On effective index approximations of photonic crystal slabs

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As a means to assess the quality of effective index approximations in simulations of photonic crystal slabs, we consider a reduction of 2-D Helmholtz problems for waveguide Bragg gratings to 1-D wave propagation, and compare with rigorous 2-D reference solutions. Variational procedures permit to establish a reasonable effective index profile even in cases where locally no guided modes exist.

Introduction

The propagation of light through slab-like photonic crystals (PCs) is frequently described in terms of effective indices (effective index method EIM, cf. e.g. Refs. [1, 2, 3]). One replaces the actual 3-D structure by an effective 2-D permittivity, given by the propagation constants of the slab modes of the local vertical refractive index profiles. Though the approach is being described usually for the approximate calculation of waveguide modes, it is just as well applicable to propagation problems. Our aim is to check the approximation by analogous steps that reduce finite 2-D waveguide Bragg-gratings, which in turn can be seen as sections through 3-D PC membranes, to 1-D problems, which are tractable by standard transfer matrix methods. A 2-D Helmholtz solver ([4], reference) allows to solve the 2-D problem rigorously, i.e. to assess the quality of the EIM approximation.
The EIM-viewpoint becomes particularly questionable if locally the vertical refractive index profile cannot accommodate any guided mode, as e.g. in the holes of a PC membrane. We check numerically a recipe [1, 5] to uniquely define an effective permittivity even for these cases, based on a variational view on the EIM.

Variational effective index approximation

The 2-D frequency domain propagation of TE-polarized light with vacuum wavelength λ and wavenumber $k = 2\pi/\lambda$ through a dielectric structure with relative permittivity $\varepsilon(x,z)$ is governed by the scalar equation

$$(\partial_x^2 + \partial_z^2 + k^2\varepsilon)\, E_y = 0 \tag{1}$$

for the single electric field component E_y that is oriented perpendicular to the x- (vertical) z- (horizontal) plane of interest.
In view of the effective index approximation we select a vertical reference permittivity profile $\varepsilon_\mathrm{r}(x)$, for which a guided slab mode $\phi(x)$ satisfies the 1-D mode equation
$(\partial_x^2 + k^2(\varepsilon_\mathrm{r} - n_\mathrm{eff}^2))\,\phi = 0$ with effective mode index n_eff. What follows is based on the assumption that ϕ constitutes a reasonable approximation for the vertical field shape on the entire horizontal axis, i.e. that the optical field is given by $E_y(x,z) = \psi(z)\,\phi(x)$, with a yet to be determined function ψ.
By employing a functional form [1, 6, 7, 5] of Eq. (1) and looking for conditions for variational stationarity with respect to ψ, one can extract an equation

$$(\partial_z^2 + k^2\varepsilon_\mathrm{eff})\,\psi = 0 \tag{2}$$

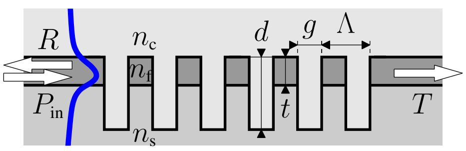
for the field dependence on the horizontal coordinate with effective permittivity [1, 5]

$$\varepsilon_{\text{eff}}(z) = n_{\text{eff}}^2 + \int (\varepsilon(x,z) - \varepsilon_{\text{r}}(x))\, \phi^2(x)\, \mathrm{d}x \Big/ \int \phi^2(x)\, \mathrm{d}x\,. \tag{3}$$

Note that, depending on the actual local refractive index contrast, $\varepsilon_{\text{eff}} = N_{\text{eff}}^2$ can well turn out to be negative. This then implies an imaginary effective index N_{eff}, along with evanescent wave propagation, in the respective regions. Below we refer to the computational approach given by Eqs. (1)–(3) as "variational effective index method" vEIM.
Eq. (2) governs the 1-D propagation through a dielectric multilayer stack with permittivity $\varepsilon_{\text{eff}}(z)$; one has thus replaced the original 2-D problem by an effective 1-D problem. Analogous expressions can be derived for different polarization [8], and based on variational forms [1, 4] of the full 3-D Maxwell equations. The procedures are analogous to what has been applied in the context of scalar [8] and vectorial [9] mode solvers.

Results

Figures 1–3 summarize results of the former procedure for a series of short, high-contrast 2-D configurations. The parameter set of Figure 1 could represent a deeply etched, air-covered Si_3N_4 film on a SiO_2 substrate. Figure 2 addresses a thin Si membrane with periodic air holes. Figure 3 looks at a resonance in an air-clad Si/SiO_2 grating with a central defect.



$n_c = 1.0$, $n_f = 2.0$, $n_s = 1.45$,
$t = 0.2\mu$m, $\Lambda = 0.21\mu$m,
$g = 0.11\mu$m, $d = 0.6\mu$m.

