Scattering by abrupt discontinuities on photonic nanowires: closed-form expressions for domain reduction

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Abstract: Semiconductor and metallic nanowires are attractive building blocks for a nanoscale integrated photonic platform. The scattering coefficients of the optical or plasmonic waveguide mode by 3-dimensional nanowire abrupt discontinuities including splices and endfaces are important figures of merit for realistic estimation of the coupling, lasing, or sensing performance. To tackle with such computationally challenging problems, we derive simple closed-form expressions based on linear equations and overlap integrals of normal modes to realize domain reduction and efficient analytical modeling. For the reflection coefficients at nanowire/waveguide endfaces, the analytical expressions incorporating all the bound modes and a few dozen leaky modes are highly accurate; whereas for the transmission coefficients at nanowire/waveguide splices, the model can be further simplified because only the input and the interested output bound modes need to be considered. Exhaustive validations using fully-vectorial simulation results as reference data show that the model is accurate and versatile for fundamental and high-order TE or TM modes, and for various architectures including high-index-contrast dielectric and plasmonic configurations, 3-D geometries or 2-D equivalents, and various operating wavelengths from ultraviolet to visible and the optical telecommunication bands in the infrared. Our model will facilitate the structure design and theoretical investigation of nanowire/waveguide photonic devices, especially lasers, resonators, sensors and couplers.

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1. Introduction

Semiconductor or metallic nanowires, emerging as a powerful class of materials, open up substantial opportunities for novel nanoscale photonic devices including photodetectors, waveguides, lasers, resonators, chemical and gas sensors, solar cells and nonlinear optical converters [1–4]. Among these nanowire building blocks, waveguides, resonators, lasers and sensors have been attracting intensive attention [5–11]. Compared with the optical modes of high-index semiconductor nanowires in purely dielectric systems, the effective mode areas of plasmonic modes are reduced to deep-subwavelength for a metallic nanowire on dielectric substrate [12] or a semiconductor nanowire on metal-insulator film (referred to as the MIS configuration) [13–17]. For a nanowire resonator or laser that relies on a Fabry-Pérot (F-P) cavity formed by endface reflection [5, 18, 19], as illustrated in Fig. 1(a), the endface reflectivity is the key parameter to estimate the quality factor and the gain threshold [17, 20, 21]. For the nanowire gratings [22] used in optical filters, spectral splitters [23] or distributed feedback (DFB) cavities [24, 25], as shown in Fig. 1(b), and the coupling between nanowires or between a nanowire and a launching or out-coupling optical fiber/waveguide [26, 27], as shown in Fig. 1(c), the reflection and transmission coefficients at the waveguide splice are key figures of merit for the design and optimization. Since the reflection and transmission coefficients of a grating could be obtained using efficient models starting from the elementary scattering coefficients at a single splice [28], in this work, we only address the scattering problems by a nanowire endface or splice, as illustrated by Figs. 1(a) and 1(c), respectively. The calculation of such scattering coefficients is a rather difficult task because it is a three-dimensional (3-D) real problem [29], which involves diffraction at edges and strongly depends on the mode type, operation wavelength, and the nanowire size [17, 20].

To deal with these problems, fully-vectorial numerical methods, such as the finite element method (FEM) [30] and finite-difference time-domain method (FDTD) [20, 21], have been widely adopted. With these pure simulation methods, fully-vectorial simulation should be performed first, then the reflection and transmission coefficients are usually obtained by calculating the S-parameters in the post-processing step. S-parameters are extracted from the fields at the planes of the ports, more precisely, from the field overlap integral between the simulated fields at the ports and the eigen-modes of the waveguides. However, 3-D calculations using these advanced numerical tools are very challenging, especially in time and memory demands. To tackle this challenge, various analytical methods have been proposed mainly for 2-D problems, and only very few could be extended to the 3-D case but the reliability has not been validated [29]. The main difficulty, as summarized in [29], comes from the “open” nature of the problem, i.e., infinite cross-sections and continuous sets of normal modes. The open system becomes a closed one by surrounding the actual geometry with perfectly-matched layers (PMLs) [31]. This truncation method is better than those by enclosing the system with metallic walls, which suffer from windowing errors [29] and are...
not suitable for plasmonic configurations. Quite recently, closed-form expressions based on the Bloch-mode orthogonality have been derived for waveguides and metallic metamaterials [32]. However, the basic assumptions that the interface is illuminated by the fundamental mode and that the two sides have only slightly different parameters [32], hinder the model from applications in nanowire photonics featuring high index contrast and sometimes multimode.

