Contribution to the modeling of coupled resonator optical waveguides in photonic crystals

Nikolaos Avaritsiotis*
National and Kapodistrian University of Athens
Department of Informatics and Telecommunications
nickava@di.uoa.gr

Abstract. In this dissertation, coupled resonator optical waveguides are analyzed and a new analytical model to study their spectral properties is developed. Coupled mode theory and plane wave expansion are employed in order to study the spectral properties of CROWs and a new semi-analytical model is derived. This semi-analytical model is used for the derivation of an analytical solution for the device’s resonant frequencies. The model not only provides a useful tool in the design of CROW based devices but also presents a useful physical insight for the device under investigation. The semi-analytical model is also used in several types of coupled cavity devices, as is a SCISSOR, and is compared with other methods, such as FDTD, in order to test the validity and accuracy of the results. All approximations and assumptions that lead to a simplification of the model are being discussed. Furthermore the relation between fabrication imperfections and the performance of photonic crystal CROWs is examined based on our semi-analytical model. A statistical study of such imperfections is enabled owing to the calculation of the coupling coefficients derivatives. The model is used to study the spectral influence of imperfections of different strengths and types on various coupled cavity devices.

Keywords: Photonic crystal waveguide, CROW, SCISSOR, Coupled mode theory, FDTD, frequency response, geometric perturbations.

1 Dissertation Summary

In this dissertation the technology of photonic crystals is chosen as the technology platform to study optical integrated nanophotonic devices. Photonic crystals are periodic structures created by materials with different dielectric constants that are periodically placed in space. Photonic crystals are classified in 1D, 2D and 3D according to their dielectric constant periodicity in space. One of the most important features of photonic crystals is the presence of photonic band gaps in their dispersion diagrams. More specifically a photonic band gap is a range of frequencies for which light cannot propagate inside the structure. Therefore many useful photonic crystal
devices can be constructed with photonic band gaps, preventing light from propagating in certain directions with specified frequencies [1].

Coupled Resonator Optical Waveguide (CROW) devices in photonic crystals may find important applications in future integrated nanophotonic circuits. These devices represent a new kind of waveguides not depending on the principles of total internal reflection nor on Bragg reflectors to guide light [2]. Waveguiding is performed by the coupling of neighboring resonators appropriately placed in order to ensure loose coupling [2]. CROWs can be manufactured by several kinds of resonators such as Fabry-Perot resonators, photonic crystal cavities, micro rings and micro disks and may function with different ways of coupling between these resonators giving rise to several designs and applications. In this dissertation the photonic crystal cavities were chosen to construct CROWs and Side Coupled Integrated Spaced Sequence of Optical Resonators (SCISSORs) [3].

Several methods are going to be developed in order to study these structures. The role of these methods is very important so as to understand the way in which light propagates through these structures and in addition to theoretically analyze and design them. Arithmetic methods that directly solve Maxwell’s equations in the time domain (Finite Difference Time Domain, FDTD) [4] or in frequency domain (Finite Difference Frequency Domain, FDFD) [5] can overview the evolution of electromagnetic fields and may be successfully applied to devices like CROWs and SCISSORs. Unfortunately they present several drawbacks such as need for enormous computational power and time for the simulation of complicated structures. The Mode Matching method [6] can analyze the properties of such structures having as only prerequisite the analysis of the structure in supercells. Another similar method that is going to be fully analyzed in this dissertation is the Couple Mode Theory (CMT) [7].

Firstly a closed form formula for the calculation of the transfer function of a Photonic Crystal (PC) CROW coupled to an input and an output PC waveguide will be derived [8]. Coupled Mode Theory is initially used for the derivation of a semi analytical transfer function model [11]. This semi-analytical model is compared to the results of an in-house FDTD tool (also used in [13]) and good agreement is obtained. Using this semi-analytical model and taking into account only adjacent cavity and/or waveguide coupling, a simpler analytical model is obtained for the first time, providing a closed form formula for the transfer function of the device regardless of the number of cavities. This analytical model may be used to quickly estimate the transfer function of the device once the coupling coefficients are estimated. Using the analytical model, the resonant frequencies of the device were also obtained. This model can provide a useful tool in the design of CROW-based filters and other similar devices [8].

