

Efficient Computation of TM- and TE-Polarized Leaky Modes in Multilayered Circular Waveguides

Dries Vande Ginste, *Member, IEEE*, Hendrik Rogier, *Senior Member, IEEE*, and Daniël De Zutter, *Fellow, IEEE*

Abstract—In combination with the Perfectly Matched Layer (PML)-paradigm, eigenmode expansion techniques have become increasingly important in the analysis and design of cylindrical and planar waveguides for photonics applications. To achieve high accuracy, these techniques rely on the determination of many modes of the modal spectrum of the waveguide under consideration. In this paper we focus on the efficient computation of Transverse Magnetic (TM) and Transverse Electric (TE) polarized leaky modes for multilayered cylindrical waveguides. First, quasi-static estimates are derived for the propagation constants of these modes. Second, these estimates are used as a starting point in an advanced Newton iteration scheme after they have been subjected to an adaptive linear error correction. To prove the validity of the computation technique it is applied to technologically important cases: vertical-cavity surface-emitting lasers (VCSELs) and a monomode fiber.

Index Terms—Multilayered circular waveguides, mode matching methods, perfectly matched layers, leaky modes, Béranger modes, vertical-cavity surface-emitting laser (VCSEL), monomode fiber

I. INTRODUCTION

Perfectly Matched Layers (PMLs) [1], [2] were originally conceived to serve as absorbing boundary conditions in electromagnetic field solvers, such as FDTD [3]. In recent years, the PML-paradigm [4], [5] has led to new and rather unexpected applications concerning full-wave analysis and design of complex electromagnetic structures, in particular layered media. This paradigm allows to convert an open waveguide that consists of an open stack of dielectric layers, into a closed waveguide. The presence of the PML ensures that the closed waveguide accurately mimics the behavior of the original open waveguide. Whereas the modal spectrum of the original open waveguide comprises a continuous set of radiating modes, the closed waveguide only exhibits discrete sets of modes. This paradigm resulted in fast analysis techniques for planar microwave structures [6]–[9] as well as in modal analysis methods for acoustic waveguides [10]. In the field of photonics, the PML-paradigm has led to vectorial eigenmode expansion techniques. These techniques have proven to be very useful in the analysis of optical slab waveguides, such as laser facets [11], [12], modelled as layered planar media. Optical cylindrical waveguides have also been studied, e.g. waveguide discontinuities appearing in vertical-cavity surface-emitting lasers (VCSELs) [13] and bending losses in optical fibers [14].

The determination of many modes, up to very high mode numbers, appearing in the modal spectrum of the waveguides under consideration is indispensable to be able to develop mode matching techniques with high accuracy. Formalisms to efficiently compute all these modes' propagation constants have been proposed in the literature for microwave and optical waveguides [15]–[20]. Often, the focus is on finding the leaky modes. These modes can be used in eigenmode analyses of open waveguides, albeit for a limited set of applications, since the leaky modes correspond to *improper* solutions of the dispersion relation [14]. The term “improper” is used to indicate that these modes do not satisfy the radiation condition [21]. In the case of a waveguide that is closed through application of the PML-paradigm, the leaky modes are *proper* solutions of the dispersion relation and together with the guided modes and the so-called Béranger (or PML) modes, they form a complete set [5], [22].

In this paper we focus on the computation of the leaky modes' propagation constants of both open and closed multilayered cylindrical waveguides presented in Fig. 1. We propose a two-step approach: first, accurate quasi-static estimates are calculated and second, these estimates are used in a Newton iteration scheme after being subjected to an adaptive linear error correction to rapidly and very precisely determine the propagation constants. It is important to mention that in [17] a computation technique has been presented for single-layered cylindrical waveguides which is also based on quasi-static estimates. However, it is not at all straightforward to extend the technique presented in [17] to general multilayered *cylindrical* waveguides. In [16], [23] a rapid technique for the determination of the leaky modes' propagation constants in multilayered *planar* media was proposed, following a similar two-step approach as presented in this paper, but without the linear error correction. In comparison to multilayered cylindrical media, the quasi-static estimates pertaining to multilayered planar media are easier to derive and more accurate. This is due to the particular form of the dispersion relations of planar media that mainly consist of exponential functions. In the cylindrical case, a large-argument expansion of Bessel functions is required, reducing the accuracy. So, in the cylindrical case discussed in this paper, extra care needs to be taken to maintain high accuracy. We focus on the transverse magnetic (TM) and the transverse electric (TE) polarized leaky modes of open waveguides and waveguides closed through application of the PML-paradigm. Hybrid modes are still more complex. Their analysis would lengthen this paper to an unacceptable size.

Applications of the technique can be found in the analysis or the design of technologically important cylindrical wave-

Electromagnetics Group, Department of Information Technology, Ghent University, Sint-Pietersnieuwstraat 41, 9000 B-Gent, Belgium. E-mail: dries.vande.ginste@intec.UGent.be, Tel.: +32 9 264 33 54, Fax: +32 9 264 99 69.

guides. Therefore, the method has been illustrated by calculating the leaky modes' propagation constants for (i) AlAs-AlOx apertures in VCSEL cavities and (ii) a typical monomode fiber. These examples have also been considered in [13], [17], [24], but, due to the limitations of the technique applied in these papers, a single cylindrical layer consisting of a homogeneous dielectric together with an *infinite* cladding had to be assumed. The new method presented here alleviates this restriction, making it better suited to address real-life applications, such as VCSEL cavities and fibers with additional layers and/or a cladding of *finite* dimensions.

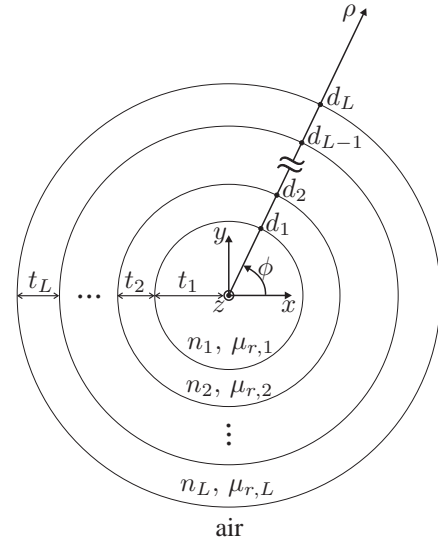
The outline of this paper is as follows. In Section II the formalism to calculate the leaky modes' propagation constants is proposed. The cylindrical waveguide configurations under consideration are defined in Section II-A and the corresponding dispersion relations are given in Section II-B. Next, quasi-static estimates are derived (Sections II-C and II-D). These estimates are used as starting points of an efficient computation procedure, as explained in Section II-E. The theory is illustrated by a set of examples in Section III. Finally, conclusions are summarized in Section IV.

In the sequel, all sources and fields are assumed to be time-harmonic with angular frequency ω and time dependencies $e^{j\omega t}$ are suppressed.