In this work, we derive close-form expressions for the scattering coefficients by 3-D nanowire abrupt discontinuities including splices and endfaces. The derivation takes into account of bound (guided) and leaky modes calculated with PMLs truncated system, and the normal mode orthogonality. Compared with pure simulation methods such as FEM and FDTD, the derived model based on linear equations and overlap integrals of several dozen normal modes is highly efficient due to domain reduction. The reduction of the computational cost is manifest especially for 3-D scattering problems. The analytical model will be quantitatively validated by comparing with fully-vectorial computations of several typical examples, for fundamental and high-order modes, for TE an TM modes, and for various architectures, including high-index-contrast dielectric and plasmonic configurations, 3-D geometries or 2-D equivalents. The model will be further simplified for transmission coefficients by discussing the contribution and choice of leaky modes.

2. Theoretical model

Before we address the optical scattering problem by nanowire abrupt discontinuities, let us retrospect some fundamental theories of optical waveguides. According to the completeness theorem of normal modes, the total forward-propagating electromagnetic fields are expressible as a summation over discrete bound and leaky modes, together with the space-wave fields [33],

\[
\begin{align*}
|\mathbf{P}\rangle &= \sum_{j=1}^{M_{\text{bn}}} a_j |\mathbf{P}_j\rangle \exp(ikn_{\text{eff},j}^0z) + \sum_{k=1}^{M_{\text{ln}}} b_k |\mathbf{P}_k\rangle \exp(ikn_{\text{eff},k}^0z) + |\mathbf{P}_\text{sw}\rangle, \\
\end{align*}
\]

(1)

where \(k = \frac{2\pi}{\lambda}\), \(M_{\text{bn}}\) and \(M_{\text{ln}}\) are the numbers of bound and leaky modes, respectively, and \(|\mathbf{P}_\text{sw}\rangle\) denotes the space-wave fields. The ranges of bound-mode and leaky-mode effective indices \(n_{\text{eff}}^b\) and \(n_{\text{eff}}^l\) for purely dielectric waveguides are given by [33],

\[
\begin{align*}
\max\{n_{\text{cl},j}, n_{\text{sub}}\} < \text{Re}\left(n_{\text{eff}}^b\right) < n_{\text{co}}, \\
0 < \text{Re}\left(n_{\text{eff}}^l\right) < \max\{n_{\text{cl},j}, n_{\text{sub}}\},
\end{align*}
\]

(2)

respectively, where \(n_{\text{co}}\), \(n_{\text{cl}}\) and \(n_{\text{sub}}\) are the refractive indices of the core, cladding and substrate, respectively. For plasmonic waveguides, the effective index ranges for bound and leaky modes are more complex though the relationship of \(\text{Re}\left(n_{\text{eff}}^b\right) < \text{Re}\left(n_{\text{eff}}^l\right)\) holds. Sometimes one may need to inspect the field distributions to distinguish the bound modes and leaky modes.

To set up a generalized theoretical model that is applicable for the scattering coefficients by 3-D nanowire/waveguide abrupt discontinuities including both splices and endfaces, we should take into account of both bound and leaky modes. For the sake of simplicity, discrete bound and leaky modes are expressed in the same form as \(\sum_{j=1}^{M} a_j |\mathbf{P}_j\rangle \exp(ikn_{\text{eff},j}^0z)\) with \(M = M_{\text{bn}} + M_{\text{ln}}\) and \(0 < \text{Re}\left(n_{\text{eff},j}\right) < n_{\text{max}}\). Furthermore, by setting \(n_{\text{max}}\) to be a bit larger than the maximum refractive index of the dielectric/semiconductor in the waveguide system, both purely dielectric and plasmonic configurations could be handled with the same model.
Without loss of generality, we assume that the incident mode is the $p$th-order bound mode, as illustrated in Fig. 2(a). The reflected and transmitted fields are represented by a superposition of discrete bound and leaky modes. Using the field continuity relations at $z = 0$, we have

$$\left| \mathbf{P}_p^I \right> + \sum_{m=1}^{M_2} r_{pm} \left| \mathbf{P}_m^R \right> = \sum_{m=1}^{M_1} t_{pm} \left| \mathbf{P}_m^T \right>,$$

