Modified step-theory for investigating mode coupling mechanism in photonic crystal waveguide taper

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Abstract: In this paper, the mathematical model of the modified step-theory is derived based on the platform of two-dimensional photonic crystal structure that is infinitely long in third dimension. The mode coupling mechanism of photonic crystal tapers is theoretically studied using the modified step-theory. The model is verified by comparing the transmission spectrum obtained for the input/output defect coupler where it shows a good match of less than 5% discrepancy. The modified step-theory is applied to different taper structures to investigate the power loss during the transmission. The power loss at the relative position of the taper provides an explanation as to which taper designs give the highest coupling efficiency.

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OCIS codes: (130.0130) Integrated Optics; (230.7380) Waveguides, channelled; (250.5300) Photonic integrated circuits

References and links

1. Introduction

Photonic crystals (PCs) are regular array of structures that are periodic in one or more dimensions. The periodic structures forbid electromagnetic waves propagation within a frequency range, which is known as photonic bandgap (PBG) in all directions. Since the last two decades, extensive research has been focused on photonic crystals because of its ability in controlling and molding the flow of electromagnetic lightwave, as an analogy to manipulate electrons flow in conventional semiconductor [1]. When defects are introduced to the crystal lattice, its applications widen, which results in the innovation of many highly compact integrated photonic devices such as photonic crystal waveguides (PCWGs), wide angle beam splitters, waveguide bends and photonic crystal cavity filters [2-6].

Photonic crystal waveguides is one of the key components because it forms a medium for transmission power and low radiation loss.
have to face many challenges in the design and analysis, fabrication process and experimental measurement techniques. These technical difficulties have also posed challenges for the commercialization of the photonic crystal devices. However, the most critical problem that arises from the small size of photonic crystal devices is to couple sufficient amount of light to the narrow waveguide. In designing photonic crystal devices, this is the most important step because poor coupling results in low transmission of power to the waveguide, which in turn affects the functionality and reliability of the optical devices. For this reason, photonic crystal tapers [8-14] have been designed to couple light source of larger cross-sectional size to the narrow PCWG. Light is tapered to the narrow guide by either structural means [8-12] or by varying the size of unit lattice to provide mode conversion [13-14]. The former uses the structural shape of the taper to slowly match the mode profile of the light source to PCWG while the latter uses progressively-variation geometry to achieve adiabatic mode conversion.

Many different methods [15-20] are used to calculate the coupling efficiency and transmission loss in tapered waveguide transmission. Among all, the coupled mode theory, perturbation method, multipole method and beam propagation method are commonly used. The coupled mode theory and the perturbation theory [15-16] are able to converge fast for analysis of weak geometrical waveguide variation. However, stronger perturbation requires higher-order corrections, which may affect the convergence to exact solution. For high-index contrast waveguide, the multipole method [17-18] can be applied to analyze the eigenmodes with high numerical accuracy but it does not allow perturbative formulation. The beam propagation method [19-20] can give high accuracy but needs very fine resolution. This can be computationally demanding.

The step-theory [21-24] is used to calculate transmission efficiency in conventional tapered waveguide by dividing it into vertical strips called steps. By matching the field components at the boundary between steps, the transmitted amplitude can be obtained. The theory can handle tapered waveguide with small or moderate variation in the cross sectional size with very high convergence [24]. For large geometrical variation, the theory can still converge moderately. Additionally, the method also demonstrates the analysis of intermodal coupling mechanism in the tapering section with respect to the relative position. Many steps are required for calculation of the transmission amplitude, which increases the computational time and resources. However, for applications in photonic crystal tapered structure, this problem is reduced as shown in the later part of the paper. This method also requires the propagation constants for all the guided modes in each step to be known, which is quite hectic for very large number of modes.

The objective of this paper is to modify the step-theory and applied it to investigate the coupling mechanism in photonic crystal tapered waveguide. The paper will applied it to several taper designs in photonic crystal and also provides an explanation as to why some taper curvature has higher coupling efficiency than the other. The paper will be organized as followed. In the next section, the fundamental of photonic crystal waveguide is briefly introduced. Section three shows the detail derivation of the modified step-theory for its application in photonic crystal taper waveguide. In the subsequent section, the method is verified with the structure designs in [9]. Section five discusses the numerical results with special focus in abrupt step waveguide, step taper waveguide and smooth linear and nonuniform taper design. Lastly, the paper concludes the results obtained.

2. Fundamentals of light propagation in photonic crystal waveguide

The field profile for any uniform planar waveguide can be described in term of the eigenfields of the normal waveguide modes. The solution of the normal modes is given as [25]

$$E = E_0\xi(z) e^{i\beta z}$$

(1)

where $E_0$ is the real amplitude of the propagating $E$-field at a position $x$. $\xi(z)$ is the $z$ dependent field distribution of the guided mode. $\xi$ is dependent on the width and the mode
number of the waveguide. \( \beta \) is defined as the propagation constant of the guided mode and the electromagnetic wave is propagating in the \( x \) direction.

For light to be guided in photonic crystal, two conditions must be satisfied. First, the mode considered is in the bandgap of a photonic crystal. Second, the mode in operation must be truly guided and does not radiate out. For photonic crystal waveguide, the waveguide solution is more complex due to the presence of the periodicity profile in the crystal lattice. Assuming a two-dimensional crystal structure in the \( x \) and \( z \) direction, the field mode of a periodic function has the following relationship [2]

\[
E_{k',k}(r) \propto \exp(ik'_x x) \times \exp(ik'_z z) \times u_{k',k}(x, z)
\]  

(2)

where \( u_{k',k}(x, z) \) is a periodic function in \( x \) and \( z \) direction. The periodicity in \( x \) and \( z \) direction leads to a \( xz \) dependent for \( E \)-field, which is a product of plane wave with a \( xz \)-periodic function. This is known as Bloch’s theorem.