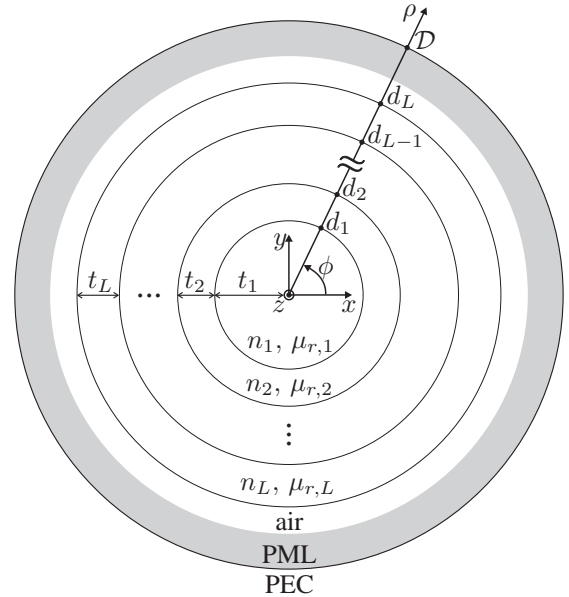
II. FORMALISM TO EFFICIENTLY COMPUTE LEAKY MODES IN OPEN AND PEC-BACKED PML-CLOSED MULTILAYERED CIRCULAR DIELECTRIC WAVEGUIDES

A. Geometry

Consider the multilayered circular waveguides consisting of L dielectric layers, as shown in Fig. 1. In these configurations, each dielectric layer l , $l = 1, \dots, L$, is characterized by its thickness t_l and a refractive index $n_l = \sqrt{\epsilon_{r,l}}$, where $\epsilon_{r,l}$ is the relative permittivity of the layer. In general, a magnetic contrast between the layers is possible, hence, each layer is also characterized by its relative permeability $\mu_{r,l}$. In cylindrical coordinates (ρ, ϕ, z) , with $\rho = \sqrt{x^2 + y^2}$, the interface between layer l and layer $l+1$ is found at a radial distance $\rho = d_l = \sum_{q=1}^l t_q$, $l = 1, \dots, L$. In the case of an open waveguide (Fig. 1(a)), the outside layer of the geometry is an air-filled half-space, indicated by the layer number $l = L+1$, a refractive index $n_{L+1} = 1$, and a relative permeability $\mu_{r,L+1} = 1$. In Fig. 1(b), the PML-paradigm [4], [5] has been applied. The waveguide is closed by means of a PML that is backed by a perfect electrically conducting (PEC) cylindrical wall. Using the complex coordinate stretching formalism [2], it can be shown that this procedure is mathematically equivalent to enclosing the L dielectric layers of the waveguide and a part of the $(L+1)$ th layer of air in a PEC cylinder with *complex* radius \mathcal{D} . This complex thickness \mathcal{D} is chosen such that the PML provides damping along the direction perpendicular to the layer interfaces, i.e. the radial direction ρ . This is achieved by a thickness with a real part $\Re(\mathcal{D}) > 0$ and an imaginary part $\Im(\mathcal{D}) < 0$. Due to the reflectionless absorption of waves impinging upon the PML, the structure of Fig. 1(b) closely mimics the behavior of the original, open structure of Fig. 1(a).



(a) Case 1: open waveguide



(b) Case 2: waveguide closed by a PEC-backed PML

Fig. 1: Multilayered circular waveguide geometries

B. Generalized reflection coefficient and dispersion relation

To derive the dispersion relation for the waveguides presented in Fig. 1, the concept of generalized reflection coefficient is used, as defined in [25]. Of course, for the PEC-backed PML-closed waveguide presented in Fig. 1(b), the method of [25] is adapted to take the closed character of the waveguide into account. For both circular geometries of Fig. 1, waves can be expanded into cylindrical harmonics with different $e^{-j\nu\phi}$ dependencies, where the integer number ν indicates the ν th harmonic. In order not to overload this paper, only axially symmetric ($\nu = 0$) transverse magnetic (TM) and transverse electric (TE) (with respect to the z -axis) polarized

modes are considered, and no hybrid modes. The modal fields have a $e^{-j\beta_{\text{TX}}z}$ -dependency where β_{TX} is the TX-polarized transverse modal propagation constant. Here, and in what follows, TX stands for TM and TE (X=M,E). For both waveguides of Fig. 1, the generalized reflection coefficient [25] for TM- and TE-polarized waves at the interface between region l and $l+1$, $l = 1, \dots, L$, is given by

$$\tilde{R}_{\text{TX}}^{l,l+1} = R_{\text{TX}}^{l,l+1} + \frac{T_{\text{TX}}^{l+1,l} \tilde{R}_{\text{TX}}^{l+1,l+2} T_{\text{TX}}^{l,l+1}}{1 - R_{\text{TX}}^{l+1,l} \tilde{R}_{\text{TX}}^{l+1,l+2}}. \quad (1)$$

The expressions for the reflection coefficients $R_{\text{TX}}^{l,l+1}$ and $R_{\text{TX}}^{l+1,l}$ and for the transmission coefficients $T_{\text{TX}}^{l,l+1}$ and $T_{\text{TX}}^{l+1,l}$ result from lengthy calculations, which are summarized in the appendix for both waveguides. They depend of course on the material parameters n_l and $\mu_{r,l}$ and the layer thicknesses t_l , as well as on the modal propagation constants β_{TX} . As can be expected, these latter typically appear in radial wavenumbers $k_{\rho,l} = \sqrt{k_0^2 n_l^2 \mu_{r,l} - \beta_{\text{TX}}^2}$ for each layer $l = 1, \dots, L+1$, where the free-space wavenumber is $k_0 = (\omega/c)$ and c is the speed of light. Since $k_{\rho,l}$ is only defined up to a sign, we demand that $\Im(k_{\rho,l}) \leq 0$. Using propagation constants β_{TX} located in the fourth quadrant of the complex β -plane, i.e. $\Re(\beta_{\text{TX}}) \geq 0$ and $\Im(\beta_{\text{TX}}) \leq 0$, propagation of the modes in the $+z$ -direction with a bounded mode profile is assured. Expression (1) for the generalized reflection coefficient should be used recursively starting from the top layer $l = L$, taking into account that $\tilde{R}_{\text{TX}}^{L+1,L+2} = 0$, working our way down to the generalized reflection coefficient $\tilde{R}_{\text{TX}}^{1,2}$. Denoting the denominator of the generalized reflection coefficient $\tilde{R}_{\text{TX}}^{1,2}$ as $N_{\text{TX}}(\beta_{\text{TX}})$, the TX-polarized dispersion relation of the waveguides under consideration is given by

$$N_{\text{TX}}(\beta_{\text{TX}}) = 0. \quad (2)$$

The propagation constants β_{TX} of the modes are found as the zeros of this dispersion relation.

Besides leaky modes, also Béranger modes exist within a multilayered PEC-backed PML-closed waveguide. As stated in [17], most of the field of these Béranger modes is concentrated inside the PML, while strong attenuation is found in the dielectric layer. Hence, a similar procedure as presented in [17] for a single-layered waveguide can be followed to determine the Béranger modes' propagation constants of multilayered waveguides. Therefore, this will not be repeated here. For the leaky modes, the situation is more complex when considering a multilayered waveguide. Since the field of the leaky modes is concentrated in the dielectric layer(s) of the waveguide, the fact that we consider multiple layers in this paper has a large influence and the procedure of [17] has to be altered.