(3)

which is valid for the tangential field components. In Eq. (3), $M_1$ and $M_2$ are the total numbers of bound and leaky modes for the input (I) and output (II) configurations, respectively, $r_{pm}$ and $t_{pm}$ denote the reflection and transmission scattering coefficients, to be more precisely, the cross conversion coefficients from the incident $p$th-order bound mode to the reflected and transmitted $m$th-order normal modes, respectively.

Fig. 2. (a) Schematics of the theoretical modeling. (b)-(f) Five typical examples used to validate the theory: 2-D (b) transmission and (c) radiation problems for the high-index-contrast dielectric waveguide; (d) a 2-D radiation problem of hybrid plasmonic mode in the metal-insulator-semiconductor (MIS) configuration; 3-D radiation problems of a nanowire (e) of circular cross section (with radius $R$) and vertically sitting on silica substrate or (f) of triangular cross section (with edge length $L$) and horizontally lying on silica substrate.

Taking into account of the orthogonality relationships between bound and leaky modes [33], and the normalization of each bound modes and leaky modes [32],

$$\langle \mathbf{P}_n | \mathbf{P}_m \rangle = \int_S (\mathbf{E}_n \times \mathbf{H}_n - \mathbf{E}_n \times \mathbf{H}_n) \cdot \mathbf{z} \text{d}S = 0 \quad \text{if } m \neq -n,$$

$$\langle \mathbf{P}_n | \mathbf{P}_m \rangle = 0,$$

$$\langle \mathbf{P}_n | \mathbf{P}_n \rangle = 4,$$

and projecting Eq. (3) onto the four sets of known bases $\left| \mathbf{P}_n^I \right>$, $\left| \mathbf{P}_m^R \right>$ with $n = 1, 2, ..., M_1$ and $\left| \mathbf{P}_n^I \right>$, $\left| \mathbf{P}_m^T \right>$ with $n = 1, 2, ..., M_2$, we obtain

$$r_{pm} \langle \mathbf{P}_n^I | \mathbf{P}_m^R \rangle = \sum_{m=1}^{M_2} t_{pm} \langle \mathbf{P}_n^I | \mathbf{P}_m^T \rangle,$$

(5a)

$$\langle \mathbf{P}_n^I | \mathbf{P}_m^R \rangle = \sum_{m=1}^{M_1} t_{pm} \langle \mathbf{P}_n^I | \mathbf{P}_m^T \rangle,$$

(5b)
\[ \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle + \sum_{m=1}^{M_1} r_{pm} \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle = 0, \quad (5c) \]

\[ \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle + \sum_{m=1}^{M_1} r_{pm} \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle = t_{pm} \langle \mathbf{P}_n^u | \mathbf{P}_m^u \rangle. \quad (5d) \]

Note that the orthogonality and normalization in Eq. (4) use \( \mathbf{E} \times \mathbf{H} \) products instead of usual Poynting \( \mathbf{E} \times \mathbf{H} \) products because of the presence of PMLs [31] and leaky modes [33, 34]. The conventional trouble on the overlap integrals of leaky modes, which will diverge because these modes have infinite fields at infinity [35], is also solved elegantly by using PMLs [31]. By eliminating \( t_{pm} \) in Eqs. (5a) and (5b), we obtain the close-form expression of \( r_{pm} (n = 1, 2, \ldots, M_1) \)

\[ 4 \{ \mathbf{r} \} = [\mathbf{A}_1][\mathbf{A}_2]^{-1} \{ \mathbf{b}_1 \}, \quad (6) \]

where \( \{ \mathbf{r} \} = \{ r_{p1}, r_{p2}, \ldots, r_{pM_1} \}^T \), \( \mathbf{A}_1 (n,m) = \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle \), \( \mathbf{A}_2 (n,m) = \langle \mathbf{P}_n^i | \mathbf{P}_m^i \rangle \), \( \mathbf{b}_1 (n) = \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle \), and \( n = 1, 2, \ldots, M_1, m = 1, 2, \ldots, M_2 \).