Photonic crystal guided mode field resembles modes in conventional waveguide [26-27]. This is because the dispersion band diagram for the conventional waveguide is similar to the photonic crystal waveguide for rod structure. A good approximation will be a case of a metallic waveguide of width \( b \), on which an artificial periodicity of \( d \) is imposed. The equation for the mode field of the guided modes is given as [26]

\[
E = E_0 \sin \left( \frac{m \pi}{b} \left( \frac{x}{b} + \frac{1}{2} \right) \right) \exp \left[ -i \psi(x) \right]
\]

(3)

The modal field distribution is based on a sine function, which is dependent on the mode number, \( m \) and the width of the waveguide, \( b \). For \( m = 1 \), this refers to the fundamental even mode where larger values imply higher order modes. When \( m = 1, 3, 5, \ldots, (2\nu+1), \ldots \), it corresponds to even modes with a cosine mode profile that is symmetrical about the \( x \) direction. When \( m = 2, 4, 6, \ldots, (2\nu), \ldots \), it corresponds to odd modes with a sine profile that is asymmetrical about the \( x \) direction. The constant \( b \) is dependent on the structure of the lattice arrangement. It corresponds to the width of the periodicity imposed waveguide, which is usually in multiples of the lattice constant. \( \psi \) is the phase coefficient, which is dependent on the artificial periodicity of \( d \) given as

\[
\psi(x) = \left( \beta + \frac{2\pi \eta}{d} \right) x \quad \eta = 0, \pm 1, \pm 2, \ldots,
\]

(4)

where \( \beta \) is the wave vector of the wave and \( \eta \) is the propagation direction. For periodic structure, the modes are also characterized by the Bloch modes. The integer \( \eta \) is related to the folding of the bands at wave vector, \( k = 2\pi \eta d \), which is at the first Brillouin zone of the photonic crystal. The phase coefficient is conserved in the direction of propagation. The mode field for guided mode in Eq. (3) is used for the derivation of modified step-theory, which is discussed in the next section.

3. Mathematical model of Modified step-theory

The modified step-theory is an extension of the original step-theory in calculating the amplitude of the transmitted modes in periodic photonic crystal waveguide. Eq. (2) is used to describe the mode field of the guided modes in the derivation of the original step-theory. In the modified step-theory, Eq. (3) is used instead to account for the periodicity and discontinuous dielectric boundary in photonic crystal structures. The equations for calculating the transmission amplitudes and coupling constant are presented in this section. Subsequently, the modified step-theory is used to calculate the transmission and reflection loss in an iterative manner from one step to another until the end of the taper in the next section.

Before deriving the modified step-theory, a few assumptions are made. Firstly, the coupling between reflected modes is negligible. This will simplify the derivation and for
gradual taper, reflection is very low with negligible coupling and adiabatic condition is achieved. Secondly, the mode coupling of reflected and transmitted radiation onto the guided modes is small and negligible. This is especially true for the reflected radiation in the case of gradual slow taper where there is only forward transmitted radiation, which is very small because near adiabatic or adiabatic condition is achieved. Thirdly, intermodal loss for short taper can be neglected because the reflection loss of the higher order mode is the main loss, as the taper becomes narrower. The higher order modes are cut-off and reflected backward.

Consider a simple case where there are two guided modes, \( i \) and \( j \) traveling in a two-dimensional photonic crystal waveguide of width \( b \) and artificial periodicity of \( d \). Both modes travel to a narrower waveguide of width \( b' \) with the same periodicity. The wider waveguide is labeled as the \( n \)th step with subscript \( n \), while the narrower waveguide is labeled as the \((n+1)\)th step with subscript \( n+1 \). Using Eq. (3) for the description of the mode field for \( i \) and \( j \), the incident, reflected and transmitted components for the \( E \) and \( H \) field at the boundary between steps are matched and the amplitude of transmitted mode \( j \) in the \((n+1)\)th step is given by

\[
A_{jn+1} \exp(-i \psi_{jn+1}) = c_{ij} A_{in} \exp(-i \psi_{in}) + c_{ji} A_{jn} \exp(-i \psi_{jn})
\]  

(5)

where \( A_{in} \) refers to the ratio of the modal field amplitude of the \( i \)th mode at the \( n \)th step, in the presence of mode conversion to the initial incident amplitude that corresponds to the fundamental mode and has a unit power. Similar assignments are given for \( A_{jn+1} \) and \( A_{jn} \). The coupling constant \( c_{ij} \) between mode \( i \) and \( j \) is given as

\[
c_{ij} = \frac{\psi_{jn} G}{\psi_{in}} \frac{I_{jn, jn+1}}{\sqrt{I_{jn, in} I_{jn+1, jn+1}}}
\]

(6a)

where

\[
G = \frac{2 \beta_{jn} \beta_{jn+1} + 2 \beta_{in+1} \beta_{jn+1} + \gamma + 2 \gamma \beta_{jn} + \gamma \beta_{jn+1} + \gamma \beta_{jn+1}}{\left( \beta_{jn} + \beta_{jn+1} + \gamma \beta_{jn} + \beta_{jn+1} + \gamma \right)}
\]

(6b)

and

\[
\gamma = \frac{4 \pi \eta}{d}
\]

(6c)

where the purpose of \( \gamma \)is to account for the Bloch modes in periodic structure for convergence in high index contrast material. When \( \gamma \) is set to zero, Eq. (6b) is simplified to the case of the conventional waveguide. The field overlap integral \( I_{in,jn+1} \) is given by

\[
I_{in,jn+1} = \int \sin \left[ m_{jn} \pi \left( \frac{z}{b} + \frac{1}{2} \right) \right] \sin \left[ m_{jn+1} \pi \left( \frac{z}{b'} + \frac{1}{2} \right) \right] dz
\]