C. Approximations for the propagation constants of the leaky modes

The procedure starts by computing quasi-static estimates of the propagation constants. These are found as zeros of a properly approximated version of the dispersion relation (2). For an open waveguide, the zeros are located in the improper Riemann sheet (where $\Im(k_{\rho,l}) > 0$) and for a PEC-backed

PML-closed waveguide they are located in the proper Riemann sheet (where $\Im(k_{\rho,l}) \leq 0$). Anyway, under the quasi-static approximation, the numbers β_{TX} are exactly the same in both cases, hence, we only focus on open waveguides here.

An approximate version of the dispersion relation (2) is found as follows. First, it is safe to assume that the layer thicknesses t_l , $l = 1, \dots, L$, form commensurable numbers. This means that for each distance d_l , $l = 1, \dots, L$, there exists an integer i_l such that $d_l = s i_l$, where s is a fixed real number. In all practical applications, such an s can be found. This allows to introduce the following notation:

$$u = e^{2jk_{\rho,l}s}. \quad (3)$$

Second, large-argument expansions for the Bessel functions [26], appearing in the expression for the reflection and transmission coefficients $R_{\text{TX}}^{l,l+1}$, $R_{\text{TX}}^{l+1,l}$, $T_{\text{TX}}^{l,l+1}$, and $T_{\text{TX}}^{l+1,l}$ (see (A-1)–(A-4)) are introduced. Third, we invoke the quasi-static approximation

$$k_{\rho} \approx k_{\rho,1} \approx k_{\rho,2} \approx \dots \approx k_{\rho,L+1} \approx j\beta_{\text{TX}}. \quad (4)$$

This quasi-static approximation is valid for high mode numbers m , i.e. for large values of $|\beta_{\text{TX}}|$. The reader notices that (4) leads to $\Im(k_{\rho}) > 0$ for propagation constants β_{TX} situated in the fourth quadrant of the complex plane. Here, for an open waveguide, this guarantees the location of the propagation constants in the correct Riemann sheet, i.e. the improper sheet. These three steps result in the following expressions for the reflection and transmission coefficients:

$$R_{\text{TX}}^{l,l+1} \approx -2j \frac{(\alpha_{\text{TX}}^{l+1} - \alpha_{\text{TX}}^l) u^{-i_l}}{(\alpha_{\text{TX}}^{l+1} + \alpha_{\text{TX}}^l) + j(\alpha_{\text{TX}}^{l+1} - \alpha_{\text{TX}}^l) u^{-i_l}}, \quad (5)$$

$$R_{\text{TX}}^{l+1,l} \approx -\frac{j}{2} \frac{(\alpha_{\text{TX}}^{l+1} - \alpha_{\text{TX}}^l)(u^{i_l} + u^{-i_l})}{(\alpha_{\text{TX}}^{l+1} + \alpha_{\text{TX}}^l) + j(\alpha_{\text{TX}}^{l+1} - \alpha_{\text{TX}}^l) u^{-i_l}}, \quad (6)$$

$$T_{\text{TX}}^{l,l+1} \approx 2 \frac{\alpha_{\text{TX}}^l}{(\alpha_{\text{TX}}^{l+1} + \alpha_{\text{TX}}^l) + j(\alpha_{\text{TX}}^{l+1} - \alpha_{\text{TX}}^l) u^{-i_l}}, \quad (7)$$

$$T_{\text{TX}}^{l+1,l} \approx 2 \frac{\alpha_{\text{TX}}^{l+1}}{(\alpha_{\text{TX}}^{l+1} + \alpha_{\text{TX}}^l) + j(\alpha_{\text{TX}}^{l+1} - \alpha_{\text{TX}}^l) u^{-i_l}}, \quad (8)$$

where $\alpha_{\text{TM}}^l = n_l^2 = \epsilon_{r,l}$ and $\alpha_{\text{TE}}^l = \mu_{r,l}$. The approximated dispersion relation for the leaky modes is now easily constructed. Starting from the top interface between layers L and $L+1$ and applying (1) with the above definitions (5)–(8), the generalized reflection coefficient at the bottom interface can be written as a rational function in u :

$$\tilde{R}_{\text{TX}}^{1,2} \approx \frac{M_{\text{TX}}(u)}{N_{\text{TX}}(u)}. \quad (9)$$

The denominator $N_{\text{TX}}(u) = 0$ now corresponds to the approximated dispersion relation, and it can be easily shown that this is a polynomial of degree i_L of the following form:

$$N_{\text{TX}}(u) \approx 1 + \text{l.o.t.}(u) - j \frac{1 + \alpha^L}{1 - \alpha^L} u^{i_L} = 0, \quad (10)$$

where the lower order terms $\text{l.o.t.}(u)$ are of a degree smaller than i_L and larger than zero.

For general waveguides, the terms $\text{l.o.t.}(u)$ cannot be neglected and the complete dispersion relation (10) with the

lower order terms has to be used to compute the quasi-static estimates. Thereto, first, the zeros of $N_{\text{TX}}(u) = 0$ are determined using fast polynomial root finding techniques [27]. This leads to i_L zeros u_p , $p = 1, \dots, i_L$. Second, each u_p yields a separate branch of propagation constants corresponding to leaky modes, given by

$$j\beta_{\text{TX}} \approx k_\rho \approx \frac{1}{2js} \log |u_p| + \frac{1}{2s} \arg(u_p) + \frac{m\pi}{s}, \quad (11)$$

for a high mode order m . Assuming that there is always a dielectric contrast in at least one of the layers of the waveguide, i.e. there is at least one refractive index $n_l \neq 1$, the above described procedure is always valid for the TM-modes. Similarly, for the TE-modes, the procedure is only valid provided $\mu_{r,l} \neq 1$ for at least one layer. In many practical applications, there is no magnetic contrast between the layers, yielding reflection coefficients for the TE-modes that are equal to zero at all interfaces (see (5) and (6)). Therefore, the particular case without magnetic contrast will be investigated below.

D. Particular case: absence of magnetic contrast

In the absence of magnetic contrast, all layers have a relative permeability $\mu_{r,l} = 1$, $l = 0, \dots, L$, and more accurate approximations of (A-1) and (A-2) for the TE-polarized reflection coefficients have to be made. Therefore, together with the definition (3) and the large argument expansions for the Bessel functions, instead of (4), the *second-order* quasi-static approximation

$$k_{\rho,l} \approx j\beta_{\text{TE}} - j \frac{k_0^2 n_l^2}{2\beta_{\text{TE}}} = k_\rho + \frac{k_0^2 n_l^2}{2k_\rho} \quad (12)$$

is introduced into the expressions of the TE-polarized reflection and transmission coefficients (see (A-1)–(A-4)), yielding

$$R_{\text{TE}}^{l,l+1} \approx j \frac{k_0^2}{k_\rho^2} \frac{(n_{l+1}^2 - n_l^2) u^{-i_l}}{2 - j \frac{k_0^2}{2k_\rho^2} (n_{l+1}^2 - n_l^2) u^{-i_l}}, \quad (13)$$

$$R_{\text{TE}}^{l+1,l} \approx \frac{j}{4} \frac{k_0^2}{k_\rho^2} \frac{(n_{l+1}^2 - n_l^2) (u^{i_l} + u^{-i_l})}{2 - j \frac{k_0^2}{2k_\rho^2} (n_{l+1}^2 - n_l^2) u^{-i_l}}, \quad (14)$$

$$T_{\text{TE}}^{l,l+1} \approx \frac{2}{2 - j \frac{k_0^2}{2k_\rho^2} (n_{l+1}^2 - n_l^2) u^{-i_l}}, \quad (15)$$

$$T_{\text{TE}}^{l+1,l} \approx \frac{2}{2 - j \frac{k_0^2}{2k_\rho^2} (n_{l+1}^2 - n_l^2) u^{-i_l}}. \quad (16)$$

