Single mode condition for shallow silica–titania rib waveguides

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Received: 1 June 2018 / Accepted: 14 September 2018 / Published online: 19 September 2018
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Abstract
A single mode condition for silica–titania rib waveguides is proposed in this work. It is applicable to rib waveguides having rib height sufficiently small to sustain fundamental modes in slab waveguides adjacent to the rib. The relationships binding rib waveguide dimensionless morphological parameters for which the secondary order, HE and EH, horizontal modes leak outside the rib, rendering rib waveguides single mode, were determined by using the film mode matching method. A new criterion function is proposed for approximation to these relationships. It is shown that the proposed single mode condition gives significantly better results than the one proposed by Soref. Furthermore, it is shown that the fundamental EH mode can also leak outside the rib. This requires to complement the single mode condition, what can be accomplished by using the proposed criterion function. The studies also showed that a Soref’s correction factor significantly depends on rib waveguides aspect ratio.

Keywords Integrated photonics · Optical design · Rib optical waveguides · Single-mode conditions

1 Introduction
Currently, there are two major directions for development of integrated optics. A research effort within a scope of the first direction is focused on photonic integrated circuits (PIC) characterized by high integration level. Those devices are in most cases fabricated based on silicon-on-insulator (SOI) or indium phosphide (InP) technology platforms and find their application in telecommunication industry (Lipka et al. 2016; Smit et al. 2014). The second direction of PICs development involves planar optical waveguide chemical and biochemical sensors (Lambeck et al. 2006; Kozma et al. 2014). A technology platform of silicon nitride (Si$_3$N$_4$) or silicon oxynitride (SiO$_x$N$_y$) waveguides is frequently utilized for fabrication of such devices (Kaźmierczak et al. 2009; Romero-Garcia et al. 2013). In many cases, these sensors use an evanescent wave spectroscopy technique (Midwinter 1971; Lukosz
1995; Delezoide 2014). Application of this technique makes some requirements about the design of planar optical measurement transducers. Considering transducers employing phase detection, one of these conditions is to ensure that they conform to single mode operation conditions.

Rib waveguides are one of the most important components of PICs. They may serve two different functions. Being a part of planar optical measurement transducers, they are involved in detection of a measurand via interaction with a sensitive film. In this case PICs usually integrate planar interferometers, which convert an optical phase shift to light intensity changes (Lukosz 1995; Schmitt et al. 2006). The second function of rib waveguides is to lead an optical wave to and off components integrated in PICs, as well as to couple planar structures to optical fibers (Zaoui et al. 2014). The problem of how to choose morphological parameters of rib waveguides, so that they are single mode is very important from two reasons. Planar optical measurement transducers operating on a basis of a phase detection scheme require single mode waveguides to achieve high interferometric contrast (Leblanc-Hotte et al. 2016). Moreover, if homogeneous and surface sensitivities of planar optical waveguides are going to be maximized, then these waveguides should be single mode and should have uniform refractive-index profile and high refractive index contrast (Karasiński 2004; Karasinski and Rogozinski 2008).

In addition to the three aforementioned, well known and established technology platforms, there is also a platform that uses silica–titania (SiO$_2$:TiO$_2$) planar waveguides fabricated on glass substrates using a sol–gel method (Karasinski and Rogozinski 2005; Karasinski et al. 2011). This type of waveguides has the undoubted advantage of having very low optical losses, which is a result of amorphous nature of the silica–titania composition. They can work in both visible and infrared part of the electromagnetic spectrum. Moreover, sol–gel based silica–titania planar waveguides show very good stability of their parameters over long-time periods. It should be noted that they are composed of titanium dioxide embedded in silica matrix. Metal oxides such as TiO$_2$, ZnO, ZrO$_2$ or Ta$_2$O$_5$ cannot be oxidized and are resistant to hydrolysis and corrosion processes (Ramsden 1993). In this article are presented results of numerical analysis which allowed to formulate the single mode conditions for silica–titania rib waveguides on glass substrates in air ambient.