(7)

The detail derivations of the equations for the coupling and transmission calculation are attached as in Appendix A. The field overlap integral account for the common field distribution between the incident and transmitted field profile at different steps. As the width of the taper waveguide varies along the direction of propagation, the values of \( b \) change. Therefore, the integral varies and is evaluated for every transmission between the steps. For the case of multiple modes propagating in the waveguide, the general expression for the transmitted \( j \)th mode is given as the sum of all the field profile of the incident mode which is given as

\[
A_{jn+1} \exp(-i \psi_{jn+1}) = \sum c_{ij} A_{in} \exp(-i \psi_{in})
\]

(8)

Based on the real and imaginary part of Eq. (7), the transmitted amplitude for the \( j \)th mode is given by

\[
A_{jn+1} = \left[ \left( \sum c_{ij} A_{in} \cos \psi_{in} \right)^2 + \left( \sum c_{ij} A_{in} \sin \psi_{in} \right)^2 \right]^{\frac{1}{2}}
\]
where $\psi$ is the phase coefficient that is defined as

$$\psi_{n+1} = \tan^{-1}\left(\frac{\sum_i c_i A_m \sin \psi_{in}}{\sum_i c_i A_m \cos \psi_{im}}\right)$$

According to Eqs. (9) and (10), the transmission and reflected amplitude of the various modes due to mode coupling in a taper waveguide are obtained using modified step-theory. In this paper, a symmetrical structure of taper waveguide is discussed, it is sufficient to consider only even propagating modes. Based on Eqs. (9) and (10), the coupling efficiency can be calculated using the instantaneous modes transmission that is propagating in any part of the taper. The modified step-theory for two-dimensional photonic crystal waveguide can be extended to three-dimensional structure. For the three-dimensional simulations, Eq. (3) is modified to include the mode field description in the third dimension. The structure is divided into finite planes which is similar to steps in two-dimensional structure. The coupling constant, $c_{ij}$ and transmission amplitudes, $A_{jn+1}$ are again derived for the three-dimensional photonic crystal tapered waveguide structures. The three-dimensional model of the modified step-theory will be discussed in other papers.

In this paper, the simulations are based on two-dimensional photonic crystal structures. However, it is noted that actual experimental structures [11, 28] are three-dimensional due to fabrication limitations. Hence, vertical radiation losses due to finite height structure need to be taken into consideration. Actual experimental devices are subjected to fabrication process control, where non uniformity in the lattice dimensions across the whole crystal can arise. This results in additional scattering losses and maybe a shift in the transmission spectrum [11]. Coupling losses between the tapered devices and source cannot be avoided. These problems cause disagreement in the results obtained from simulation and experiment. However, careful optical characterization or inclusion of loss terms in simulation can reduce the differences. In the next section, the modified step-theory is verified and compared with [9].

### 4. Verification of the Modified step-theory

In this section, the modified step-theory is applied to obtain the transmittance for each of the normalized frequency spectra of the taper structure. Before applying the theory, Eqs. (5) - (10) are verified by comparing with the numerical simulation results obtained in [9] with the taper structure shown in Fig. 1(a). The tapered structure consists of a smooth input linear taper structure at the entrance on the left end, which is obtained by just shifting the position of the rods accordingly in the $z$ direction. There is also a row of linear defects in the input tapering area which acts as a linear chain of waveguide resonators for the propagation of lightwave. The input taper is then joined by an identical taper but with increasing width towards the other end. A twin head input/output photonic crystal taper is then formed.

For this case study, the modified step-theory is applied to deal with decreasing number of modes at the input taper coupler. The number of modes increases as the taper opens up at the other end. When applying the equations to the taper, the centre part of the waveguide can be left out because there is no change in the width. The propagating loss is assumed to be negligible and coupling losses are due mainly to the variation in width. With the addition of line defects for guiding, the modified step-theory gives a good approximation by obtaining beta values of the defect waveguide at each step. In calculating the beta values, the taper are divided into steps, which corresponds to a unit cell of waveguide. By solving the master wave equation and plotting the band diagram, the beta values at each frequency for each mode can be obtained. Those beta values are then substitute into Eq. (6) and using Eq. (7) to run
iteratively to obtain the transmittance for each frequency and the transmission spectrum is shown in Fig. 1(b).

![Image](image_url)

**Fig. 1.** (a) Structure of the linear defect photonic crystal waveguide with input taper and output taper (b) Comparison of transmission spectra by scattering method and modified step-theory

In Fig. 1(b), the solid line refers to the transmission spectrum that is calculated using the scattering method [9]. The circle dots are the simulated result that is calculated using the modified step-theory. The graph shows a very good agreement between the simulation results obtained by the modified step-theory and the scattering method. From Fig. 1(b), the spectrum at the band edge (< 0.23 and > 0.257) fluctuates due to the low group velocity propagation that results from the presence of Fabry-Perot oscillation between the side-wall of the taper. The average transmission at the middle of the bandgap (between 0.23-0.257) is greater than 90% which implies that adiabatic transmission is achieved. This means that there is very little coupling to the higher order modes and maximum power transfer is maintained in the fundamental mode throughout the whole taper structure. Hence, it is shown that the modified step-theory can be used to calculate both the input and output coupling tapers. Additionally, it can also be used to calculate tapered waveguide linear defects with high accuracy. In other words, the modified step-theory is capable of calculating the transmission spectra of complex photonic crystal taper waveguide and obtains result with high accuracy.

5. Numerical results and discussions

In this section, the modified step-theory is applied to investigate the effect of different input taper waveguide designs on the coupling efficiency. The study begins with a simple case of an abrupt step waveguide. The method is then applied to a step taper waveguide. After this, a more complex linear and non-uniform taper waveguide is analyzed using the modified step-theory.