Similarly, we obtain the close-form expression of \( t_{pm} (n = 1, 2, \ldots, M_2) \) by eliminating \( r_{pm} \) in Eqs. (5c) and (5d),

\[ -4 \{ \mathbf{t} \} = \{ \mathbf{b}_2 \} + [\mathbf{C}_1][\mathbf{C}_2]^{-1} \{ \mathbf{b}_2 \}, \quad (7) \]

where \( \{ \mathbf{t} \} = \{ t_{p1}, t_{p2}, \ldots, t_{pM_2} \}^T \), \( \mathbf{C}_1 (n,m) = \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle \), \( \mathbf{C}_2 (n,m) = \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle \), \( \mathbf{b}_2 (n) = -\langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle \), \( \mathbf{b}_1 (n) = \langle \mathbf{P}_n^u | \mathbf{P}_m^i \rangle \), and \( n = 1, 2, \ldots, M_2, m = 1, 2, \ldots, M_1 \).

Specially, if only the fundamental bound modes of both the input and output sides are considered, Eqs. (6) and (7) are reduced into

\[ r_{11} = -\langle \mathbf{P}_1^u | \mathbf{P}_1^i \rangle / \langle \mathbf{P}_1^i | \mathbf{P}_1^u \rangle, \]
\[ -4t_{11} = \langle \mathbf{P}_1^u | \mathbf{P}_1^i \rangle - \langle \mathbf{P}_1^u | \mathbf{P}_1^i \rangle / \langle \mathbf{P}_1^i | \mathbf{P}_1^u \rangle \]

which is exactly the same as Eqs. (4) and (5) in [32]. Note that there is a typo error in Eq. (5) of [32], as its left side should be \( -4t_{11} \) instead of \( 4t_{11} \). We should also note that in this work we use bra ket notation instead of a more standard notation following [33] so as to facilitate the comparison with [32].

By solving the linear equations expressed by Eqs. (6) and (7), the reflection and transmission scattering coefficients are obtained efficiently. Since all the bound and leaky modes are normalized, the corresponding reflection and transmission efficiencies are then obtained with \( R_{pm} = |r_{pm}|^2 \) and \( T_{pm} = |t_{pm}|^2 \), respectively. Under most circumstances, one usually needs the scattering coefficients of only the bound modes. Specially, for the scattering at nanowire/waveguide endfaces, only the reflection coefficients of specific bound modes are of interest.

We should emphasize that \( [\mathbf{A}_1]^{-1} \{ \mathbf{b}_1 \} \) and \( [\mathbf{C}_2]^{-1} \{ \mathbf{b}_2 \} \) should be calculated using the matrix left division operation, i.e., \( [\mathbf{A}_1] \{ \mathbf{b}_1 \} \) and \( [\mathbf{C}_2] \{ \mathbf{b}_2 \} \), respectively, which can be easily and efficiently done in MATLAB-based codes. Since there is no need to calculate the inverse of a matrix, the restriction of \( M_1 = M_2 \) is removed. In other words, the derived model does not require the two sides to be truncated with the same rank, making it more reliable than those requiring \( M_1 = M_2 \) [29].
Note that we ignore the evanescent radiation modes with imaginary values of the effective indices (i.e., \( \text{Re}(n_{\text{eff}}) = 0 \)) that do not propagate in the \( z \)-direction. As pointed out in [34], such modes are almost never used in practical calculations. We should also note that there is no further approximation during the derivation of Eqs. (6) and (7), making the closed-form expressions versatile for calculating the reflection and transmission coefficients at nanowire/waveguide splices and the reflection coefficients at endfaces, for fundamental and high-order modes, and for various architectures, including high-index-contrast purely dielectric and plasmonic configurations, 3-D geometries and 2-D equivalents.