## 2 Single mode condition

A single mode condition (SMC) for rib waveguides has a form of an inequality that operates on quantities related to rib waveguides morphological parameters, which characterize their transversal sizes: a parent-slab thickness $H$, a rib width $w$ and a rib height $t$ (see Fig. 1 in Sect. 3). This inequality is very often expressed in terms of a dimensionless rib width $u$ and a dimensionless side-slab thickness $r$, which are defined by Eqs. (2) and (3). The first SMC was derived by Petermann (1976), who derived it by using the effective index method, EIM, (Hocker and Toulios 1970; Chiang 1986). This condition, further referred to as “EIM SMC”, is given by the formula:

\[
 u < r/(1 - r^2)^{1/2}
\]

(1)

where $u$ and $r$ are defined by the following equations (Pogossian et al. 1998):

\[
 u = \frac{w + 2r \sqrt{k^2 (n_f^2 - n_c^2)} - 1/2}{H + q}
\]

(2)
where \( n_f, n_s \) and \( n_c \) are refractive indices of a silica–titania guiding film, a substrate and a cover, respectively. A parameter \( \gamma \) depends on a polarization, \( \gamma_{c,s} = 1 \) for HE\(_{pq}\) modes (quasi-TE), \( \gamma_{c,s} = (n_{c,s}/n_f)^2 \) for EH\(_{pq}\) modes (quasi-TM), \( k = 2\pi/\lambda \) where \( \lambda \) is a wavelength.

Soref et al. (1991) added a single correction constant \( a_S \), to the right-hand side of (1) and showed that HE\(_01\) and EH\(_01\) modes leak to side-slab waveguides rendering rib waveguides single mode for HE and EH polarizations, respectively. The Soref’s SMC is given by the formula:

\[
u < a_S + r/(1 - r^2)^{1/2}
\]

where \( n_f, n_s \) and \( n_c \) are refractive indices of a silica–titania guiding film, a substrate and a cover, respectively. A parameter \( \gamma \) depends on a polarization, \( \gamma_{c,s} = 1 \) for HE\(_{pq}\) modes (quasi-TE), \( \gamma_{c,s} = (n_{c,s}/n_f)^2 \) for EH\(_{pq}\) modes (quasi-TM), \( k = 2\pi/\lambda \) where \( \lambda \) is a wavelength.

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\[
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\]

A function on the right-hand side of (5) is further referred to as the Soref’s criterion function. The Soref’s SMC is restricted to a range of \( r \geq 0.5 \), because in this range effective indices of fundamental side-slab modes were higher than any higher-order vertical modes of rib waveguides. The rib waveguides, considered in this work, guide only fundamental vertical modes. For that reason the restriction on \( r \) results from a relationship between effective indices of side-slab fundamental modes and rib waveguide second-order horizontal modes. A necessary condition that must be satisfied is that the side-slab is not cut-off. As a result the SMC derived in this work is limited to shallow rib waveguides.