5.1 Abrupt Step Waveguide and Step Taper Waveguide

For the abrupt step waveguide, the modified step-theory is used to explain the coupling mechanism at the interface between two waveguides with different widths. Then an advanced structure of tapered waveguide is considered by cascading all the step waveguides together. The structure is known as a photonic crystal step taper waveguide. The modified step-theory determines the transmission of the step waveguide by iteratively calculating the coupling efficiency from one step to another, until the last step which is the photonic crystal waveguide.

The structure of the photonic crystal described is a two-dimensional photonic crystal with square lattice arrangement. It consists of high refractive rods that are infinitely long in the third dimension surrounded by air medium. The material of the rods is silicon with refractive index of 3.45 at optical wavelength of 1.55 μm. \( a \) is the lattice constant, \( r \) is the radius of the rods and the \( r/a \) ratio is 0.2. Using plane wave calculation for high refractive index rods, a...
A photonic bandgap exists in normalized frequency range of 0.274 - 0.429 for TM polarization but there is no bandgap for TE polarization. The transverse magnetic (TM) polarization is defined to have magnetic field in \( x-z \) plane and the electric field is perpendicular to the plane while vice versa for the transverse electric (TE) polarization.

The mode coupling characteristic of the abrupt step waveguide is analyzed using the modified step-theory. A linear row of the rods is removed from the crystal to create a single row defect photonic crystal waveguide. On the left half of the waveguide, two additional rows are removed and the final structure is shown in Fig. 2. The wider waveguide is the first step while the narrower waveguide is the second step. For each of the waveguide, the mode profile and the number of modes supported are different. The number of rows of rods removed generally corresponds to the number of localize modes in the bandgap. For the narrower waveguide, the projected band diagram is shown in Fig. 3(a). There exists a single localized mode in the bandgap, and therefore the waveguide only supports a single guided mode. Since the waveguide has even symmetry, the mode field distribution of the fundamental guided mode is an even mode as shown in Fig. 3(a). The band diagram of the wider waveguide has three localized modes in the bandgap supporting three guided modes as shown in Fig. 3(b). The three modes are characterized into two even modes and an odd mode by plotting the field distributions. Depending on the frequency use, the number of modes supported may not be the same for all frequencies. For example, when the frequency is 0.368, the photonic crystal waveguide can only support two modes. Of the two modes, the mode with higher wave vector, \( k \) is the fundamental even mode while the other is the higher order odd mode. For the higher frequency of 0.4, the wider waveguide can support all the three guided modes.

![Fig. 2. Structure of two PCWG cascaded together to form a abrupt step waveguide with different widths](image)

The projected band diagram is obtained using plane wave expansion and supercell method. For convergence and high accuracy, the supercell must be defined such that it has a size of \( q \) rows \( \times 1 \) column rods as shown in Fig. 2. Only one column of rods is needed because the wave vector is conserved in the direction of propagation. \( q \) is the number of rows of rods to be considered in the supercell such that the eigenvalues converge and accurate band diagram is obtained. For this paper, the \( q \) value of 15 is sufficient to serve for this purpose.
Fig. 3. (a) Projected band diagram of the waveguide with single line defects (b) Projected band diagram of the waveguide with three line defects. The red line is odd mode while the black lines are even modes.

Coupling between even and odd mode is not possible due to the difference in the mode field distribution. To illustrate this, the larger waveguide is excited with two different modes distributions, an even and an odd mode. Figure 4(a) shows that the even fundamental mode is coupled to the even single mode waveguide while in Fig. 4(b), the odd mode has zero transmission to the even single mode. This shows that the coupling is only possible between the modes of the same symmetry. Besides calculating the transmitted field amplitude, the modified step-theory can also be used to calculate coupling of the even to odd mode using the overlap integral in Eq. (7).

Fig. 4. (a) Field transmission of the even fundamental mode to the narrower waveguide (b) Transmission of the odd second order mode to the narrow waveguide. Because odd mode cannot couple to even mode, there is no transmission.

The beta values of the odd and even modes can be calculated from the dispersion diagram for both waveguides. In this case, the beta values are taken from the dispersion diagram for the frequency of 0.368. For the wider waveguide, the beta values are 0.940k₀ for the fundamental mode and 0.707k₀ for the odd mode where k₀ is the free space wave vector from Fig. 3(a) and (b). The narrower waveguide has a propagation constant of 0.7334k₀. Using the modified step-theory, the power transmitted from the input power of unity with the even mode is 0.6559. The result is obtained using the exact scattering method. The difference between the two values differ by less than 2%. This shows a good match between the modified step-theory and the scattering method. When the input is excited by the odd mode, the transmission is zero. The scattering method gives a value of 3 × 10⁻⁵. The reason for this small value is due to scattered stray light that is calculated using the scattering method. However, the value
detected by the scattering matrix is close to zero. Therefore, it can be concluded that the odd and even mode do not couple to each other.

From the step waveguide, a more advanced waveguide structure which is known as the step taper waveguide is created by cascading step waveguide of different width and fixed length together as shown in Fig. 5. This taper structure is similar to the design shown in [8]. This taper design is simple and is a good approximation of the classical taper waveguide. The input width is $18a$ which gives a width of approximately $10 \mu m$. This corresponds to the modal diameter of single mode optical fibre source. The taper is known as a “step” taper because the side-wall of taper resembles that of a step staircase. Each step has a fixed length but different width as shown in Fig. 5. In Fig. 5, each step is fixed at a length of $3a$ with the largest width of $18a$ at the input and $2a$ at the output of the taper. By varying the length of the step, the total length of the taper is changed. The change in the taper length can result in a more gradual or abrupt mode transition which affects the coupling efficiency of the taper.