These new expressions (13)–(16) for the reflection and transmission coefficients in geometries without magnetic contrast are now used in the construction of the generalized reflection coefficient $\tilde{R}_{\text{TE}}^{1,2}$. During this process, terms with factors $\left(\frac{k_0}{k_\rho}\right)^\eta$ with $\eta > 2$ are omitted in the spirit of the second-order approximation. This leads to a new approximated dispersion relation $N_{\text{TE}}(u) = 0$ of the following form:

$$N_{\text{TE}}(u) \approx 1 + \text{l.o.t.}(u) + \frac{4j}{k_0^2 (1 - n_L^2)} u^{i_L} = 0. \quad (17)$$

Given this dispersion relation (17), it is clear that the procedure explained in the previous section, i.e. finding the roots of the polynomial leading to quasi-static estimates, cannot be applied as the coefficients of the polynomial in u (17) now also depend on $k_\rho \approx j\beta_{\text{TE}}$. As an alternative, for high mode numbers m , we propose the following solution for the propagation constants of the m th TE-polarized leaky mode:

$$j\beta_{\text{TE}} \approx k_\rho \approx \frac{m\pi}{s i_L} + A + \frac{j}{s i_L} \log \left(\frac{m\pi}{s i_L} + A \right). \quad (18)$$

It is now verified, a posteriori, that (18) is a good choice and that A is a constant independent of the mode number m . Substitution of (18) into (3) yields

$$u = e^{\frac{2jm\pi}{i_L}} e^{2jAs} \left(\frac{m\pi}{s i_L} + A \right)^{-\frac{2}{i_L}}, \quad (19)$$

where A yet remains to be determined. Introducing (19) and the first two terms of (18) into (17) yields

$$1 + \text{terms } \mathcal{O}\left(\frac{1}{m^\xi}\right) + \frac{4j}{k_0^2 (1 - n_L^2)} e^{2jAs i_L} \approx 0. \quad (20)$$

For large m , the terms of order $\mathcal{O}\left(\frac{1}{m^\xi}\right)$ can be neglected as $\xi > 0$, yielding the following solution for A :

$$A = -\frac{j}{s i_L} \log \left(\frac{k_0 \sqrt{1 - n_L^2}}{2} \right) + \frac{\pi}{4s i_L}, \quad (21)$$

which is indeed a constant independent of the mode number m , making the proposed solution (18) valid. Inserting (21) into (18) approximately results in

$$j\beta_{\text{TE}} \approx k_\rho \approx \frac{j}{s i_L} \log \left(\frac{(4m+1)\pi}{2s i_L k_0 \sqrt{1 - n_L^2}} \right) + \frac{(4m+1)\pi}{4s i_L}, \quad (22)$$

which are valid second-order quasi-static approximations for the TE-polarized dispersion relation in absence of magnetic contrast.

Still, more accurate approximations can be obtained. Let us introduce (18) and (19) into the common denominator of (13)–(16). This yields

$$\begin{aligned} & 2 - j \frac{k_0^2}{2k_\rho^2} (n_{l+1}^2 - n_l^2) u^{-i_l} \\ & \approx 2 - j \frac{k_0^2}{2} (n_{l+1}^2 - n_l^2) \frac{e^{-ji_l \frac{2m\pi}{i_L}} e^{-ji_l 2As}}{\left(\frac{m\pi}{s i_L} + A \right)^{2\left(1 - \frac{i_l}{i_L}\right)}}. \end{aligned} \quad (23)$$

Two cases should now be distinguished. First, consider $i_l < i_L$, viz. $l = 1, \dots, L-1$. The second term in the right-hand side of (23) decreases quickly for increasing m and hence, it can be neglected for large m . Second, for $i_l = i_L$, this term becomes independent of m and it should be retained. So, it can be seen that for $l < L$ the reflection coefficients $R_{\text{TE}}^{l,l+1}$ (13) and $R_{\text{TE}}^{l+1,l}$ (14) are of order $\mathcal{O}\left(\frac{1}{m^\xi}\right)$ and tend to zero as $\xi > 0$. In the same way, the transmission coefficients $T_{\text{TE}}^{l,l+1}$ (15) and $T_{\text{TE}}^{l+1,l}$ (16) for $l < L$ tend to one. Hence, the second-order quasi-static estimates of the TE-polarized leaky modes of a multilayered waveguide

without magnetic contrast only depend on the reflection and transmission coefficients at the interface where $\rho = s i_L = d_L$. This means that, in contrast to the general case described in Section II-C, the lower order terms l.o.t.(u) in the dispersion relations (17) can be neglected and the waveguide can be replaced by a single-layered waveguide of thickness $d_L = s i_L$ with refractive index n_L . The dispersion relation of this waveguide is given by

$$1 + \frac{4j}{\frac{k_0^2}{k_\rho^2}(1 - n_L^2)} e^{2jk_\rho s i_L} = 0. \quad (24)$$

The reader notices that this result (24) could also be found by noting that, given (20), the terms l.o.t.(u) in (17) can be omitted for high mode numbers m . Closed-form solutions of the approximate TE-polarized dispersion relation (24) exist, yielding the following accurate second-order quasi-static estimates

$$j\beta_{\text{TE}} \approx k_{\rho,L} \approx -\frac{j}{s i_L} W\left(m, \pm \frac{1-j}{2\sqrt{2}} k_0 s i_L \sqrt{1 - n_L^2}\right), \quad (25)$$

where each m is integer and corresponds to a different branch of the LambertW function $W(\cdot, \cdot)$ [28]. Due to the nature of this approach, the solution (25) is similar to the result presented in [17] for the TE-polarized estimates for a single-layered waveguide.