Furthermore, for 3-D (or 2-D) scattering problems, all one needs to do is to solve the bound and leaky modes of the corresponding 2-D (or 1-D) cross-section waveguide, which can be easily done using various conventional numerical tools such as FEM, FDTD and aperiodic Fourier modal method (aFMM), to calculate the overlap integrals between these normal modes, and then to solve the linear equations of Eqs. (6) and (7). As the numerical cost of the linear equations is negligible, the major cost is for the solving of normal modes and their overlap integrals. This will greatly reduce the time and memory requirements because of domain reduction, especially for 3-D real problems. Moreover, as we will elaborate later, the efficiency of the model can be further improved without loss of prediction accuracy by further truncating the leaky modes properly, and the model can be further simplified for transmission coefficients at nanowire/waveguide splices.

3. Results and discussion

To validate the quantitative accuracy and the versatility of the analytical model, exhaustive comparisons with fully-vectorial numerical calculations will be performed for scattering problems at nanowire/waveguide splices and endfaces, for fundamental and high-order modes, for TE and TM modes, and for various architectures including purely dielectric and plasmonic configurations, 3-D real geometries and 2-D equivalents, and various operating wavelengths from ultraviolet to visible and the optical telecommunication bands in the infrared. We should emphasize that this work is intended not to investigate all the nanowire/waveguide splices and endfaces architectures mentioned in literatures, but to quantitatively validate the derived model, which will pave the way for the structure design and theoretical investigation with a great reduction of the computational cost. Due to the space limitations, here we only provide several typical examples including scattering at 2-D and 3-D splices or endfaces, as illustrated in Figs. 2(b)–2(f).

Throughout the paper, the fully-vectorial numerical calculations of the original scattering problems are all performed using the aFMM with the actual geometry being truncated by PMLs [36–38]. After the fields are obtained via pure simulations, the reflection and transmission coefficients of bound modes are then extracted from the field overlap integral according to the mode orthogonality (please refer to [39] for details). In the analytical model, the bound and leaky modes of the cross-section waveguides are also solved using the aFMM. We should emphasize that although all the calculations are done with the aFMM in this work, the pure simulation of the original scattering problem and the solving of the corresponding domain-reduced eigen-mode problems could also be done with conventional numerical methods such as FEM and FDTD, which can be realized with numerous commercial software. However, no matter which numerical tools, commercial or home-built, are used, it has been well accepted that the numerical cost for the solving of 2-D (or 1-D) normal modes is much smaller than that for the fully-vectorial calculation of the original 3-D (or 2-D) scattering problem. In other words, domain reduction reduces the numerical cost.

To further reduce the computational cost of the model, we will try to make use of a subset of leaky modes, which are selected according to the imaginary parts of the effective indices. By doing this, we provide a quantitative discussion on the contributions of leaky modes in the model. For the sake of clarity, we refer to the subset of leaky modes with \( \text{Im}(n_{\text{eff}}) < 1 \) as 'leaky 1', \( \text{Im}(n_{\text{eff}}) < 3 \) as 'leaky 3', and so on. Note that we select leaky modes based on the
imaginary parts instead of the mode number. This is because, given the range of leaky modes, the mode number varies with the parameters of PMLs, as pointed out in [31]. In our normal mode solving results using the aFMM with the PML coefficient of $(f_{\text{PML}})^{-1} = 5(1 + i)$ [38], the numbers of leaky modes for ‘leaky 1’ and ‘leaky 3’ are only a few dozen for 2-D and 3-D cases, specifically, ranging from 20 to about 60.

3.1 Validation with 2-D scattering problems

Let us first consider a 2-D scattering problem as illustrated in Fig. 2(b). As the scattering problem of a multimode waveguide is more complex than that of a single-mode one, we set the parameters to be $h = 0.8 \, \mu m$, $n_S = 3.45$, $n_{\text{sub}} = 1.5$, and $\lambda = 1.2 \, \mu m$, so that the incident waveguide is of multimode. Note that, the right-side configuration changes as $\Delta + h$ increases, from supporting no bound mode at all if $\Delta = -h$ or if $\Delta + h$ is small enough, to being of single mode and multimode. For the latter two cases, the scattering problem can be treated as the 2-D counterpart of the 3-D real transmission problem, as shown in Fig. 1(c); whereas for the former cases, Fig. 2(b) becomes a radiation problem, which can be treated as the 2-D approximation of the 3-D real radiation problem, as illustrated in Fig. 1(a).