The modified step-theory is applied to the step taper waveguide using the above process at the boundary between steps. The difference is that the taper is divided into more steps to calculate the power transmission. An iterative calculation of the transmitted power from the first step to the last step gives the coupling efficiency of the taper. The first step is the one with the largest width and the subsequent steps are smaller in decreasing order. The $9^{th}$ step is actually the single mode photonic crystal waveguide. The difference is that to calculate the transmission from the wider to the narrower end of the taper, the value of $b$ changes as the width changes. For the step taper waveguide, the complexity increases as greater number of modes are involved compared to the step waveguide.

![Fig. 5. Lattice layout of the “step” taper waveguide](image)

By using the supercell and plane wave calculation method, the band diagram for each of the step are plotted. The propagation constants of the localized mode in each step are taken from the band diagram at the frequency of consideration. As the number of steps is fixed, the modified step-theory is only applied at each boundary where the width changes. When the width at the boundary between steps changes, mode coupling mechanism is affected because the beta values changes. The power transmission for the step taper is calculated. As shown in Fig. 6, the coupling efficiency increases as the taper length increases. This is because the taper structure becomes more gradual with slightly less abrupt mode conversion.
For the single step length of 6a (a total taper length of 48a), the transmitted power is 74% only. This coupling efficiency is higher compared to the butt coupled power of 23%. However, this is not sufficient for waveguide device and integrated waveguide circuit. Therefore, the taper has to be lengthened for more power transmission to increase the coupling efficiency. However, from Fig. 6, the power transmission is observed to increase at a slower rate. This is because the uneven side-wall increases the amount of reflected light. The scattering loss at the corners of the abrupt steps also reduces the amount of the light coupled in the forward mode. Even with length of 48a, adiabatic condition for the step taper is still not achieved. The magnetic field distribution of the taper at length of 48a is shown in Fig. 7. There are a lot of inter-modal coupling due to the scattering and reflection from the abrupt corner, which excites the higher order modes and hence cannot achieve adiabatic behavior. This reduces the transmitted power because the higher order modes are reflected at the narrower part of the taper. When the taper gets narrower, it supports only the lower order modes which propagate through the taper. Therefore, it is not good to couple to the higher order modes.

Figure 8 shows the transmitted power for the fundamental mode at each position of the taper for taper length of 24a and 40a using the modified step-theory. For the step structure, the transmitted power has a discrete step function as the power coupling only occurs at the boundary between steps. When the light propagates through the taper, the transmitted power begins to reduce because of the uneven side-wall and scattering at the corner of the steps. The higher order even modes are excited and some power is transferred to them. Due to the abrupt
change in the width of the taper, the power carried by the higher order mode is reflected rather than transferred to the lower order mode. Lower power is received in the photonic crystal waveguide. For the shorter taper length, the wave propagation is abrupt and fast tapering of the tapered waveguide induces a lot of intermodal coupling. However, when the taper length increases, the transmitted power increases because of more gradual change in the width of the taper.

The step taper design is a simple implementation of the taper structure on the photonic crystal lattice in two-dimension. However, this design cannot provide sufficient coupling transmission due to the abrupt step discontinuity. This uneven side-wall leads to a substantial amount of reflection and scattering loss and hence high coupling loss. The design of the taper is modified to obtain a structure with smoother side wall in order to obtain higher power coupling. The design is modified by shifting of the crystal lattice to produce a smoother wall taper. In the next section, the modified step-theory will be used to explain the coupling characteristics of the different taper designs.

6.2 Smooth linear and nonuniform taper design

The structure of the smooth linear and nonuniform tapers is defined as [12]

\[
z(x) = d_i + (d_o - d_i) \left( 1 - \frac{x}{L} \right)^{\alpha} - 1
\]  \hspace{1cm} (11)

where the \( \alpha \) parameter determines the different curvature of the taper waveguide. \( d_i \) and \( d_o \) are the input and output width of the taper respectively. \( L \) is the total length of taper. The different taper structures are obtained by shifting the rods in the crystal lattice using Eq. (11) with respect to the centerline. Based on [12], the convex shape taper with \( \alpha = 0.5 \) gives the highest coupling efficiency of 97.5 % at a taper length of 20.52 \( \mu \)m. The linear taper with \( \alpha = 1 \) and concave taper \( \alpha = 2 \) give a coupling efficiency of 91.2 % and 90.5 % respectively due to higher reflection loss. The results of the coupling efficiency for different taper curvature are discussed in depth using the modified step-theory. The transmitted power for the three different taper curvatures at varied length is shown in Fig. 9.

The modified step-theory is used to evaluate the power loss of tapers with different curvatures at each relative position of the taper. Figures 10(a), (b) and (c) show the power loss versus the relative position for the linear, convex and concave tapers at length of 9.69 and 18.24 \( \mu \)m. From Figs. 10(a) and (b), the power loss at the relative position of the taper show almost the same trench. The reason for the similar loss trench is due to the more abrupt change in the taper slope at the boundary between the taper and PCWG. The abrupt change results in the scattering of light between the taper and PCWG. Therefore, this causes an
increase in the power loss shown Fig. 10(a) and (b). For the convex taper in Fig. 10(b), the more abrupt change in the curvature causes an even sharper increase in the power loss.