As previously stated CROWs and SCISSORs are well suited for coupling of mode analysis, which usually requires much less computational resources compared Finite Difference Time Domain (FDTD) schemes. Coupled mode models [10] also provide a useful physical insight in the device operation. Therefore in this dissertation is derived a general coupled mode theoretic model for the treatment of coupled cavity devices incorporating various phenomena such as dispersion, frequency variation of the coupling coefficients, non-adjacent cavity coupling and waveguide mode self coupling [14]. The model is validated comparing its results against the FDTD method [13] and the strength of the underlying assumptions is highlighted. Overall it was
shown that the CMT model can provide an adequate device description offering a tangible manner of calculating the transfer function and a useful physical insight.

Finally the relation between fabrication imperfections and the performance of a photonic crystal Coupled Resonator Optical Waveguide (CROW) is studied [12]. A semi-analytical model is presented, which calculates the perturbation of the coupling coefficients through their derivatives with respect to the geometric characteristics of the rods of the photonic crystal lattice. To account for random perturbations in finite devices, Finite Difference (FD) methods require very small grid size in order to capture small geometric perturbations. To obtain reliable statistical results, many perturbed devices must be calculated rendering such simulations intractable. This alternative approach, based on a previously developed coupled mode model [8], is applied to the calculation of the derivatives of the coupling coefficients with respect to the rod radii and positions. Once these derivatives are calculated, the transfer functions of a large number of devices with randomly perturbed geometric characteristics using Taylor’s expansion, are estimated and the results are analyzed discussed.

2 Results and Discussion

2.1 Electromagnetic field equations

\[ E = \sum_n a_n E_n + \sum_l a_l E_{fl} + \sum_l a_{sl} E_{bl} \]

\[ H = \sum_n a_n H_n + \sum_l a_l H_{fl} + \sum_l a_{sl} H_{bl} \]

where \( E_n, H_n \) are the electric and magnetic modal fields of the \( n \)th isolated cavity modes \((1 \leq n \leq N)\), \((E_{fl}, H_{fl})\) and \((E_{bl}, H_{bl})\) are the forward and backward propagating modes of the \( l \)th waveguide \((l=1 \text{ or } 2)\). Due to the symmetry of the device in Fig. 1a,
the role of the input and output waveguide may be interchanged. The waveguide \( l = 1 \) will be considered as the input waveguide. In addition, \( a_n \) and \( d_n \) denote the excitation coefficients of the \( n \)th cavity mode and the forward and backward isolated propagating mode of the \( l \)th waveguide respectively. Assuming that \( z \) is the propagation direction of the waveguide modes, \( a_n \) and \( d_n \) are generally considered \( z \)-dependent [15], while the cavity mode amplitudes \( a_n \) are assumed not to depend on \( z \) [16]. The Bloch’s theorem will be used in order to express the waveguide mode fields as [17]. The propagation constant \( \beta_{\text{isol}} \) will be considered positive for the forward \((m=f)\) and negative for the backward \((m=b)\) propagating mode and the Bloch functions \( e_{\text{isol}} \) and \( h_{\text{isol}} \) are periodic vector functions with the same periodicity \( a \) as the input/output waveguides along the \( z \) direction. Since the waveguides are considered the same, at a given frequency \( \omega \), the propagation constants will be \( \beta_{f1} = \beta_{b1} = -\beta_{b2} = \beta \). The waveguide modes are normalized and the forward and backward propagating modes obey the orthogonality relations as in [15].

In the same way the cavity modes obey a similar set of equations,

\[
\nabla \times E_n = j\omega \mu H_n \\
\n\nabla \times H_n = -j\omega \varepsilon_n E_n
\]

(3)  

(4)  

where \( \varepsilon_n(r) \) is the isolated dielectric constant distribution of \( n \)th cavity alone and \( \omega_0 \) is the isolated mode resonant frequency. Assuming a lossless structure, one may chose the electric fields for the cavity modes to be purely real \( E_n^* = E_n \) resulting in purely imaginary magnetic field, \( H_n^* = -H_n \) as discussed in [18].