All SMCs for rib waveguides that have been formulated to date (Petermann 1976; Soref et al. 1991; Powell 2002; Jinsong and Jinzhong 2004; Seong et al. 2005; Xuejun et al. 2009; Dorin and Ye 2013; Ziyang et al. 2016), base on searching for such morphological parameters at which effective indices of higher order rib waveguide modes leak into the fundamental side-slab mode of corresponding polarization. They have one of the following forms: \( u < S(r) \) (Petermann 1976; Soref et al. 1991; Jinsong and Jinzhong 2004), \( u < S(r,H) \) (Seong et al. 2005; Xuejun et al. 2009; Dorin and Ye 2013; Ziyang et al. 2016) and \( u < S(r,H,t,w) \) (Powell 2002), where \( S \) is the criterion function. The function \( S \) in its most favorable form depends only on \( r \), which is a dimensionless parameter. Up until now investigations aimed either directly at SMCs (Soref et al. 1991; Hauffe et al. 1999; Powell 2002; Lousseau et al. 2004; Jinsong and Jinzhong 2004; Xuejun et al. 2009) or focused on other properties of rib waveguides in the context of SMCs (Vivien et al. 2002; Seong et al. 2005; Milosevic and...
Matavulj 2008; Dorin and Ye 2013) were mainly carried out for SOI rib waveguides. However, rib waveguides fabricated using other material platforms were also studied: GeSi-Si (Soref et al. 1991), polymer-silica (Hauffe et al. 1999), GaAs-AlGaAs (Ferguson et al. 2006), Si$_3$N$_4$-SiO$_2$ (Grote and Bassett 2016), Yb-YAG/YAG (Ziyang et al. 2016). Investigation of single mode conditions were carried out using the EIM method (Petermann 1976; Soref et al. 1991), the Film Mode Matching method, FMM, (Hauffe et al. 1999; Vivien et al. 2002; Xuejun et al. 2009; Dorin and Ye 2013; Ziyang et al. 2016), the Beam Propagation Method, BPM, (Powell 2002; Jinsong and Jinzhong 2004; Lousteau et al. 2004; Ferguson et al. 2006) and the Finite Element Method (Laurentis et al. 2007; Huang et al. 2016). The rib waveguides investigated in this work were fabricated using the sol–gel method and a dip coating technique (2005-01-Karasiński, 2011-01-Karasiński). They have substantially higher aspect ratio ($w/H > 8$), than those investigated by the researchers cited in this paper ($w/H < 4.5$). A new type of the criterion function $S$ is proposed. It depends only on dimensionless side-slab thickness $r$, and gives significantly better results than the criterion function derived by Soref et al. (1991).

3 Investigated structure

The schematic diagram of the structure investigated in this work is shown in Fig. 1. A vertically-walled, silica–titania rib waveguide is deposited on a BK7 glass substrate. The rib waveguide is characterized by three independent geometrical parameters: $w$, $t$ and $H$. A thickness of the parent-slab and the side-slab are linked by the equation: $H - h = t$.

Analysis was carried out for a single wavelength $\lambda = 0.635 \, \mu$m, at which refractive indices of the silica–titania waveguide film, the BK7 glass substrate and the cover are $n_f = 1.8186$, $n_s = 1.5150$, $n_c = 1.0000$, respectively.

4 Method

A single mode condition presented in this work was derived based on analysis of effective index (modal) characteristics of rib waveguides and side-slab waveguides. Modal characteristics of guided modes were calculated as a function of the rib height $t$. For this purpose was utilized the FMM method implemented in the FIMMWAVE 6.3 solver from Photon Design. Dirichlet boundary conditions were set on boundaries of the computational domain. Principal components of $HE_{pq}$ modes ($E_x$ and $H_y$) and $EH_{pq}$ modes ($E_y$ and $H_x$) are vanishing at these boundaries. This is the rigorous and semi-analytical method giving very accurate results when applied to vertically-walled rib waveguides. A schematic diagram of subsequent analysis steps is presented in Fig. 2.

The analysis presented in this paper is based on a search of points at which modal characteristics of rib waveguides and side-slab waveguides are intersecting. Lousteau et al. (2004) showed that such methodology is sufficient because the rib waveguides analyzed in this work do not support higher order vertical modes (e.g. $HE_{pq}$ or $EH_{pq}$ where $p > 1$), but only modes characterized by $p = 0$ and $q = 0,1$. Modal characteristics were calculated as a function of the rib height $t$ which is considered a basic morphological parameter. If the parent-slab thickness is a constant parameter then there is one fixed modal characteristic of the side-slab waveguide associated with a set of characteristics of rib waveguides, which are characterized by constant parent-slab thickness and varying rib width $w$. Sample modal characteristics are presented in

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Fig. 2 Schematic diagram of the analysis process. Morphological parameters are described in Fig. 1.