E. Efficient computation procedure to exactly determine the propagation constants of the leaky modes of open and PEC-backed PML-closed waveguides

To now efficiently compute the *exact* values of the leaky modes' propagation constants of open or PEC-backed PML-closed multilayered circular waveguides, the quasi-static estimates β_{TX} , described in the previous sections, are used as a starting point. Using the original, pertinent dispersion relations $N_{\text{TX}}(\beta_{\text{TX}}) = 0$ (2) for the open or the PEC-backed PML-closed waveguide, the exact propagation constants β_{TX} can be determined by performing some additional Newton iterations [29]

$$\beta_{\text{TX}}^{\text{new}} \leftarrow \beta_{\text{TX}}^{\text{old}} - \frac{N_{\text{TX}}(\beta_{\text{TX}}^{\text{old}})}{\left. \frac{d}{d\beta} N_{\text{TX}}(\beta) \right|_{\beta=\beta_{\text{TX}}^{\text{old}}}}. \quad (26)$$

This approach, also used in [16], yields good results for sufficiently high mode numbers. Compared to the quasi-static estimates for the leaky modes of multilayered *planar* dielectric waveguides described in [16], however, the quasi-static estimates presented here are less accurate. This is due to the fact that for *circular* waveguides we have to invoke the large argument expansions of the Bessel functions. Nevertheless, it is possible to implement a more accurate and robust scheme by considering the estimates *branch per branch*, starting from the highest mode numbers. The difference between the asymptotic approximation and the actual propagation constant (obtained via (26)) for mode m is used as a constant error term to correct the value of the asymptotic estimate for mode order $m - 1$ along the same branch, i.e. this difference is

added to the asymptotic estimate for mode $m - 1$ to yield a better approximation. As a consequence, a smaller number of additional Newton iterations (26) will be needed. It turned out to be even more advantageous to apply a so-called *linear error correction*. Now, the asymptotic estimate for mode order $m - 2$ is corrected using the values of both mode orders $m - 1$ and m of the same branch. In this way the number of required Newton iterations becomes minimal, leading to a very efficient technique.

III. NUMERICAL EXAMPLES

The technique to compute the propagation constants of leaky modes, presented in Section II, is now validated and illustrated by means of several numerical examples. We focus on two technologically important cases, i.e. VCSEL cavities on the one hand and a monomode fiber on the other. These are both non-magnetic waveguides, as is most often the case in practical applications. A comparison with a slow but accurate principle of argument method (PAM) [30] is made. All calculations were carried out in Mathematica 6.0 on a Pentium T7400 Centrino Duo 2.16 GHz machine with 2 GB RAM.

A. VCSEL cavities

	VCSEL cavity 1	VCSEL cavity 2
t_1	0.5 μm	0.8 μm
n_1	2.9	2.9
t_2	0.5 μm	0.7 μm
n_2	1.55	1.55
n_3	1	1
s	0.5 μm	0.1 μm
i_1	1	8
i_2	2	15

TABLE I: Material parameters (layer thicknesses t_l and refractive indices n_l) for two VCSEL cavities consisting of two dielectric, non-magnetic layers.

Consider two waveguides with material parameters as provided in Table I. These structures correspond to the AlAs-AlOx apertures in VCSEL cavities described in [13], [31]. For a free-space wavelength $\lambda_0 = k_0/2\pi = 1 \mu\text{m}$, corresponding to an angular frequency of $\omega = 2\pi 300 \text{ THz}$, the location of the TM-polarized propagation constants of a selected number of leaky modes are given in Figs. 2(a) and 2(b) for VCSEL cavity 1 and 2 respectively. The quasi-static solutions with linear error correction are indicated by circles. These are computed by calculating the roots of the polynomial $N_{\text{TM}}(u) = 0$, as presented in (10), combined with (11) and by applying linear error correction, branch per branch, starting from the highest mode orders. The exact locations of the propagation constants (crosses on Fig. 2(a) and 2(b)) are determined by performing additional Newton iterations (26), starting from the quasi-static estimates after linear error correction. We have also determined the exact locations using the PAM approach. For the modes shown in Fig. 2, which are all high-order modes, they coincide perfectly with the ones found with our technique (up to the here considered 10 digits of accuracy). As for VCSEL cavity 1,

the degree of the polynomial (10) is $i_L = 2$, in Fig. 2(a) two branches of leaky modes can be clearly distinguished. For VCSEL cavity 2, $i_L = 15$, and it is rather difficult to identify the corresponding 15 branches visually in Fig. 2(b). From

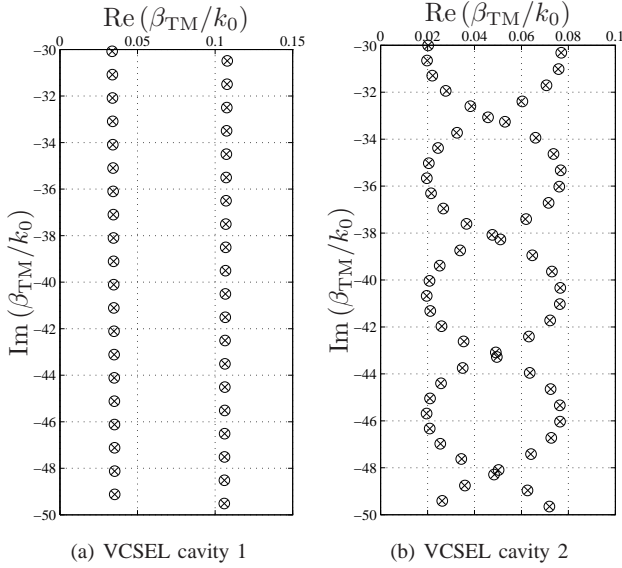


Fig. 2: Propagation constants β_{TM} of a selected number of TM-polarized leaky modes of the VCSEL cavities 1 and 2 (Table I). Circles (\circ): quasi-static approximations with linear error correction. Crosses (\times): Exact locations.

both branches of leaky modes of VCSEL cavity 1, a selected number of quasi-static estimates with linear error correction and the exact propagation constants (obtained after a number of Newton iterations), as well as the relative error between these two, are presented in Table II. The results obtained with a PAM are exactly the same as the ones obtained after performing additional Newton iterations, hence, they are not shown in the table. Note that in this table — and in the remainder of this paper — no distinction between the branches is made to number the modes. They are collectively indexed such that the imaginary part of the propagation constant of mode m is smaller than the imaginary part of the propagation constant of mode $m-1$, for all m . For VCSEL cavity 1, using the new technique, it took 30 seconds of CPU time to calculate the propagation constants of the first 500 TM-polarized leaky modes up to 10 digits precision. To do the same with the PAM, 10986 seconds of CPU time were needed. Hence, the new technique leads to a speedup factor of ca. 360. For VCSEL cavity 2, similar speedups are obtained. It is clear from the above that a high accuracy can be rapidly obtained, especially for the high-order modes. The accuracy of the method is further illustrated in Figs. 3(a) and 3(b), where the effect of the linear error correction for VCSEL cavities 1 and 2 respectively is demonstrated. This is done by showing the relative error between the estimates (with and without linear error correction) on the one hand and the exact propagation constants on the other hand. The two bottom curves are the curves with the crosses, the two top ones those with the circles. The reader notices that applying linear error correction for

each branch of modes, leads to far more accurate estimates. Hence, starting from these accurate estimates, the number of required additional Newton iterations (26), e.g. to obtain an accuracy of 10 digits of precision, is low. For VCSEL cavity 1, for mode numbers m larger than 100, a maximum of only 4 additional Newton iterations is needed to assure 10 digits of precision. For VCSEL cavity 2, for mode numbers m larger than 100, a maximum of 5 additional Newton iterations (26) is needed to assure 10 digits of precision. On the one hand, this number of additionally required Newton iterations decreases for increasing mode numbers. On the other hand, as can be seen from Fig. 3, the relative error starts increasing quite drastically for low order mode numbers. This is due to the fact that the linearly corrected quasi-static approximation is no longer good. The location of such low order modes, with an imaginary part that is larger than, say $-5k_0$, can be found easily with a PAM, keeping in mind that, although being more robust for these low order modes, this method is more elaborate and time-consuming.