2.2 Coupled Mode Equations

In order to derive the coupled mode equations for the waveguide and cavity modes of the structure, the Lorentz’s reciprocity theorem [18] will be used. This theorem relates two electromagnetic fields \( (E_a, H_a) \) and \( (E_b, H_b) \) obeying Maxwell’s equations in media with dielectric constant distributions \( \varepsilon_a \) and \( \varepsilon_b \) respectively. Using the corresponding reciprocity equations presented in [18], the following coupled system of equations is derived:

\[
\frac{df_1}{d\tau} = Wf_1 + Cf_2
\]

(5)  

where the vectors \( f = (f_1, f_2, \ldots, f_N) \) contain the amplitudes of the waveguide and cavity mode respectively, while the matrices \( W = [w_{pq}] \) and \( C = [c_{pq}] \) are determined by the coupling coefficients of the modes,

\[
w_{pq} = j\omega \delta \int \sum \left( \varepsilon - \varepsilon_n \right) E_p \cdot E_q^* \\
c_{pq} = j\delta \left\{ \mu \left( \omega - \omega_0 \right) \int \sum \mathbf{H}_q \cdot \mathbf{H}_p^* \right\} + j\delta \left\{ \varepsilon \left( \omega - \varepsilon_n \omega_0 \right) \int \sum \mathbf{E}_q \cdot \mathbf{E}_p^* \right\}
\]

(6)  

(7)
where $\delta_1=1$ and $\delta_2=-1$. The coefficients $w_{pq}$ correspond to the coupling of the waveguide modes inside the cavities, while $c_{pq}$ are determined by the coupling of the waveguide modes with the cavity modes. As previously stated we apply Bloch’s theorem [1] to express the forward waveguide mode as $E_1 = e_1 \exp(j\beta z)$, where $\beta$ is the propagation constant of the mode and $e_1$ is the Bloch function which is periodic along $z$. In order to obtain the cavity coupled mode equations, the reciprocity equations can be applied in this case considering the vector functions $F_n = E \times H_{cn}^* + E_{cn}^* \times H$, where $1 \leq n \leq N$.

The following equations are then derived:

$$\int_0^L dz S a + K b = 0$$

In (8) the integration is performed along the propagation direction from the input ($z=0$) to the output ($z=L$) of the device. The matrices $S=[s_{pq}]$ and $K=[\kappa_{pq}]$ are defined by:

$$s_{pq} = j\mu(\omega-\omega_b) \int S H_{cp}^* H_q + \int S (\epsilon \omega - \epsilon_{cp} \omega_b) E_{cp}^* E_q$$

$$\kappa_{pq} = j\mu(\omega-\omega_b) \int V H_{cp}^* H_q + \int V \left( \epsilon \omega - \epsilon_{cp} \omega_b \right) E_q E_{cp}^*$$

where elements $\kappa_{pq}$ are the coupling coefficients between the cavity modes and $s_{pq}$ much like $c_{pq}$ are determined by the coupling of the waveguide modes with the cavity modes.

### 2.3 Estimation of the transfer function

The previous equations provide a framework for the estimation of the transfer function of the structure. The power transfer function is defined as $T(\omega) = |a_1(L)/a_1(0)|^2$ and is determined by the ratio of the amplitudes of the forward propagating mode at the device output and input. In [8] we have shown how under certain simplifying assumptions (e.g. assuming $W=0$) the transfer function of the CROW can be obtained. However, in this case a more generalized transfer function derivation will be shown for the case of a SCISSOR (Fig. 1b). Because of the term corresponding to $W$, (5) is not directly amenable to integration as in [8] and for this reason we consider the $2 \times 2$ matrix $U$, obeying the differential equation:

$$\frac{\partial U}{\partial z} = W U$$

Given its value $U(0)$ at $z=0$, $U$ can be calculated numerically by approximating the derivative in (11) with a finite difference. If $W$ is small enough, then it can be easily shown that $U$ is approximated by:
\[ U(z) \equiv I + \int_0^z dz' W(z') \]  \hspace{1cm} (12)

where it is assumed that \( U(0) = I \). We substitute \( a = Uc \) in (5) in which case we obtain:

\[ \frac{dc}{dz} = U^{-1}Cb \]  \hspace{1cm} (13)