Fig. 3. There are some specific values of the rib height \( t \) at these graphs. The first, \( t_{\text{sst}} \), is the rib height at which effective indices of rib waveguide modes are equal to the effective index of a fundamental side-slab mode of corresponding polarization. The second, \( t_{\text{cff}} \), is the rib height at which a given rib waveguide mode is cut-off. Only \( t_{\text{sst}} \) values are needed to determine the SMC for rib waveguides whose side-slab waveguides are guiding modes. In Fig. 4 are presented exemplary characteristics \( t_{\text{sst}}(w) \). These characteristics were transformed into a space of dimensionless variables \( u(r) \) and approximated by a new type of the criterion function \( S \), given by the equation:

\[
u = S(r) = a + b \cdot r / (1 - r^2)^c
\]  

where \( a, b, c \) are approximation coefficients that depend on constant family parameter \( H \). The function (6) becomes identical to the Soref’s criterion function if \( b = 1 \) and \( c = 0.5 \). It gives very good approximation to \( u_{\text{sst}}(r) \) characteristics as is shown in the next section. Moreover, it only depends on dimensionless side-slab thickness \( r \) and have three coefficients which must be obtained by fitting, while the function \( u = a + b \cdot r / (1 - c \cdot r^2) + d \cdot r \) proposed in Jinsong and Jinzhong (2004) have four such coefficients. For each approximated \( u_{\text{sst}}(r) \) characteristic the approximation error was calculated using the following equation:

\[
E = \frac{1}{M} \sum_{i=1}^{N} \left| \frac{u_i - u_{ai}}{u_i} \right|
\]  

Fig. 3 Effective indices of a rib waveguide as a function of the rib height \( t \) for \( HE \) modes (a) and \( EH \) modes (b). \( t_{\text{sst}}^{00}, t_{\text{sst}}^{01} \)—rib heights for which effective indices of rib and side-slab waveguide modes are equal, \( t_{\text{cff}}^{00}, t_{\text{cff}}^{01} \)—rib heights for which effective indices of rib and side-slab waveguide modes decrease down to the refractive index of the substrate \( n_s \). Morphological parameters are described in Fig. 1.

Fig. 4 Exemplary characteristics of SMC conditions for rib waveguides whose side-slab waveguides are guiding modes.
where $u_i$ are values of $u_{sst}$ characteristics, $u_{ai}$ are values of criterion functions approximating $u_{sst}$. $M$ is a number of points on $u_{sst}$ characteristics.

Each modal characteristic was calculated in a range from 0 to $H$ for 150 points. Values of criterion functions (5) and (6) were evaluated for $H$ varying from 135 nm to 240 nm every 15 nm. The rib width varied from 1.0 µm to 2.0 µm every 0.02 µm. Derivation and approximation of $u_{sst}$ characteristics for several values of the parent-slab thickness allowed to extend a dimensionless rib width range within which the SMC was derived.

### 5 Results and discussion

The sample modal characteristics of $HE$ and $EH$ modes of a silica–titania rib waveguide as well as $TE_0$ and $TM_0$ modes of the associated side-slab waveguide are presented in Fig. 3. Characteristics are plotted using a solid, bold line if a given mode is guided. One can observe that considering $HE$ modes, this rib waveguide is single mode for $t \in (0, t_{sst}^{01})$ because effective indices of the secondary order horizontal mode, $HE_{01}$, are greater than effective indices of the side-slab $TE_0$ mode if $t > t_{sst}^{01}$. The presence of rib makes the rate of decline of rib waveguide modes slower than is observed for side-slab waveguide modes. Considering $EH$ modes, the rib waveguide is single mode for $t \in (t_{sst}^{00}, H)$, whereas for $t \in (0, t_{sst}^{00})$ it does not guide modes of this polarization. That is because of two reasons: (i) effective indices of the secondary horizontal mode, $EH_{01}$, are less than effective indices of the side-slab $TM_0$ mode in entire range of variation of $t$ and (ii) the fundamental mode, $EH_{00}$, leaks into the side-slab for $t < t_{sst}^{00}$. It can furthermore be noted that there are no $t_{sst}^{00}$ values for $HE_{00}$ modes in entire considered parent-slab thickness range, whereas for $EH_{00}$ modes $t_{sst}^{00} < 4$ nm.