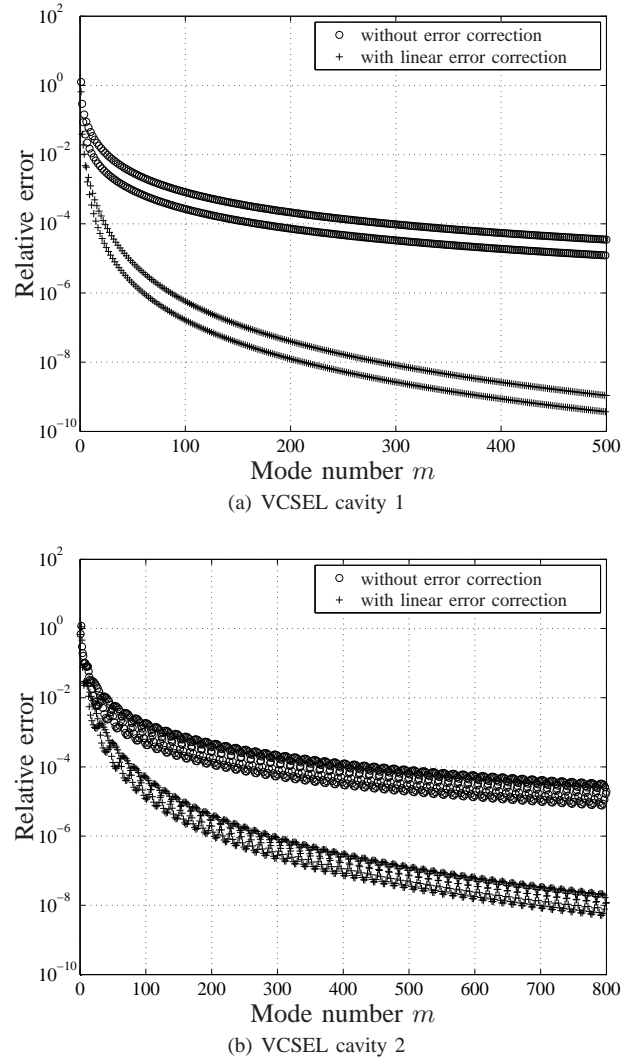


Fig. 3: Relative error on the estimated quasi-static propagation constants β_{TM} of VCSEL cavities 1 and 2 (Table I). Circles (\circ): analytical estimates. Plus signs ($+$): linearly corrected estimates.

mode number m	β_{TM}/k_0 : quasi-static approximations with linear error correction	β_{TM}/k_0 : exact values	relative error
10	$0.1130153 - j 7.2951684$	$0.1119906 - j 7.3042000$	$1.24 \cdot 10^{-3}$
11	$0.0352484 - j 7.7459141$	$0.0358785 - j 7.7485492$	$3.50 \cdot 10^{-4}$
50	$0.1082974 - j 27.4851664$	$0.1083013 - j 27.4853739$	$7.55 \cdot 10^{-6}$
51	$0.0334020 - j 28.0695995$	$0.0333966 - j 28.0696495$	$1.79 \cdot 10^{-6}$
100	$0.1057097 - j 52.5181019$	$0.1057113 - j 52.5181322$	$5.78 \cdot 10^{-7}$
101	$0.0355355 - j 53.1290048$	$0.0355338 - j 53.1290130$	$1.58 \cdot 10^{-7}$
250	$0.1036129 - j 127.5398356$	$0.1036131 - j 127.5398377$	$1.65 \cdot 10^{-8}$
251	$0.0374738 - j 128.1676009$	$0.0374736 - j 128.1676016$	$5.68 \cdot 10^{-9}$

TABLE II: Quasi-static estimates with linear error correction and exact values of the normalized propagation constants β_{TM}/k_0 of a selected number of leaky modes of VCSEL cavity 1 (Table I), and the relative error between them.

The TE-polarized eigenmodes of VCSEL cavity 1 are also presented. Again a free-space wavelength $\lambda_0 = 1 \mu\text{m}$ is used. The locations of a selected number of TE-polarized propagation constants in the complex β -plane are shown in Fig. 4. There are two branches of leaky modes, which was also predicted by (25). One branch of propagation constants is calculated using the plus sign in the argument of the LambertW function, the other branch corresponds to the minus sign. Comparing the precision of the estimates without error correction and with linear error correction for this TE-case leads to similar conclusions as for the TM-case. Also, a significant speedup is obtained. With the new technique, it took 27 seconds to determine the propagation constants of the first 500 TE-polarized leaky waves up to 10 digits of precision. Doing the same with the PAM took 8281 seconds, and hence, the speedup factor is ca. 300. For the TE-modes of VCSEL cavity 2, similar results as for VCSEL cavity 1 are obtained.

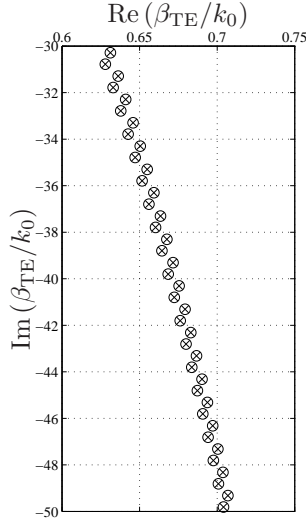


Fig. 4: Propagation constants β_{TE} of a selected number of TE-polarized leaky modes of VCSEL cavity 1 (Table I). Circles (○): quasi-static approximations with linear error correction. Crosses (×): Exact locations.

B. Monomode fiber

In the final example, the TM-polarized leaky modes' propagation constants of a monomode fiber with characteristics shown in Table III, leading to a numerical aperture $\text{NA} = 0.17$,

Monomode fiber	
t_1	$4.5 \mu\text{m}$
n_1	1.5096
t_2	$58.5 \mu\text{m}$
n_2	1.5
n_3	1
s	$4.5 \mu\text{m}$
i_1	1
i_2	14

TABLE III: Material parameters (layer thicknesses t_l and refractive indices n_l) for a monomode fiber consisting of two dielectric, non-magnetic layers, and with a numerical aperture $\text{NA} = \sqrt{n_1^2 - n_2^2} = 0.17$.