Fig. 9. Transmission vs taper length plots for $\alpha$ values of 1, 2 and 0.5

Fig. 10. (a) Power loss vs relative position for (a) linear taper (b) convex taper and (c) concave taper at 9.69 and 18.24 $\mu$m

For the concave taper, the loss trend is slightly more interesting. From Fig. 10(c), the loss is higher at the front part of the taper that is due to the fast reduction in taper width. There is high inter-modal coupling between the fundamental even mode and the higher order modes. This results into large reflection of the higher order modes and contributes to the high power loss. However, towards the back of the taper, the loss increment begins to slow down and even drops. The power loss starts to drop at about relative position of 0.7. This is because the
slope of concave taper is more gentle, which reduces inter-modal coupling. At the end of the taper, the number of modes is also lesser and hence that contributes to the reduction in power loss. For the concave taper, the back has fitted well to the PCWG and this explains the absence of the sharp increase at the end of the taper compared to Fig. 10(a) and (b). Even though the concave taper fits smoothly to the waveguide, the transmission is still lower than the convex or linear taper due to higher power reflection at the front part of the taper.

To develop a detailed explanation on the power transferred and mode coupling mechanisms of the three taper designs, the transmitted power for the fundamental mode is plotted in Fig. 11. The power for the fundamental mode is obtained using the modified step-theory. In Fig. 11(a), the power transmission of the fundamental mode decreases along to the taper position. This coincides with Fig. 10(a) where the power loss slowly increases until the end of the taper. The power decreases faster for the shorter taper than the longer taper because the width of taper changes more abruptly, which causes more coupling to higher order modes. This results in more power reflected as the lightwaves travel to the narrow part of the taper, hence causes the transmitted power to drop.

![Graphs](a) (b) (c)

Fig. 11. Power transmission of the fundamental mode for (a) linear taper (b) convex taper (c) concave taper at length 9.69 and 18.24 μm

For the case of the convex and concave tapers, the same observation is concluded at the longer taper length in Figs. 11(b) and 11(c) respectively. For the convex taper, the fundamental mode power decreases very slowly at the front part due to the slow tapering. The coupling to the higher order modes is very small and hence gives high power transmission. At the end of the taper, due the abrupt increase in the slope of the taper, the power transmission drops more significantly. This is because faster tapering causes back reflection and excitation of the higher order modes. However, at longer taper length of 18.24 μm, the power loss
remains constant throughout the whole taper because of its gradual curvature. The back of the convex taper becomes more gentle which reduces inter-modal coupling and hence lower reflection loss. For the concave taper, the power of the fundamental mode drops fast in the front part of the taper due to the fast change in the curvature. From the relative position of approximately 0.7, the power drop starts to slow down. This is due to the gentle curvature and good fit of the structure to the PCWG.

The other phenomenon observed in Fig. 11 is the presence of power fluctuations, along the relative position of the taper. These fluctuations are due to the inter-modal coupling between the fundamental mode and the higher order modes, which indicate either too much or too little power is transferred from one mode to another. The upward "bumps" indicate that more power is transferred to the fundamental mode. On the other hand, the downward "bumps" indicate that there is more power coupled to the higher order modes. In Fig. 11(a), for taper length of 9.69 µm, more fluctuations are observed and scattered at different parts of the taper. At the taper length of 18.24 µm, the power transmission is more stable, indicating less inter-modal coupling and power loss.

For the linear taper mentioned in the previous paragraph, the fluctuations are scattered along the different parts of the taper. For the convex taper, the fluctuations occur towards the end of the taper when the slope of the taper becomes steeper. The inter-modal coupling mechanism between the fundamental mode and higher order modes is shown in Fig. 11(b). For taper length of 9.69 µm, the fluctuations are more vicious due to steeper slope. When taper length is 18.24 µm, except for a few small fluctuations, the major fluctuations have almost disappeared. This is because the slow tapering of convex curvature reduces coupling of higher order modes. Therefore, the coupling efficiency reaches 90% or more for the convex taper. For the concave taper, fluctuations are observed in the front part of the taper due to the fast reduction of the taper width. The presence of the inter-modal coupling reduces the amount of power coupling to PCWG. Even at longer taper length of 18.24 µm, the power transmitted is only approximately 0.8.

For the convex taper, “saturation” transmission is achieved at the length of 20.52 µm [12]. Figure 12 shows the relationship between the power change and the relative position of the three types of taper at the length of 20.52 µm. For the linear taper, the transmitted power is more stable because of lesser fluctuations. The field distribution of the linear taper is shown in Fig. 13(a). The structure is approaching the adiabatic region as there are only some inter-modal modes coupling. From the field distribution, some part of the taper has only single mode and the transmitted power is 89%. By extending the length of the taper to 25.08 µm, the linear taper will achieve adiabatic condition with a transmission efficiency of 91.2%. The remaining losses come from the mode field mismatch between Gaussian input and the waveguide mode as well as scattering loss at the end of the taper.
Fig. 13. Field distribution for the different taper at 20.52 μm. (a) Linear taper (b) Convex taper (c) Concave taper
For the convex taper, the power is almost constant with virtually no ripples, which shows that the coupling to higher order mode is almost eliminated. The field distribution of the convex taper is also plotted in Fig. 13(b). The lightwaves maintain visibly monomode throughout the whole convex taper which shows that the adiabatic condition is achieved for the convex taper at the length of 20.52 μm and the transmitted power is 97.5 %. For the concave taper, some coupling losses are observed due to fast changing curvature. From Fig. 13(c), it is far from adiabatic. This can be solved by lengthening the concave taper. However, lengthening the concave taper will reduce the compactness of the taper and hence not feasible.

Based on the discussions, the modified step-theory has very high convergence for waveguide with moderate cross sectional variation. Even for short and abrupt tapered waveguide, it gives moderate convergence with reasonable accuracy as shown in Fig. 6. Compared to the other semi analytical methods [15-20], the modified step-theory is better because it analyzes the intermodal coupling mechanism and describes the modes behavior in the tapering section. It can be applied to a wider range of taper curvature and designs. The modified step-theory is a better choice for providing an in depth analysis of photonic crystal tapered waveguide structure compared to other numerical methods [29-30].