Furthermore if $EH$ modes and variation of the rib width are considered, one can see in Fig. 4b that rib waveguides can be single mode in two separate intervals of the rib height. This happens in an interval $(w_1, w_2)$. One can see from characteristics presented in this graph that for $w = w_1$ the side-slab becomes cut-off ($t = t_{eff}^0$), whereas for $w = w_2$ a cut-off rib height of the secondary order horizontal mode reaches its maximum value ($t_{eff}^1 = H$). The difference between $t(w)$ characteristics for $HE$ and $EH$ modes stems from the fact that for a given value of the parent-slab thickness, $HE$ modes are further from cut-off than $EH$ modes. A cut-off thickness, $H_{eff}$ of parent-slab $TE_0$ and $TM_0$ modes are 85 and 131 nm.
respectively. Second order horizontal modes are not cut-off for sufficiently thick parent-slab waveguides in entire considered rib width range, as one can see in the case of $HE_{00}$ modes, which is why there is no $t_{01}$ characteristics in Fig. 4a.

Single mode conditions are formulated in the $(r, u)$ coordinate system. In the Fig. 5 are presented characteristics from Fig. 4 transformed into this system. A bold, solid line in Fig. 5b is an approximation to a $u_{sst}$ characteristic of the $EH_{00}$ mode, whereas bold, dash lines are approximations to $u_{sst}$ characteristics of second order horizontal modes: $EH_{01}$ and $HE_{01}$. There are no $u_{sst}$ characteristics of the $HE_{00}$ mode in the entire considered parent-slab thickness range. One can see that the proposed function (6) is much better approximation to $u_{01}^{\text{sst}}$ characteristics than the Soref’s criterion function (5). Approximation curves obtained using (5), are plotted using dash-dot lines. The difference in approximation quality is particularly evident when $EH_{01}$ modes are considered. The EIM SMC (1), gives the poorest approximation to $u_{00}^{\text{sst}}$ characteristics. Furthermore, in the case of $EH$ modes this condition gives better approximation to $u_{00}^{\text{sst}}$. The $u_{01}^{\text{eff}}$ of the $EH_{01}$ mode wasn’t approximated.

Characteristics $u_{sst}(r)$ derived for subsequent values of the parent-slab thickness, are presented on both graphs in Fig. 6 and in Fig. 7a. In order to avoid obscuration of solid lines representing approximation curves, only selected markers were plotted. One can see
that the proposed criterion function (6) gives very good approximation not only to $u_{ss}$ characteristics of secondary order, horizontal modes, but also to the $HE_{00}$ mode. The characteristics $u_{ss}$ of $HE_{01}$ and $EH_{01}$ modes exist in a narrower interval of the dimensionless side-slab thickness by comparing it to these determined by other researchers: $r \geq 0.5$ (Soref et al. 1991; Powell 2002; Jinsong and Jinzhong 2004; Xuejun et al. 2009), $0.5 \leq r \leq 0.7$ (Hauffe et al. 1999), $0.5 \leq r \leq 0.8$ (Lousteau et al. 2004). In the case of silica–titania rib waveguides discussed in this work, the lower and upper limits of these intervals depend on the polarization and parent-slab thickness. However for the secondary order horizontal modes all of them are in the range of $0.84 \leq r \leq 0.98$. A shift of a lower limit of this range from 0.5 to $\approx 0.84$ stems from the fact that investigated rib waveguides are relatively thin. In this respect it is to be noted that a cut-off thickness of $TE_{1}$ and $TM_{1}$ modes of the parent-slab are 400 nm and 447 nm, respectively. When analysing side-slab waveguides modal characteristics as functions of the dimensionless side-slab thickness $r$, one can observe that in the entire considered parent-slab thickness range, side-slab waveguides are cut-off for $r \leq 0.62$. A relationship between $r$ and $t$ is given by the equation:

$$r = 1 - \frac{t}{H} \left( 1 + \frac{1}{kH} \left( \frac{\gamma_{c}}{\Delta_{c}} + \frac{\gamma_{s}}{\Delta_{s}} \right) \right)^{-1}$$

(8)

where $\Delta_{s,c} = \left( n_{s,c}^{-2} - n_{s,c}^{-2} \right)^{1/2}$. A description of the remaining symbols is given in the footnotes of Fig. 1 and Eq. 4. A family of such characteristics for $TE_{0}$ modes is presented in Fig. 7b. As expected, a dimensionless side-slab cut-off thickness ($n_{eff}=n_s$) significantly depends on the parent-slab thickness. However, the lower and upper limits of intervals within which $HE_{0j}$ modes are leaking into side-slabs slightly depend on the parent-slab thickness. It is depicted by bold line segments of side-slab effective index characteristics which are corresponding to $u_{ss}$ characteristics presented in the adjacent graph.