![Fig. 3. Comparison of aFMM pure simulated results (black lines) and model predictions (symbols) for the scattering problem illustrated by Fig. 2(b) with the fundamental TE mode incidence: (a) $|r_{11}|$, (b) $|t_{11}|$, (c) arg($r_{11}$), and (d) arg($t_{11}$). 'o' is for model without leaky modes, '+' for model with ‘leaky 1’, ' ' + ' for model with ‘leaky 3’, and ' ' + ' for model using only the interested incident and transmitted modes. The missing points at $\Delta = 0 \, \mu m$ in (a) and (d) are due to $|r_{11}| = 0$ and arg($t_{11}$) = 0, respectively. The calculations were performed with $h = 0.8 \, \mu m$, $n_S = 3.45$, $n_{\text{sub}} = 1.5$, and $\lambda = 1.2 \, \mu m$.](image-url)
Fig. 4. Comparison of aFMM pure simulated results (black lines) and model predictions (symbols) for the scattering problem illustrated by Fig. 2(b) with the 2nd-order TE mode incidence: $|r_{21}|$, $|r_{22}|$, $|r_{23}|$, $|t_{21}|$, $|t_{22}|$, and $|t_{23}|$. The missing points at $\Delta = 0$ in (a)–(c) are corresponding to $|r_{22}| = 0$, $|r_{21}| = 0$, and $|r_{23}| = 0$, respectively. The calculations were performed with the same parameters as Fig. 3 except for $p = 2$.

Figure 3 shows that, under the incidence of the fundamental TE mode (i.e., $p = 1$), the reflection and transmission coefficients $r_{11}$ and $t_{11}$ are precisely predicted by the model with 'leaky 3', i.e., the subset of leaky modes with $\text{Im}(n'_{\text{eff}}) < 3$. The high accuracy, not only in amplitude but also in phase, keeps over a very large range of $\Delta$, including the special cases that there are no bound modes for the right-side configuration if $\Delta = -h$ or if $\Delta + h$ is small enough. The model predictions using 'leaky 1' are also very accurate, whereas those without leaky modes are only accurate for $t_{11}$. In other words, the more leaky modes used in the model, the higher accuracy of the model prediction on reflection coefficients; whereas the transmission coefficients are always highly predictable by the model even without any leaky modes. These conclusions are applicable for the case of the 2nd-order TE mode incidence (i.e., $p = 2$), as shown in Fig. 4, and other cases such as the incidence of the fundamental TM mode or higher-order TE or TM modes (not shown due to space limitations).

Knowing that the transmission coefficient $t_{pn}$ is almost independent from the leaky modes, we further speculate that it is also independent from all the other bound modes except the directly related incident $p^{th}$-order and output $n^{th}$-order bound modes. Under this assumption, Eq. (7) is simplified into

$$-4t_{pn} = \left(\frac{\langle P^a_{-p} \mid P^i_p \rangle - \langle P^a_{-p} \mid P^i_p \rangle \langle P^a_n \mid P^n_p \rangle}{{\langle P^a_n \mid P^n_p \rangle}}\right),$$

where $p = 1, 2, ..., M_1$ and $n = 1, 2, ..., M_2$. Figures 3 and 4 show that Eq. (9) yields almost the same results as Eq. (7), validating our speculation. As a matter of fact, Eq. (9) can be treated as another form of the classical approximate expression for the coupling efficiency $\eta$ at an interface between two waveguides, which is derived directly from the overlap integral of the input and output fields [34], and $\eta_{pn} = |t_{pn}|^2$. In other words, if only the transmission coefficient $t_{pn}$ is of interest, all one needs to do is to solve the eigen-fields of the $p^{th}$-order and $n^{th}$-order bound modes for the incident and output waveguides, respectively, and then make use of Eq. (9) for efficient calculation.