6. Conclusions

In this paper, the mode coupling mechanism of photonic crystal tapers is rigorously studied using the modified step-theory. The taper waveguide is divided into many vertical steps and solved for the fields at the boundary between each step to obtain the coupling coefficient and transmitted amplitudes. The mathematical model is verified by comparing the transmission spectra using the same structure as in [9]. The numerical simulation results show that the spectra calculated by the modified step-theory are consistent with [9]. This shows that the modified step-theory can calculate the transmission for both input and output coupling taper as well as linear defects tapered waveguide with high accuracy. The modified step-theory is then applied to different design of photonic crystal taper to discuss the variation in the coupling efficiency. In the first case of abrupt step waveguide, the results obtained by the modified step-method for the even and odd mode propagation are highly consistent with the results obtained by the scattering method. This shows that the modified step-theory works well for multimode propagation in step waveguide. The method is then applied to step taper waveguide to obtain a coupling efficiency of 74% for a taper length of 48a. The modified step-method is also used to calculate the power transmission along the taper. Large inter-modal coupling which is caused by the presence of abrupt discontinuities and scattering at the corners of the side-wall is observed. The smooth linear and nonuniform taper is created to obtain higher coupling efficiency. For the convex taper, lesser inter-modal coupling is observed due to its large receiving curvature. This provides an explanation for the fundamental mode with high power throughout the whole taper compared to the linear and concave taper. From the power transmission along the taper, the degree of inter-modal coupling can also be deduced by observing the fluctuations in the plot. For the linear taper, the fluctuations are most scattered along the taper with moderate amplitude. For the convex taper, it is mostly found in the latter part with smaller amplitude. For the concave taper, it is found in the front part, fluctuating viciously and indicating high inter-modal coupling. This method converges for a rather wide range of photonic crystal tapered waveguide designs with reasonable accuracy. The downside of the method is perhaps obtaining the propagation constant for the propagating modes at each step. As a result, the modified step-theory is very useful for modeling and analysis of the coupling mechanism in tapered waveguide. It is also simple to use for the design and optimization of more complex photonic crystal tapered waveguide structure.

Acknowledgments

The authors express their sincerest gratitude to Steven G. Johnson of MIT for his useful discussion and friendly advice.
Appendix A

In this appendix, the derivation of the modified step-theory is shown in details. Starting from classical Maxwell’s equation, in the absence of field current and source, the electric and magnetic field in electromagnetic waves are related in the equation given as

\[ \nabla \times E = -\mu \frac{\partial H}{\partial t} \]  \tag{A1}

\[ \nabla \times H = \varepsilon \frac{\partial E}{\partial t} \]  \tag{A2}

where \( \mu \) and \( \varepsilon \) are the permeability and permittivity of the material in which the field exist. Assuming linear and lossless material, the complex field \( E \) and \( H \) can be expanded to a set of harmonic modes with complex time exponential \( e^{i\omega t} \). Rearranging Eqs. (A1) and (A2) and substituting the field harmonics, the equation for the electric field is given as

\[ \nabla \times (\nabla \times E) = \left(\frac{\omega}{v}\right)^2 E \]  \tag{A3}

where \( v \) is the speed of electromagnetic waves in the material with refractive index, \( n \) given by

\[ v = \frac{1}{\sqrt{\varepsilon \mu}} = \frac{c}{n} \]  \tag{A4}

For \( H \) field, similar expression can be obtained. By applying vector properties for the \( E \) field and Coulomb’s law, the curl of the curl symbol can be removed and be replaced by \( \nabla^2 \) to form the scalar wave equation given as

\[ \nabla^2 E = \left(\frac{\omega}{v}\right)^2 E \]  \tag{A5}

where \( \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \)

Considering the electromagnetic waves propagating along the \( x \) direction in a planar channel waveguide extending the \( x \) and \( z \) direction. The wave solution for the electric field is described by the normal modes given as [25]

\[ E = E_0 \xi(z) \times e^{i\beta x} \]  \tag{A6}

where \( \beta \) is the propagating constant of the waves traveling in the waveguide and \( \xi(z) \) is the \( z \) dependent field distribution of the guided mode. \( E_0 \) is the real amplitude of the propagating electric field. As mentioned in section 2, photonic crystal waveguide mode field resembles modes in conventional waveguide [26-27]. A close approximation is to consider it to be a case of a metallic waveguide of width \( b \), on which an artificial periodicity of \( d \) is imposed. The equation for the mode field of the guided modes is given as

\[ E = E_0 \sin \left( m \pi \left( \frac{z}{b} + \frac{1}{2} \right) \right) \exp \left[ -i \psi(x) \right] \]  \tag{A7}

where the phase coefficient, \( \psi \) is given as

\[ \psi(x) = \left( \beta + \frac{2\pi \eta}{d} \right) x \quad \eta = 0, \pm 1, \pm 2, \ldots \]  \tag{A8}
Before deriving the equations, the field distribution in Eq. (A7) is replaced by the symbol $\zeta$ so as to give a clearer deriving process. Consider there are two modes, $i$ and $j$ are propagating at the $x$ direction. Both modes travel to a narrower waveguide of width $b'$ with the same periodicity. The wider waveguide is labeled as the $n$th step with subscript $n$, while the narrower waveguide is labeled as the $(n+1)$th step with subscript $n+1$. Matching the boundary conditions between the $n$th and $(n+1)$th steps, the incident, reflected and transmitted field components are given as

$$E_{in} \zeta_{m} \exp(-i \psi_{in}) + E_{jn} \zeta_{n} \exp(-i \psi_{jn}) + E_{in} \zeta_{in} \exp(i \psi_{in}) + E_{jn} \zeta_{jn} \exp(i \psi_{jn}) + E_{ref} = E_{in1} \zeta_{in1} \exp(-i \psi_{in1}) + E_{jn1} \zeta_{jn1} \exp(-i \psi_{jn1}) + E^{trans}$$  \hspace{1cm} (A9)