The above equation can now be readily integrated with respect to \( z \), in order to obtain:

\[ a(L) = U^{-1}(L) \left[ a(0) + \left( \int_0^L dz U^{-1}C \right) b \right] \]  \hspace{1cm} (14)

where we used the fact that \( c = U^{-1}a \). The vector \( b \) can be estimated by (8), if one performs integration by parts. We assume a matrix \( A \) such that:

\[ \Lambda(z) = \int_0^z dz' S(z') U(z') + P \]  \hspace{1cm} (15)

where \( P \) is a constant matrix. Taking into account that \( Sa = (\partial A/\partial z)c \), we can write:

\[ \int_0^L dz Sa = \Lambda(L)c(L) - \Lambda(0)c(0) - \int_0^L dz A \frac{dc}{dz} \]  \hspace{1cm} (16)

and using (13) and (8) we obtain:

\[ \Lambda(L)U^{-1}(L)a(L) - \Lambda(0)U^{-1}(0)a(0) - Gb = 0 \]  \hspace{1cm} (17)

where matrix \( G \) is determined by:

\[ G = -K + \int_0^L dz \Lambda U^{-1}C \]  \hspace{1cm} (18)

We note that in (17), the amplitudes of the cavity modes contained in \( b \) are expressed in terms of the input and output waveguide mode amplitudes \( a(L) \) and \( a(0) \). The amplitudes \( a_1(0) \) and \( a_2(L) \) of the forward and backward mode at \( z = 0 \) and \( z = L \) are determined by the incident wave conditions. Typically when calculating the transfer function, we assume that \( a_2(L) = 0 \), i.e. that there is no reflected wave at the device output. In any case, we can choose the elements of \( P \), so that only the incident amplitudes of the forward and backward modes \( a_1(0) \) and \( a_2(L) \) respectively appear in (17). To do this we require the first column of \( \Lambda(L)U^{-1}(L) \) to be zero and that the second column of \( \Lambda(0)U^{-1}(0) \) be also zero. Using some straightforward mathematic manipulations, we find that the elements of \( P_{pq} \) of \( P \) must be given by:

\[ P_{pq} = 0 \]  \hspace{1cm} (19)
where the $M = [M_{pq}]$ is the matrix $M = SU$ and $u_{pq}$ are the elements of $U$ which can be estimated numerically using (11) or (12). Given $M_{pq}$, we can use (19)-(20) to determine the elements of $P$. Assuming that $a_2(L) = 0$, then taking into account that $E(0) = I$ and that $A(0) = P$, we obtain from (17):

$$b = a_1(0) G^{-1} P^{(q)}$$  

(21)

where $P^{(q)}$ denotes the $q^{th}$ column of $P$. Equation (21) expresses the cavity mode amplitudes $b = (a_{c1}, a_{c2}, \ldots, a_{cN})$ in terms of the forward waveguide mode amplitude $a_1(0)$ at the device input. Therefore equation (14) can be used to estimate $a_1(L)$ in terms of $a_1(0)$ and $b$. The transfer function can be calculated taking into account the fact that $T(\omega) = |a_1(L)/a_1(0)|^2$.

To calculate the transfer function of a CROW, like the one depicted in Fig. 1a, using the semi-analytical form and the simplifying assumptions of [8] one first needs to estimate the coupling coefficients of the cavity/cavity and cavity/waveguide systems and hence the isolated modal fields of the waveguides and the cavities. This can be achieved through the Plane Wave Expansion (PWE) method [17]. For the calculation of the modes of the isolated cavity the number of plane waves used were 55 in each direction (resulting in a total number of 3025 plane waves) while for the waveguide modes the number of plane waves used were 15 along the propagation direction and 61 in the transverse direction. Using this method, the isolated cavity mode resonant frequency $f_0$ was calculated near $f_0/c = 0.3869$. Fig. 2 depicts the power transfer function $T = |h|^2$, obtained. The three notches of $T$ are due to the resonances of the three cavity system (Fig. 2). The amplitude of the power transfer function reaches approximately the value 0.25 at the resonant frequencies [19].