Bold lines:
QUEP (continuous, reference),
vEIM (dashed).

Thin curves:
"conventional" EIM,
$N_{\text{eff}}^{\text{holes}} = 1.0$ (continuous),
$N_{\text{eff}}^{\text{holes}} = 1.2$ (dash-dotted),
$N_{\text{eff}}^{\text{holes}} = 1.45$ (dashed).

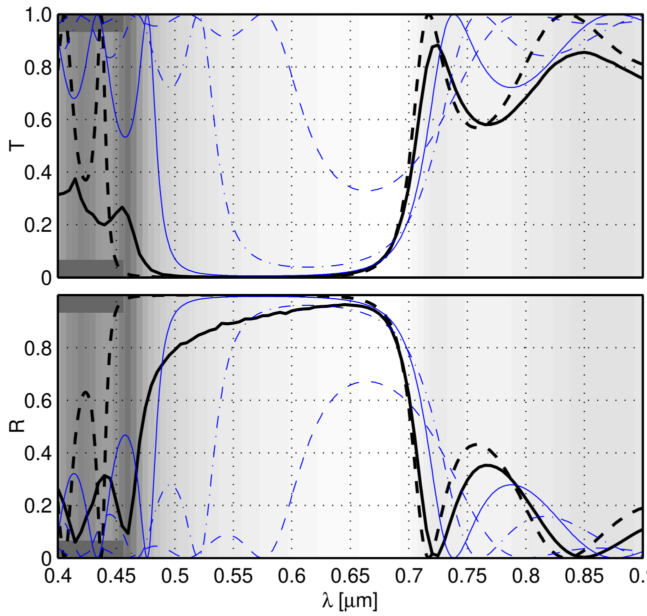
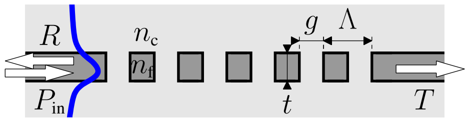
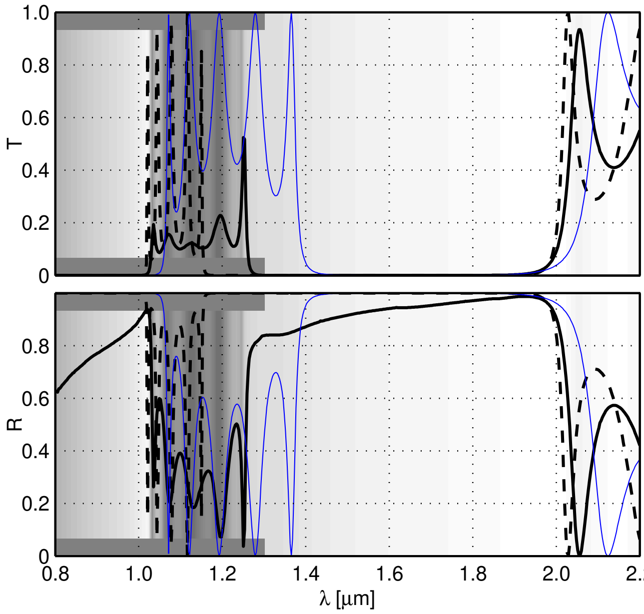


Figure 1: A deeply etched, vertically nonsymmetric waveguide Bragg grating, relative guided wave (fundamental mode) transmission T and reflection R versus vacuum wavelength λ. Both EIM and vEIM approximations rely on effective indices for the slab segments between $N_{\text{eff}}^{slab} = 1.87$ ($\lambda = 0.4\mu m$) and $N_{\text{eff}}^{slab} = 1.67$ ($\lambda = 0.9\mu m$). The vEIM effective index in the etched regions varies from $N_{\text{eff}}^{holes} = 0.82$ ($\lambda = 0.4\mu m$) to $N_{\text{eff}}^{holes} = 0.71$ ($\lambda = 0.9\mu m$). Darker shading indicates higher losses (vertical scattering) as predicted by the QUEP reference. The gray patches span the wavelength range where the slab is multimode.

In all configurations there is (at least) one guided slab mode in the non-etched regions; the corresponding vertical refractive index profile thus allows to compute a reasonable



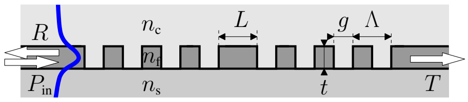
$n_c = 1.0$, $n_f = 3.4$,
$t = 0.2\mu$m, $\Lambda = 0.45\mu$m,
$g = 0.225\mu$m.



