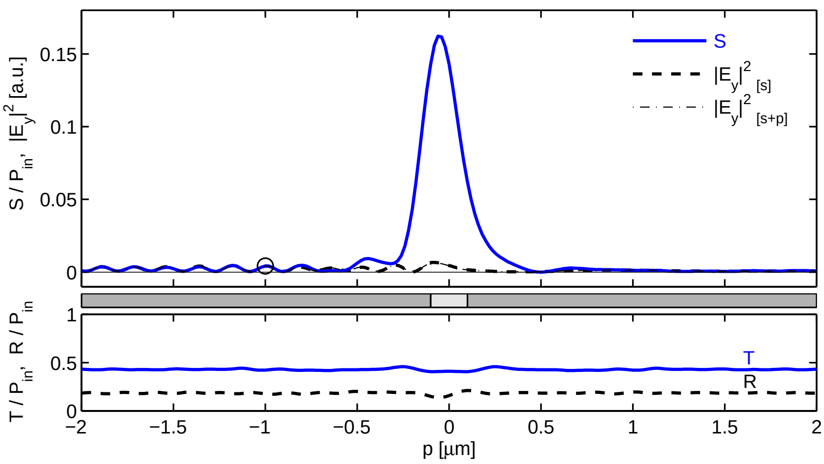

Fig. 3. Horizontal PSTM scan across the hole in the waveguide, signal S and local field intensity $|E_y|^2$ (top) versus the z-position p of the probe center. Bottom: guided power transmission T (continuous) and reflection R (dashed).

Without the probe, the hole reflects $R = 19\%$ and transmits $T = 43\%$ of the incident power; the remaining 38% are lost to nonguided, radiated fields. The superposition of the unit input and the guided reflection forms partly standing and traveling waves in the input core segment; the confined transmission leads to outwards traveling waves in the ongoing core segment. Both the reflected and transmitted parts of the confined fields undergo a transient oscillation until the lateral shapes of the waves are adapted to the particular profile of the guided mode further away from the defect. The hole acts as a strong localized source, where the radiation consists of waves with cylindrical shapes that originate from the hole, with wavelengths according to the different refractive indices in the regions below and above the waveguide core.

If the probe is moved along the sample in a region sufficiently far away ($|p| \geq 0.7\,\mu$m) from the hole, the PSTM signal follows nicely the local intensity of the predominantly evanescent waves that are present in those regions close to the sample surface. The almost periodic intensity pattern of the standing waves can be observed in the input segment. Beyond the hole, the signal corresponds to the lower constant level of the outgoing guided wave, with a shallow modulation due to the transient adaption to the precise mode profile. The radiated waves from the hole that reach the probe in these regions are partly reflected and transmitted by the vertical slab (cf. the third plot of Figure 4), but do not significantly couple to the upwards traveling mode of the probe, i.e. do not contribute to the signal.

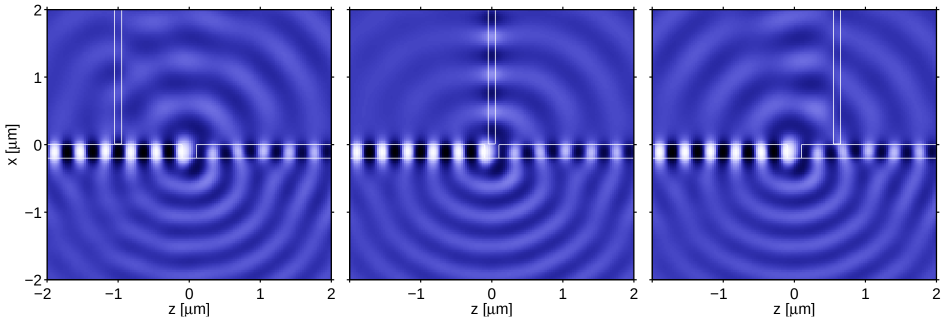

Fig. 4. Optical field around the hole in the waveguide, for probe positions $p = -1.0,\ 0.0,\ 0.6\,\mu$m. The colorscales correspond to time snapshots of the stationary physical electric field of the TE waves.

Close to the hole, however, the signal exhibits a strong peak, which obviously must be attributed to direct scattering from the hole upwards into the probe tip. Here the relation between the local field and the signal is entirely lost. Still, the peak is only moderately wider than the defect; the peak maximum is located slight off the center of the hole. If the probe is positioned directly above the defect, it collects most of the waves that are otherwise radiated into the upper half space (cf. the middle inset of Figure 4).

A series of further simulations with different types of samples have been carried out, in order to address the question in how far an experimental PSTM signal can be regarded as a quantitative "map" of the "optical field" in the device under test. We could point out several configurations where, according to the model, this simple notion definitely fails. Either the proportionality between the PSTM signal and the local intensity is entirely lost, or, even worse, the presence of the probe influences significantly the optical state of the sample. In fact, we could confirm an approximate proportionality exclusively for the constant-height scans along configurations with local single-mode standing wave patterns. Disturbance effects must be expected e.g. in any PSTM observations of high-quality resonances in photonic micro- and nano-cavities, in principle. While one should certainly be aware of these findings when executing PSTM measurements on photonic structures, we do not think it adequate, however, to attempt, only on the basis of the simplifying 2-D model, any more general quantitative characterization of experimental settings where these artefacts occur, or where they can be excluded.