![Fig. 2](image)

**Fig. 2** Transfer functions of a CROW side-coupled to two PC waveguides as obtained using either the FDTD method or the outlined CMT.

In a similar way Fig. 3 presents the results for the generalized CMT model for a SCISSOR (Fig. 1b) along with the FDTD transfer functions for validation purposes.
A single cavity SCISSOR is chosen (depicted in the inset of Fig. 3) device and various grid sizes $\Delta$ were assumed for the FDTD scheme. The cavity is spaced one rod away from the waveguide. Fig. 3 illustrates that as grid size reduces the transfer function calculated by the FDTD gradually approaches that of the CMT. For $\Delta=r_a/8$ ($r_a$ is the radius of the rod) one obtains a 0.3% difference between the values of the resonant frequencies predicted by two methods and a 15% difference in the 3 dB bandwidth of the resonance. Smaller grid sizes were not considered because they rendered the FDTD simulations quite time consuming especially in the case of sharper resonances. To estimate the modal fields with the PWE, we used 75x75 plane waves in the case of the cavity mode and 33x75 plane waves in the case of the waveguide mode along the $z$ and $y$ directions respectively. The resonant frequency of the isolated cavity mode was estimated at $f_r/c=0.3877$. A7x7 and 1x7 supercell was used in the PWE calculation in the case of the cavity and the waveguide fields.

Fig. 3 Transfer function of a single cavity SCISSOR obtained by the CMT and the FDTD scheme. For the latter method, various grid sizes $\Delta$ are considered.

2.4 Approximations of the CMT model

The CMT approach usually results in a more tangible estimation of the transfer function of the device. In [8] it was shown how this can be rigorously achieved in the case of a CROW, by ignoring the evanescent waveguide modes in the field expansion, the frequency dependence of the modal fields and secondary coupling effects. In this section some of these restrictions mentioned above will be discussed and the CMT results are going to be compared against the FDTD method.

Frequency dependence of the coupling coefficients.

Inspecting the coupled mode coefficients in (7) and (9)-(10), it is deduced that the coupling coefficients exhibit a frequency dependence since $\omega$ appears both in front of the magnetic mode overlap integral and inside the electric field overlap integral. The frequency dependence of the coupling coefficients is also due to the fact that the modal fields are given by $\mathbf{E}_i=e_1\exp(jft/c)$ [8] where both the propagation constant $\beta$ and the Bloch field $e_1$ are frequency dependent. Our simulation results have shown that taking into account the frequency dependence of the coupling coefficients can have an important bearing on the results.
Coupling Assumptions.

As previously stated, the general coupling of modes analysis accounts for the coupling of the waveguide modes inside the cavities through the matrix $W$. If this secondary coupling is ignored ($W\approx0$) the transfer function evaluations become much simpler. It is therefore interesting to investigate the influence of this waveguide mode coupling. The simulation results imply that $W$ has a rather minor bearing even in the case where the cavities are placed relatively near the waveguides. Its influence may be greater in the case of structures with weaker mode confinement, however. In addition it is interesting to consider whether adjacent cavity coupling alone is sufficient to provide an accurate estimate for the transfer function. In this case, the matrix $K$ is considered tridiagonal, i.e., $\kappa_{pq}\approx0$ when $|p-q|>1$. The simulation results indicate that coupling between non-adjacent cavities also results in a frequency detuning which may be important in the case of sharp resonances.

Expansion in terms of the cavity supermodes.

The CMT model presented in 2.2 is based on the expansion of the electromagnetic field in terms of the isolated cavity modes. This is not the only choice however. In [16], we have discussed how an $N$-cavity system can be considered as a single resonator exhibiting $N$ modes inside the bandgap, which can be referred as the “supermodes” $E_{sn}, H_{sn}$ of the cavity system in analogy to the supermodes of a waveguide coupler [20]. These modes obey Maxwell’s equations, e.g. $\nabla \times \mathbf{H}_{sn} = j\omega_n \varepsilon_n \mathbf{E}_{sn}$ where $\varepsilon_n$ is the dielectric constant of the $N$-cavity system, and $\omega_n$ is the resonant frequency of the $n^{th}$ mode. One can apply the reciprocity relations [8] again to obtain coupled mode equations similar to 2.2. The simulation results have shown that the choice of supermodes seems to produce a more accurate description for the broad resonance. However, since it involves the estimation of the cavity modes of a large resonator (coupled cavity system) such estimations may require an excessive number of plane waves.