Characteristics of the approximation error $E$ as a function of the parent-slab thickness were calculated using (7). They are presented in Fig. 8a. One can observe that error values calculated for approximation using the Soref’s criterion function (5) are several times higher than it is in the case of the proposed criterion function (6). Moreover, on the contrary to error characteristics determined for (5), approximation errors for (6) depend on the parent-slab thickness to a small extent. Approximation errors are
comparable only for a $EH_{01}$ mode and the lowest value of the parent-slab thickness for which $t_{sst}^{01}$ values exist ($H = 165$ nm). This results from the fact that in this case a rate of change of the $u_{sst}(r)$ is the lowest (see Fig. 6b). This is the case if a parent-slab thickness is close to a cut-off thickness of its fundamental mode, which is 131 nm.

The Soref’s correction factor $a_s$ significantly depends on the parent-slab thickness. Corresponding characteristics are presented in Fig. 8b. Considering both polarizations, the determined values of $a_s$ are decreasing with the increase in parent-slab thickness. In this respect, it is to be noted that an aspect ratio of rib waveguides is also decreasing. As one can see, the Soref’s correction factor monotonically depends on rib waveguides aspect ratio. It is consistent with the results obtained in by Ferguson et al. (2006), who presented result of studies on SOI rib waveguides.

The function (6) can be utilized to approximate a relationship between dimensionless rib width $u_{sst}$ and dimensionless side-slab thickness $r$ of rib waveguides fabricated utilizing other technological platforms (e.g. $Si_3N_4$–$SiO_2$, SOI). It is because a nature of $u_{sst}(r)$ functions will remain unchanged. They are continuous, increasing functions defined on some subintervals of the interval $r \in (0, 1)$. Differentiating (6) with respect to $r$, one gets:

$$\frac{du}{dr} = b \left( 1 + 2c \frac{r}{1-r^2} \right) (1 - r^2)^{-c}$$ (9)

One can see that if $b$ and $c$ are positive, the derivative is also positive in the interval $r \in (0, 1)$ making the approximating function also continuously increasing in this interval.

The single mode condition proposed in this paper is valid if rib waveguides are not capable of guiding higher order modes $HE_{pq}$ or $EH_{pq}$, which are characterized by $p > 1$ or $q > 1$. Lousteau et al. showed that the single mode condition based on approximation to $u_{sst}(r)$ is not enough if a rib waveguide guides higher order vertical modes ($p > 1$). This suggest that the same situation take place if horizontal modes are considered ($q > 1$). However the question whether the presented condition is valid for shallow rib waveguides guiding more than two horizontal modes ($p=0, q > 1$) is still open and requires further analysis that cannot be lead using analysis based only on effective index characteristics.
6 Conclusion

The derivation of a single mode condition for high aspect ratio, silica–titania rib waveguides requires a new type of the criterion function. The single mode condition proposed by Soref et al. (1991) is insufficient, especially if the parent-slab thickness is significantly higher than a cut-off thickness of its fundamental mode. The criterion function proposed in this article gives very good results in a wide range of the normalized rib width. Also fundamental rib waveguide modes can leak into slab waveguides adjacent to the rib. Within the considered range of rib waveguides morphological parameters, this is the case if $EH$ modes are considered. The proposed criterion function also gives very good approximation to the relationship between the normalized rib width and normalized side-slab thickness for which effective indices of rib waveguide $EH_{00}$ mode is equal to the side-slab $TM_0$ mode.

Acknowledgements This work was supported by Polish National Science Center under Grant DEC-2017/25/B/ST7/02232 and by the Silesian University of Technology under Grant 05/040/RGH17/0018.

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