We should emphasize that Figs. 3 and 4 also show the high accuracy of Eq. (6) with a few dozen leaky modes for the radiation problem, i.e., the special case of $\Delta = -h$. In this case, Fig. 2(b) can be treated the 2-D approximation of the endface radiation problem for a 3-D
nanowire sitting on infinite large substrate. Note that if no leaky modes are taken into account for the radiation problem, \( M_2 = 0 \) and the model will be out of function, leading to the missing of red circles at \( \Delta = -h \) in Figs. 3 and 4. In other words, leaky modes must be incorporated in the model to handle the radiation problem at a waveguide/nanowire endface.

Compared with Fig. 2(b), the configuration shown by Fig. 2(c) is more popular in F-P cavity semiconductor lasers, whose facet should be finely polished for high quality factor and high coupling efficiency into output waveguides [40]. Figures 5(a) and 5(b) show that the amplitude and phase of \( r_{11} \) for the fundamental TE mode are quantitatively predicted by Eq. (6) with 'leaky 3'. Compared with the transmission problems with results shown in Figs. 3 and 4, we note that more leaky modes need to be incorporated for such radiation problems.

More leaky modes should be incorporated in the model for plasmonic configurations compared with purely dielectric ones. Figure 2(d) illustrates a 2-D endface reflection problem of a semiconductor in an MIS configuration, which supports hybrid plasmonic modes and becomes popular in nanolasers based on propagating surface plasmon [14, 16]. By incorporating 'leaky 10', the model predictions on the amplitude and phase of \( r_{11} \) for the fundamental hybrid plasmonic (TM) mode are highly accurate; by incorporating 'leaky 3', the predictions are also very accurate, as shown in Figs. 5(c)–5(d).

Fig. 5. Comparison of aFMM pure calculated results (black lines) and model predictions (symbols) for the radiation problem in Fig. 2(c) with the fundamental TE mode incidence: (a) \( |r_{11}| \) and (b) \( \arg(r_{11}) \), and for the radiation problem in Fig. 2(d) with the hybrid plasmonic (TM) mode incidence: (c) \( |r_{11}| \) and (d) \( \arg(r_{11}) \). The calculations for (a)–(b) were performed with the same parameters as Fig. 3, and those for (c)–(d) were performed with \( n_{Ag} = 0.0157 + 3.0848i \) (Ag) [41], \( n_1 = 1.38 \) (MgF2), \( n_6 = 2.5 \) (CdS), \( h_1 = 10 \) nm, and \( \lambda = 0.5 \) \( \mu \)m.

### 3.2 Validation with 3-D scattering problems

As the 3-D real problems are still computationally challenging with purely numerical tools, it is not easy to provide many scattering results of 3-D nanowire/waveguide splices or endfaces as reference data for the validation of the theoretical model. As a result, in this work we only provide two typical examples as illustrated in Figs. 2(e)–2(f), to demonstrate the reliability of the derived analytical model. We are only interested in the endface reflectivity, which is the key parameter for realistic estimation of the threshold gain and quality factor for the nanowire laser.

Figure 2(e) illustrates the scattering at the top endface of a semiconductor (ZnO or CdS) nanowire with circular cross section and vertically sitting on silica substrate, and the parameters are set to be \( R = 60 \) nm and \( n_e = \sqrt{6} \) following [20]. Figure 2(f) shows an endface
scattering problem of a GaN nanowire with triangular cross section and horizontally lying on silica substrate, and the parameters are set to be $n_{\text{sub}} = 1.46$ (SiO$_2$), $n_i = 2.6$ (GaN) and $\lambda = 0.38 \mu$m following [42]. By comparing with 3-D fully-vectorial aFMM simulation results, Fig. 6 shows that the absolute values of endface reflection coefficients of the fundamental HE$_{11}$ modes and the TE$_{01}$ modes, as functions of the operation frequency for Figs. 6(a)–6(b) or of the nanowire size for Figs. 6(c)–6(d), are all accurately predicted by the model with 'leaky 1'. Note that this conclusion should also be valid for the endface reflection coefficients of other higher modes such as the TM$_{01}$ modes, and the cross conversion coefficients between modes.