Evanescent waves.

The simulation results have indicated that in specific cases CMT fails to provide an accurate description of very sharp resonances. This may be due to the assumptions made during its derivation. Probably the most important one is that evanescent waves are neglected in the field expansion of (1)-(2). Although coupled mode theory could in principle be expanded to include evanescent waves [21], this would lead to a cumbersome model, since the number of evanescent waves is infinite. Evanescent modes are included in FDTD, but their influence cannot be easily distinguished. To obtain some measure of the importance of evanescent modes, we resort to the Mode Matching (MM) method also developed in [6] where the PWE method was adapted to estimate evanescent waveguide modes as well.

2.5 Geometric perturbations

To account for random perturbations in finite devices a very small grid size is required in order to capture these small geometric perturbations. To obtain reliable
statistical results, many perturbed devices must be calculated. Therefore an alternative approach is proposed derived from the previously developed coupled mode model based on the calculation of the derivatives of the coupling coefficients with respect to the rod radii and positions [14]. Once these derivatives are calculated, one may estimate the transfer functions of a large number of devices with randomly perturbed geometric characteristics using Taylor’s expansion. Consequently the first step is to calculate all the coupling coefficients of the ideal device (i.e. a device free of geometric perturbations) and estimate its transfer function. To incorporate the effect of perturbations, the derivatives of the coupling coefficients need to be calculated as in [14]. Then one may generate random perturbations along the horizontal ($\Delta x$) and vertical ($\Delta z$) axis and the rod radius $\Delta R$, for each rod of each perturbed device. The derivatives in this method need to be calculated only once and can then be used to statistically study the effect of imperfections on a large number (for example 1000) of perturbed devices. The transfer functions for perturbed CROW devices with 10 cavities, for different cavity/waveguide and cavity/cavity spacing are shown in Fig. 4.

Finally simulation results calculated from 200 sample devices with $\Delta=2nm$, depicted in Fig. 5, have shown that the average of standard deviation $\sigma=\text{std}\{T(f_n)\}$, of the resonance centers $f_n$ increases with the size of the device, implying that larger CROWS are much more susceptible to fabrication imperfections.
3 Conclusions

This dissertation presented the method that was developed in order to analyze the spectral characteristics of CROW waveguides with finite cavity numbers in photonic crystals starting from Maxwell’s equations. The analysis additionally assumed an input and output waveguide coupled to the CROW structure since its spectral behavior is directly linked to the way light is coupled in and out of the structure. The simplification of the model led to an analytical equation for the calculation of the resonant frequencies of the structure directly by the calculation of its coupling coefficients. The presented method does not require excessive computational time or resources in order to produce accurate results. In addition the results were compared with the FDTD method and good agreement was observed. Furthermore this analytical method provides a better physical insight of the way cavities and waveguides interact inside the CROW and may provide a useful tool in the design of CROW-based filters and other similar devices.

An analysis of the spectral characteristics of SCISSOR devices was also performed using the proposed semi-analytical model. All parameters (i.e. frequency dependence of the coupling coefficients, adjacent cavity/cavity and cavity/waveguide coupling, CMT expansion consideration, evanescent waves) involved in the calculation of the transfer function were discussed and a better physical understanding of the analysis was provided. Many discrepancies of the CMT model for specific SCISSOR structures were therefore explained.

Finally, the influence of fabrication induced disorders in the performance of a photonic crystal CROW was numerically investigated. The semi-analytical model was also used for the calculation of the transfer function of the device in the presence of geometric perturbations of various types. The model was based on the estimation of the derivatives of the coupling coefficients of the CROW. Then, using these derivatives a large number of perturbed devices was simulated with a very small computational overhead. The statistical study of various performance issues such as the amplitude change and frequency shift of the device resonances as well as the resonance 3dB bandwidth were discussed. Using this model one may numerically estimate the relation between the device performance and the quality of the fabrication process.

4 References