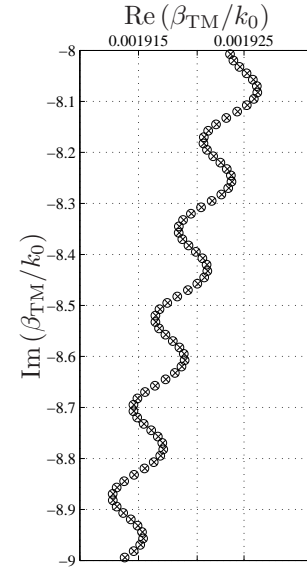


Fig. 5: Propagation constants β_{TM} of a selected number of TM-polarized leaky modes of the monomode fiber (Table III). Circles (○): quasi-static approximations with linear error correction. Crosses (×): Exact locations.

are computed. For a free-space wavelength $\lambda_0 = k_0/2\pi = 1.55 \mu\text{m}$, or thus an angular frequency of $\omega = 2\pi 194 \text{ THz}$, the location of a selected number of TM-polarized propagation constants of the leaky modes are given in Fig. 5. For this fiber, the dispersion relation corresponds to a polynomial in u of degree $i_L = 14$, leading to 14 branches of leaky modes. Fig. 6 demonstrates the effect of the linear error correction

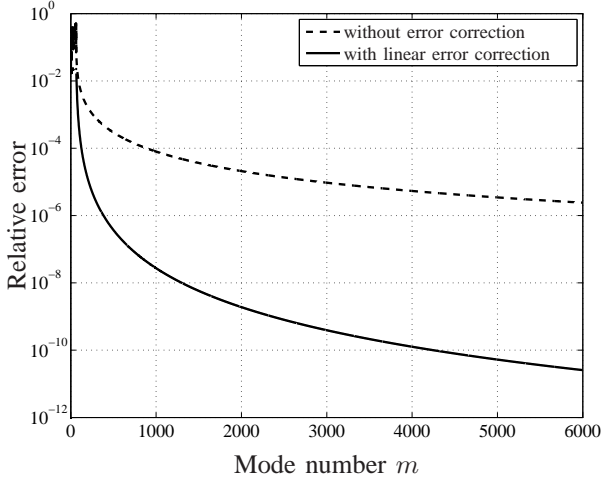


Fig. 6: Relative error on the estimated quasi-static propagation constants β_{TM} of the monomode fiber (Table III). Dashed line (---): analytical estimates. Full line (—): linearly corrected estimates.

by showing the relative error between the estimates (with and without linear error correction) on the one hand and the exact propagation constants obtained after a number of Newton iterations on the other hand. It is clear that, also in this example, applying linear error correction for each branch of modes, leads to far more accurate estimates. Hence, starting from these accurate estimates, the number of required additional Newton iterations (26), e.g. to obtain an accuracy of 10 digits of precision, is again low. E.g., for mode numbers m higher than 100, a maximum of only 6 additional Newton iterations is required to assure 10 digits of precision. This number of additional Newton iterations decreases for increasing mode numbers. E.g., for mode numbers m higher than 4284, the quasi-static estimates with linear error correction are already accurate up to 10 digits of precision and no additional Newton iterations are required.

The above examples demonstrate that the proposed technique is very efficient and accurate. Of course, the method is best suited to locate high-order modes, since the accuracy of the quasi-static approximations is the best for high mode orders. When used in a PML-based (mode matching) formalism the new method is especially advantageous, since the propagation constants of many modes need to be accurately determined and also because the method remains stable for high mode orders.

IV. CONCLUSIONS

To efficiently and accurately compute the TM- and TE-polarized leaky modes' propagation constants of open and PEC-backed PML-closed multilayered cylindrical waveguides, a two-step approach has been presented in this paper. Assuming that the layer thicknesses form commensurable numbers, which is the case in most practical applications, first, the pertinent dispersion relation of the cylindrical waveguides, expressed in terms of cylindrical Bessel functions, are carefully approximated. For higher-order modes, this leads to quasi-static estimates of the propagation constants, which are found

as the roots of a polynomial function. In the particular case of dielectric waveguides without magnetic contrast, special closed-form solutions have been derived. Second, the estimates are used as the starting point in an iterative Newton scheme to determine the exact propagation constants. In contrast to planar layered media, extra care has to be taken here to achieve a high accuracy. This is done by subjecting the quasi-static estimates to an adaptive linear error correction technique.

The proposed method has been applied to two types of technologically important multilayered cylindrical waveguides, i.e. VCSEL cavities and monomode fibers. In this way, the method is thoroughly illustrated and validated. It is important to mention that the proposed formalism is indispensable to conceive accurate mode matching techniques used for analysis and design purposes in photonics applications [13], [14].

APPENDIX

In this appendix, the reflection coefficients $R_{\text{TX}}^{l,l+1}$ and $R_{\text{TX}}^{l+1,l}$, and the transmission coefficients $T_{\text{TX}}^{l,l+1}$ and $T_{\text{TX}}^{l+1,l}$, used in the expression for the generalized reflection coefficient $\tilde{R}_{\text{TX}}^{l,l+1}$ (1) are presented. To compute these coefficients, for a PEC-backed PML-closed waveguide, the procedure presented in [25] has to be adapted. The results of this procedure for both the open and the PEC-backed PML-closed multilayered circular waveguide presented in Fig. 1 can be summarized as follows:

$$R_{\text{TX}}^{l,l+1} = \frac{X_{\text{TX}}^{l,l+1}}{D_{\text{TX}}^{l,l+1}}, \quad (\text{A-1})$$

$$R_{\text{TX}}^{l+1,l} = \frac{X_{\text{TX}}^{l+1,l}}{D_{\text{TX}}^{l+1,l}}, \quad (\text{A-2})$$

$$T_{\text{TX}}^{l,l+1} = \frac{2j}{\pi k_{\rho,l}^2 d_l} \frac{\alpha_{\text{TX}}^l}{D_{\text{TX}}^{l,l+1}}, \quad (\text{A-3})$$

$$T_{\text{TX}}^{l+1,l} = \frac{2j}{\pi k_{\rho,l+1}^2 d_l} \frac{\alpha_{\text{TX}}^{l+1}}{D_{\text{TX}}^{l+1,l}}, \quad (\text{A-4})$$

and

$$D_{\text{TX}}^{l,l+1} = \frac{\alpha_{\text{TX}}^l}{k_{\rho,l}} J_0'(k_{\rho,l} d_l) f_{\text{TX}}(k_{\rho,l+1} d_l) - \frac{\alpha_{\text{TX}}^{l+1}}{k_{\rho,l+1}} J_0(k_{\rho,l} d_l) g_{\text{TX}}(k_{\rho,l+1} d_l), \quad (\text{A-5})$$

$$X_{\text{TX}}^{l,l+1} = \frac{\alpha_{\text{TX}}^{l+1}}{k_{\rho,l+1}} H_0^{(2)}(k_{\rho,l} d_l) g_{\text{TX}}(k_{\rho,l+1} d_l) - \frac{\alpha_{\text{TX}}^l}{k_{\rho,l}} H_0^{(2)'}(k_{\rho,l} d_l) f_{\text{TX}}(k_{\rho,l+1} d_l), \quad (\text{A-6})$$

$$X_{\text{TX}}^{l+1,l} = \frac{\alpha_{\text{TX}}^{l+1}}{k_{\rho,l+1}} J_0(k_{\rho,l} d_l) J_0'(k_{\rho,l+1} d_l) - \frac{\alpha_{\text{TX}}^l}{k_{\rho,l}} J_0'(k_{\rho,l} d_l) J_0(k_{\rho,l+1} d_l), \quad (\text{A-7})$$

