Abstract

Photonics plays an important role in modern technologies, e.g. in telecommunications and sensing systems. Waveguiding structures with micro- and nano-meter scale features are the basic building blocks of photonic circuits. Large varieties of structures have been used by scientists and engineers. These range from the conventional planar and channel waveguides, which work on the basis of the total-internal-reflection (TIR) mechanism, to the more advanced structures that utilize the anti-resonance-reflection, leaky-defect-resonance, and photonic-band-gap principles to (quasi-)confine and control the light. More and more complicated structures are emerging along with the development of both theory and fabrication technologies, leading to the improvement of existing applications and enabling access to many new application areas. As the fabrication of these devices usually involves costly facilities and time-consuming procedures, modeling tools are indispensable to explore new ideas, characterize and design the devices before their realization, as well as to understand the experimental results.

This thesis reports a series of techniques the author has developed to model various waveguiding structures, including the conventional planar and channel waveguides working by, and the advanced structures working beyond the TIR mechanism. Hence, this thesis contains both the methods and their applications to model and study the standard guided-wave and the advanced leaky-wave structures. The methods include mode solvers based on finite difference method (FDM) and finite element method (FEM), furnished with transparent boundary conditions (TBCs) for both guided and leaky modes. Based on the developed techniques, structures as simple as planar waveguides up to as complicated as photonic crystal fibers (PCFs) can be modeled rigorously.

For structures with 1-D cross-section, both FDM and FEM mode solvers have been developed. For the FDM, a special discretization scheme that takes into account both the permittivity gradients and discontinuities at interfaces between different graded-index anisotropic materials of planar structures, has been developed and applied to structures with complicated index profiles like the titanium-indiffused proton-exchanged $LiNbO_3$ waveguides. For the FEM, either the one based on the variational or Galerkin approaches, simple high-order schemes capable to give 4th- or

6^{th}-order accuracy in effective indices have been developed for guided and leaky modes computation. Using the FEM mode solver; the properties of the anti-resonance reflecting optical waveguides (ARROWs), especially the anti-crossing phenomenon observed in the dispersion curves were studied. Together with the perturbation method, the FEM mode solver was also used to study the effect of a high-index medium in the proximity of a waveguiding structure. An interesting phenomenon on evolution of modes from guided to leaky and back to guided again as one varies the refractive index of the high-index medium was observed.

For structures with 2-D cross-section, a FEM scheme based on the Galerkin principle has been developed to solve the full vectorial wave-equation with a TBC that enables the computation of both guided and leaky modes in a relatively small computational domain. Using the mode solver, we investigate what happens when one varies the gap thickness of a Si_3N_4 strip waveguide with a DAST (4'-dimethylamino-*N*-methyl-4-stilbazolium tosylate) overlay. We observed in particular the evolution of modes from guided to leaky and back to guided again, from q-TM_{00} to q-TE_{10} and back to q-TM_{00} again, and from q-TE_{11} to q-TE_{10}. The vectorial leaky mode solver is well capable to handle complicated structure cross-section. It is suitable to rigorously study PCFs, including those that utilize the index-guiding mechanism as well as those that use the band-gap-guiding mechanism. Dispersion properties and confinement losses were investigated for a variety of PCFs, among others PCFs with circular or non-circular holes in the cladding, and with solid or air core. Another part of the study concerns the single-modeness of a commercial endlessly single-mode PCF. Based on the leaky mode picture, a criterion was proposed to locate its single mode operation regime. Additionally, hollow-core integrated optical waveguides were studied. A strategy, by considering the material composition of the anti-resonant bilayers to reduce the leakage loss, is reported. Low-loss hollow-core integrated optical waveguides designed based on that strategy, using silicon-compatible materials were proposed.