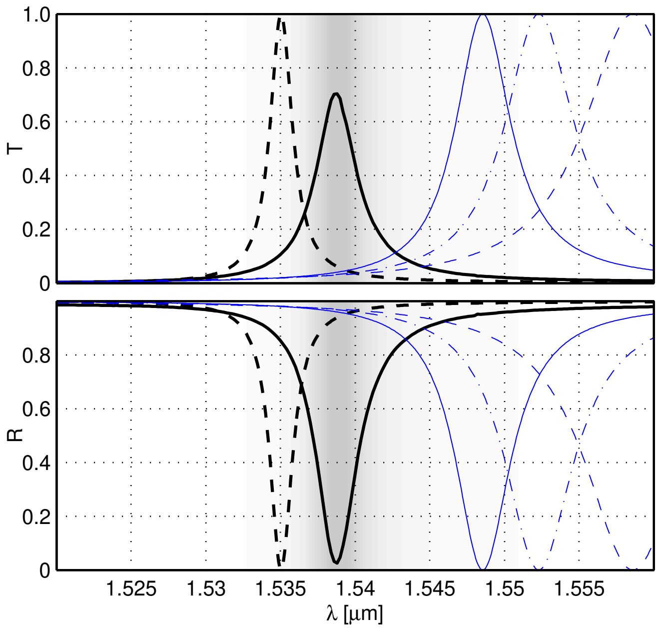
Bold lines:
QUEP (continuous, reference),
vEIM (dashed).

Thin curves:
"conventional" EIM,
$N_{\rm eff}^{\rm holes} = 1.0$.

Figure 2: High contrast vertically symmetric waveguide Bragg grating, modal transmission T and reflection R versus vacuum wavelength λ. $N_{eff}^{slab} \in [2.33_{\lambda=2.2\mu m}, 3.09_{\lambda=0.8\mu m}]$ *(vEIM and EIM),* $\varepsilon_{eff}^{holes} \in [-1.30_{\lambda=2.2\mu m}, -0.41_{\lambda=0.8\mu m}]$ *(vEIM). Cf. also the caption of Figure 1.*



$n_c = 1.0$, $n_f = 3.4$, $n_s = 1.45$,
$t = 0.220\mu$m, $\Lambda = 0.310\mu$m,
$g = 0.135\mu$m, $L = 1.515\mu$m.



Bold lines:
QUEP (continuous, reference),
vEIM (dashed).

Thin curves:
"conventional" EIM,
$N_{\rm eff}^{\rm holes} = 1.0$ (continuous),
$N_{\rm eff}^{\rm holes} = 1.2$ (dash-dotted),
$N_{\rm eff}^{\rm holes} = 1.45$ (dashed).

Figure 3: Vertically nonsymmetric waveguide grating with central defect, spectral transmission T and reflection R around a defect resonance. $N_{eff}^{slab} \in [2.75_{\lambda=1.56\mu m}, 2.77_{\lambda=1.52\mu m}]$ *(vEIM and EIM),* $\varepsilon_{eff}^{holes} \in [-0.96_{\lambda=1.56\mu m}, -0.94_{\lambda=1.52\mu m}]$ *(vEIM). Cf. also the caption of Figure 1.*

effective index which enters both the "conventional" EIM calculations and the vEIM procedures. The non-etched slab also provides the reference permittivity and vertical mode profile to evaluate Eq. (3) for the vEIM approach. All configurations have also in common that the etched regions (holes) do not support any guided modes. The "conventional" EIM approach thus requires to guess an effective index for the hole regions; results for different plausible values are compared in the figures. Note that, along with the vertical

mode profiles and with the exception of the former "guessed" values, all effective indices are wavelength dependent. The dependence appears almost linear for the present configurations; corresponding intervals are given in the figure captions.
A semianalytic Helmholtz solver (quadridirectional eigenmode propagation, QUEP [4, 10]) is applied to generate reference solutions for the present 2-D problems. We restrict to the simplest case of TE polarization as introduced before. In contrast to the EIM and vEIM approximations, the rigorous QUEP calculations cover vertically propagating waves accurately. This out-of plane scattering manifests through losses in the guided wave power balance, which can not be taken into account by the EIM and vEIM approximations. One should thus focus the comparison to those spectral regions without pronounced losses, i.e. the regions with bright background in Figures 1–3.

Concluding remarks

The previous simulations showed clearly that a treatment of a propagation problem involving a high contrast PC membrane in terms of effective indices can hardly be expected to be more than a mere qualitative, rather crude quantitative approximation. Nevertheless, situations may arise where, for various reasons, there are no options but to restrict simulations to 2-D. One should then at least invest the small effort to determine the correction term in Eq. (3), and perform the 2-D calculation for the thus established effective permittivity profile. At least for the former examples we could observe that the resulting variational effective index approximation comes closer to reality than any "conventional" EIM with educated guesses of effective indices for regions where no local modes exist.

Acknowledgments

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