where

$$f_{\text{TM}}(k_{\rho,l+1}d_l) = H_0^{(2)}(k_{\rho,l+1}d_l) - \sigma_{l+1} \frac{H_0^{(2)}(k_{\rho,l+1}\mathcal{D})}{J_0(k_{\rho,l+1}\mathcal{D})} J_0(k_{\rho,l+1}d_l), \quad (\text{A-8})$$

$$g_{\text{TM}}(k_{\rho,l+1}d_l) = H_0^{(2)'}(k_{\rho,l+1}d_l) - \sigma_{l+1} \frac{H_0^{(2)'}(k_{\rho,l+1}\mathcal{D})}{J_0(k_{\rho,l+1}\mathcal{D})} J_0'(k_{\rho,l+1}d_l), \quad (\text{A-9})$$

$$f_{\text{TE}}(k_{\rho,l+1}d_l) = H_0^{(2)}(k_{\rho,l+1}d_l) - \sigma_{l+1} \frac{H_0^{(2)'}(k_{\rho,l+1}\mathcal{D})}{J_0'(k_{\rho,l+1}\mathcal{D})} J_0(k_{\rho,l+1}d_l), \quad (\text{A-10})$$

$$g_{\text{TE}}(k_{\rho,l+1}d_l) = H_0^{(2)'}(k_{\rho,l+1}d_l) - \sigma_{l+1} \frac{H_0^{(2)'}(k_{\rho,l+1}\mathcal{D})}{J_0'(k_{\rho,l+1}\mathcal{D})} J_0'(k_{\rho,l+1}d_l), \quad (\text{A-11})$$

$\alpha_{\text{TM}}^l = n_l^2$, $\alpha_{\text{TE}}^l = \mu_{r,l}$, and $k_{\rho,l} = \sqrt{k_0^2 n_l^2 \mu_{r,l} - \beta_{\text{TX}}^2}$. In (A-5)–(A-11), $J_0(\cdot)$ is the zeroth order Bessel function, $H_0^{(2)}(\cdot)$ is the zeroth order Hankel function of the second kind, and $J_0'(\cdot)$ and $H_0^{(2)'}(\cdot)$ are their first-order derivatives respectively. The numbers σ_l allow to write the expressions (A-8)–(A-11) for both the open and the PEC-backed PML-closed waveguide compactly. They are given by:

$$\sigma_l = 0, \text{ for } l = 1, \dots, L, \\ \sigma_{L+1} = \begin{cases} 0, & \text{for an open waveguide (Fig 1(a)),} \\ 1, & \text{for a closed waveguide (Fig 1(b)).} \end{cases} \quad (\text{A-12})$$

Hence, the numbers σ_l equal zero for all dielectric layers $l = 1, \dots, L$. For the layer of air ($l = L + 1$), σ_{L+1} equals zero for an open configuration (Fig. 1(a)), and the functions $f_{\text{TX}}(k_{\rho,l+1}d_l)$ and $g_{\text{TX}}(k_{\rho,l+1}d_l)$ reduce to outgoing cylindrical waves. For the *finite* layer of air, σ_{L+1} is equal to one for the PEC-backed PML-closed configuration (Fig. 1(b)), and then the proper boundary condition at $\rho = \mathcal{D}$ is imposed via the functions $f_{\text{TX}}(k_{\rho,l+1}d_l)$ and $g_{\text{TX}}(k_{\rho,l+1}d_l)$.

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Dries Vande Ginste was born in 1977. He received the M.S. degree and the Ph.D. degree in electrical engineering from Ghent University, Gent, Belgium, in 2000 and 2005, respectively. From October 2000 until March 2006, he was with the Department of Information Technology (INTEC), Ghent University, as a Doctoral and Postdoctoral Researcher, where his research focused on fast techniques for the modeling of layered media. In June and July 2004, he was a Visiting Scientist at the Department of Electrical and Computer Engineering, University of Illinois at

Urbana-Champaign (UIUC). From April 2006 to May 2007, he was active as a Senior Consultant in a private company, i.e., Applied Logistics N.V., where he was mainly involved in the modeling of material handling systems, feasibility studies, technical-economical evaluations for clients, and where he also had commercial responsibilities. In June 2007, he joined the Department of Information Technology (INTEC) again, first as a Technology Developer in the field of high-frequency technologies for ICT applications and since July 2009 as a Postdoctoral Researcher and Lecturer. His current research interests comprise computational electromagnetics, electromagnetic compatibility, and antenna design. He is a Member of the IEEE.

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Hendrik Rogier was born in 1971. He received the Electrical Engineering and the Ph.D. degrees from Ghent University, Gent, Belgium, in 1994 and in 1999, respectively. He is currently a Postdoctoral Research Fellow of the Fund for Scientific Research Flanders (FWO-V), Department of Information Technology, Ghent University where he is also Associate Professor with the Department of Information Technology. From October 2003 to April 2004, he was a Visiting Scientist at the Mobile Communications Group of Vienna University of Technology.

He authored and coauthored about 55 papers in international journals and about 80 contributions in conference proceedings. He is serving as a member of the Editorial Boarding of IET Science, Measurement Technology and acts as the URSI Commission B representative for Belgium. His current research interests are the analysis of electromagnetic waveguides, electromagnetic simulation techniques applied to electromagnetic compatibility (EMC) and signal integrity (SI) problems, as well as to indoor propagation and antenna design, and in smart antenna systems for wireless networks. Dr. Rogier was twice awarded the URSI Young Scientist Award, at the 2001 URSI Symposium on Electromagnetic Theory and at the 2002 URSI General Assembly. He is a Senior Member of the IEEE.

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Daniël De Zutter was born in 1953. He received his M. Sc. Degree in electrical engineering from the University of Gent in 1976. From 1976 to 1984 he was a research and teaching assistant at the same university. In 1981 he obtained a Ph. D. degree and in 1984 he completed a thesis leading to a degree equivalent to the French Aggrégation or the German Habilitation. From 1984 to 1996 he was with the National Fund for Scientific Research of Belgium. He is now a full professor of electromagnetics.

Most of his earlier scientific work dealt with the electrodynamics of moving media. His research now focusses on all aspects of circuit and electromagnetic modelling of high-speed and high-frequency interconnections and packaging, on Electromagnetic Compatibility (EMC) and numerical solutions of Maxwell's equations. As author or co-author he has contributed to more than 140 international journal papers and 150 papers in conference proceedings. In 1993 he published a book titled "Electromagnetic and circuit modelling of multiconductor transmission lines" (with N. Fache and F. Olyslager) in the Oxford Engineering Science Series. He received the 1990 Montefiore Prize of the University of Liège and the 1995 IEEE Microwave Prize Award (with F. Olyslager and K. Blomme) from the IEEE Microwave Theory and Techniques Society for best publication in the field of microwaves for the year 1993. In 1990 he was elected as a Member of the Electromagnetics Society. In 1999 he received the Transactions Prize Paper Award from the IEEE EMC Society. In 2000 he was elected to the grade of Fellow of the IEEE. He is an Associate Editor for the IEEE Microwave Theory and Techniques Transactions. Between 2004 and 2008 he served as the Dean of the Faculty of Engineering of Ghent University and is now the head of the Department of Information Technology.