Beside the main propagating modes, there also exist other modes such as the transmitted radiation modes, $E^{trans}$ and the reflected radiation modes, $E^{ref}$. These two modes will vanish during the course of derivation by applying orthogonal condition. For $H$-field in $z$ direction, similar expressions can be obtained as

$$\psi_{m} E_{in} \zeta_{m} \exp(-i \psi_{in}) + \psi_{jn} E_{jn} \zeta_{jn} \exp(-i \psi_{jn}) - \psi_{jn} E_{jn} \zeta_{jn} \exp(i \psi_{jn})$$

$$H^{ref} = \beta_{jn} E_{jn} \zeta_{jn} \exp(i \psi_{jn}) + H^{ref}$$

$$= \psi_{in} E_{in1} \zeta_{in1} \exp(-i \psi_{in1}) + \psi_{jn1} E_{jn1} \zeta_{jn1} \exp(-i \psi_{jn1}) + H^{trans}$$  \hspace{1cm} (A10)

where $E^R$ refer to the real amplitude of the reflected guided mode. By multiplying Eqs. (A9) and (A10) by a transmitted mode field distribution and integrating over $x$, the unguided radiation modes are eliminated because of the orthogonality. The aim now is to obtain an iterative equation for field amplitude and phase of $j$th mode, $E_{jn+1}$ and $\psi_{jn+1}$. To do this, the expression for the reflected field of the $i$th mode must be obtained. Together with the assumption made in section 3 and multiplying Eqs. (A9) and (A10) by transmitted mode field of the $\zeta_{in+1}$ and integrating over $x$, the expression for the reflected field of mode is given as

$$E_{in} \zeta_{in} \exp(i \psi_{in}) = \left( \frac{\psi_{in} - \psi_{in+1}}{\psi_{in} + \psi_{in+1}} \right) E_{in} \exp(-i \psi_{in})$$  \hspace{1cm} (A11)

Eqs. (A9) and (A10) are multiplied by the transmitted field $\zeta_{jn+1}$ and integrating over $x$. After some algebraic manipulation and substituting the reflected field for $i$th mode with Eq. (A11), the transmitted field expression for the $j$th mode is obtained as

$$E_{jn+1} I_{jn+1, in+1} \exp(-i \psi_{jn+1}) = \left( \frac{2 \psi_{in}}{\psi_{jn} + \psi_{jn+1}} \right) \left( \frac{\psi_{in} + \psi_{in+1}}{\psi_{jn} + \psi_{jn+1}} \right) E_{in} I_{in, in+1} \exp(-i \psi_{in})$$

$$+ 2 \left( \frac{\psi_{jn}}{\psi_{jn} + \psi_{jn+1}} \right) E_{jn} I_{jn, in+1} \exp(-i \psi_{jn})$$  \hspace{1cm} (A12a)

where

$$I_{in, in+1} = \int \zeta_{in} \zeta_{jn+1} dx$$  \hspace{1cm} (A12b)

$I_{in, in+1}$ is refer as the field overlap integral of the respective modes at each side of the steps. The field amplitude in Eq. (A12a) is normalized by the amplitude of the incident field of the
respective mode, $E_m$ which has a mode power, $P_m$ of unity. The mode power, $P_m$ is related to
the unity mode field $E_m$ for the transmitted $j_{th}$ mode at the $(n+1)$th step can be expressed as

$$P_m = (E_m) \frac{\psi_{jn+1}}{2k_0} I_{jn+1, jn+1} = 1 \quad (A13)$$

where $k_0$ is the free space wave vector. All the terms of Eq. (A12a) is divided by appropriate
factor of the unity mode field and simplifying, the amplitude and phase of the $j_{th}$ mode at
$(n+1)$th step is given by

$$A_{jn+1} \exp(-i \psi_{jn+1}) = c_{ij} A_{in} \exp(-i \psi_{in}) + c_{ji} A_{jn} \exp(-i \psi_{jn}) \quad (A14)$$

where the coupling constant $c_{ij}$ is given by

$$c_{ij} = \frac{\psi_{jn} G \psi_{in}}{\psi_{in}} \frac{I_{jn+1, jn+1}}{G} \quad (A15a)$$

where

$$G = \frac{2 \beta_{jn} \beta_{jn+1} + 2 \beta_{jn} \beta_{jn+1} + \gamma^2 + 2 \gamma \beta_{jn} + \gamma \beta_{jn+1} + \gamma^2}{(\beta_{jn} + \beta_{jn+1} + \gamma)(\beta_{jn} + \beta_{jn+1} + \gamma)} \quad (A15b)$$

and

$$\gamma = \frac{4 \pi \eta}{d} \quad (A15c)$$

It can be seen that the equation depends on the propagation constant, $\beta$ and the Bloch mode of
the periodicity. The coefficient $c_{ij}$ can be obtained by substituting $i$ by $j$. For multiple modes
coupling, the general expression is given as

$$A_{jn+1} \exp(-i \alpha_{jn+1}) = \sum_i c_{ij} A_{in} \exp(-i \alpha_{in}) \quad (A18)$$

By equating the real and imaginary parts of the left and right hand side, the transmitted
amplitude is derived as

$$A_{jn+1} = \left[ \left( \sum_i c_{ij} A_{in} \cos \alpha_{in} \right)^2 + \left( \sum_i c_{ij} A_{in} \sin \alpha_{in} \right)^2 \right]^{1/2} \quad (A19)$$

and the phase is derived as

$$\alpha_{jn+1} = \tan^{-1} \left( \frac{\sum_i c_{ij} A_{in} \sin \alpha_{in}}{\sum_i c_{ij} A_{in} \cos \alpha_{in}} \right) \quad (A20)$$