Figures 6(a) and 6(c) also reveal that the endface reflectivities for the HE$_{11}$ modes increase with the operation frequency or the nanowire size, respectively. However, they approach those for the normal incidence on an infinite semiconductor/air interface, i.e., $(n_i - 1)/(n_i + 1) = 0.42$ for Fig. 6(a) with $n_i = \sqrt{6}$, and $(n_i - 1)/(n_i + 1) = 0.44$ for Fig. 6(c) with $n_i = 2.6$. Interestingly, this feature due to strong confinement of the HE$_{11}$ mode [19, 20] holds for nanowires of various cross sections.

To quantitatively illustrate by how much the computational cost can be reduced due to the domain reduction using the developed model, here we provide some data on the memory and time requirements for calculating the original 3-D scattering problem with $L = 200$ nm in Fig. 2(f) and the corresponding 2-D eigen-mode problem. Both problems are calculated using COMSOL (FEM) in a personal computer with Intel core i7-3610QN processor (2.30GHz) and 16G memory. It shows that the simulation of the original 3-D scattering problem consumes 6.07G memory and 370 seconds, whereas the computing of the corresponding 2-D eigen-mode problem only costs 0.93G memory and 22 seconds. As both the pure simulation method and the developed model need to calculate the field overlap integrals, and the solving of the linear equations of Eqs. (6), (7) and (9) is of negligible cost, it is evident that both the memory and time requirements are greatly reduced by using the developed analytical model.

We note that the 2-D approximation of this 3-D radiation example has been illustrated by Fig. 2(b) and validated by Figs. 3 and 4 with $\Delta = -h$. As a result, it is reasonable to claim...
that, Eqs. (7) and (9), although not be validated here, should also be accurate for the transmission coefficients at 3-D nanowire/waveguide splices.

4. Concluding remarks

Note that although we have restricted ourselves to the scattering problems at single interfaces including splices and endfaces, the developed model will also find applications in more complicated discontinuities problems, such as the transmission through nanowire/waveguide Bragg gratings illustrated in Fig. 1(b) and the scattering of a nanoparticle on a nanowire/waveguide [43, 44] or locating between two separate nanowire/waveguides. These complicated problems could be analytically and efficiently investigated adopting the scattering-matrix or transmission-matrix approach combining both interface and propagation matrices, where the interface matrices composed of normal modes' scattering coefficients could be calculated efficiently with the developed model.

In conclusion, we have derived simple closed-form expressions for the scattering coefficients by nanowire/waveguide splices or endfaces. By solving the bound modes and leaky modes of the corresponding 2-D (or 1-D) cross section, the overlap integrals between normal modes, and the linear equations of Eqs. (6) and (7), the numerical cost for the fully-vectorial calculation of the original 3-D (or 2-D) scattering problem has been greatly reduced. The cost of the model has been further reduced by using only a few dozen leaky modes, which are selected to be of the lowest propagation loss. Especially, if only the transmission coefficient \( t_{pn} \) or efficiency \( \eta_{pn} = |t_{pn}|^2 \) is of interest, Eq. (7) has been further simplified into Eq. (9), where only the \( p^{th} \)-order incident bound mode and the \( n^{th} \)-order output bound mode are considered.

The quantitative accuracy and versatility of the analytical model have been validated using several typical examples by comparing with fully-vectorial numerical calculations. Results have shown that the model incorporating only a few dozen leaky modes are accurate enough to calculate the reflection and transmission scattering coefficients including their real and imaginary parts, for fundamental and high-order modes, for TE and TM modes, and for various architectures including high-index-contrast purely dielectric and plasmonic configurations, 3-D real systems and 2-D equivalents, and various operating wavelengths from ultraviolet to visible and the optical telecommunication bands in the infrared.

Encouraged by the reduced numerical cost, the quantitative accuracy, the versatility and the reliability, we believe the derived analytical model will greatly facilitate the structure design and theoretical analysis of nanowire photonic building blocks as well as classical optical waveguide-based devices, especially resonators, lasers, couplers and sensors.

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