Highly Accurate Modelling of Generalized Defect Modes in Photonic Crystals using the Fictitious Source Superposition Method

Lindsay C. Botten¹*, Kokou B. Dossou¹, Stewart Wilcox², Ross C. McPhedran², C. Martijn de Sterke², Nicolae A. Nicorovici¹², and Ara A. Asatryan¹

¹Centre for Ultrahigh-bandwidth Devices for Optical Systems (CUDOS) and Department of Mathematical Sciences, University of Technology, Sydney, PO Box 123, Broadway, NSW, 2007, Australia. Tel: 61-2-9514 2247; Fax: 61-2-9514 2260; E-mail: Lindsay.Botten@uts.edu.au
²CUDOS and School of Physics, University of Sydney, NSW 2006, Australia.

Abstract - We present an exact theory for modelling the modes of two-dimensional photonic crystals with a truly infinite cladding. It builds on our previous implementation of the fictitious source superposition method for simple point defects that is based on three key ideas: the use of fictitious sources to modify response fields so defects can be introduced; the representation of the defect mode as a superposition of solutions of quasiperiodic field problems; and the reduction of the two-dimensional superposition to a highly efficient, one-dimensional average. Here we describe an elegant extension to model a compound, multiple scatterer, defect in a given layer, and then build on this to construct an arbitrary defect from multiple layers of compound defects. We demonstrate the method's accuracy and efficiency, and present two- and three-dimensional results. We also demonstrate the strengths of the method for difficult problems, such as where a mode is highly extended near cutoff.

Index Terms - defect modes, diffraction, fictitious sources, microstructured optical fibres, multiple scattering, photonic crystals, photonic crystal fibres.

I. INTRODUCTION

Though photonic band gaps—frequency ranges in which the propagation of light is suppressed through Bragg reflection—form the foundation of the technological potential of many photonic crystal¹ structures, it is the introduction of defects into an otherwise periodic medium (e.g., waveguides[2], cavity resonators[3], photonic crystal fibres[4] etc.) that allows this potential to be realized. The introduction of defects into photonic crystal structures gives rise to defect modes, the frequencies of which lie in the band gap of the surrounding PC, and which are thus localized.

Most of the modelling of defect modes in such imperfect periodic structures has been undertaken using techniques that assume a finite structure, either explicitly (as for a finite cluster of scatterers[5-7] or implicitly (as in supercell methods[8-10] which periodically replicate a finite structure). Such methods work well for modes that are strongly confined but are beset with difficulties when the mode becomes highly extended. In such cases, the computational requirements of modelling a structure that is sufficiently large to accommodate the extended nature of the mode may be overwhelming and can lead to inaccurate results.

To handle problems of this type, which typically arise in studying a mode near cutoff[11-13], we developed an exact theory for computing defect modes in a genuinely infinite 2D lattice, and have applied it to the study of the long-wavelength behaviour of microstructured optical fibres (MOFs). Our approach not only handles MOFs with an infinite cladding, but is also computationally more efficient than other techniques when the size of the structure becomes large. Accordingly, our method allows for calculations similar to those for conventional fibres, which, because of their relatively simple geometry, are also modelled with infinite claddings. Though the
cladding in realistic fibres is of course finite, it is nonetheless sufficiently large for modelling errors to be negligible. One might expect that with further technological improvements a similar situation will occur with MOF fabrication, or one might argue this has already been achieved: namely that their cladding is so large that confinement losses and other finite cladding effects are negligible, and therefore for MOFs to be well modelled as having infinite cladding.

Our original treatment[14] of the Fictitious Source Superposition (FSS) method, while being a useful tool that helped resolve the controversy about the cutoff of the fundamental mode in a MOF[15], was restricted nevertheless to modelling simple defects—specifically, a single defect in a single row of scatterers. The purpose of this paper is to extend the theory to accommodate more complex defects comprising compound defects (i.e., with a multiplicity of cylinders removed or modified) in multiple rows of an infinite photonic crystal. In Sec. II, we review the FSS method[14] for a single cylinder defect and in-plane incidence, noting that the theory extends naturally to conical incidence, and focus on the three key concepts that lie at its heart. We then outline how the basic method may be modified to handle a compound defect in a single row of the structure, and then proceed to generalize the treatment to accommodate a multiplicity of rows of compound defects. In Sec. III, we demonstrate the application and utility of the method before drawing some conclusions in the discussion of Sec. IV.

II. THEORY

A. Preliminaries and Fictitious Sources

We consider the structure in Fig. 1 and aim to model the modes of propagation of a defect constructed by removing a finite number of cylinders in adjacent rows of the regular lattice which has a lattice constant of \(d\), an interlayer spacing of \(h\) and which is characterized by its lattice vectors \(\mathbf{e}_1\) and \(\mathbf{e}_2\).

While ultimately we wish to solve problems with arbitrary propagation directions (3D problems), here, for the sake of mathematical simplicity, we will formulate the method in 2D, i.e., with propagation orthogonal to the inclusions, in either of the two fundamental \(E\) or \(H\) polarizations. We then briefly mention the generalizations that are required to convert from the 2D to the full 3D formulation. In two dimensions, the problem reduces to the solution of a scalar problem in which the field quantity satisfies a Helmholtz equation 

\[
\nabla^2 V + k_j^2 V = 0,
\]

where \(k_j\) denotes the wave number in medium \(j\).

In the exterior vicinity of each cylinder (centred on \(\mathbf{r} = \mathbf{r}_j\)), and also within its interior, we respectively expand the field in multipole expansions\[16,17\]

\[
V_e = \sum_{n=-\infty}^{\infty} \left[ a_n^j J_n(k_n \rho) + b_n^j H_n^{(1)}(k_n \rho) \right] e^{i\mathbf{k} \cdot \mathbf{r}}
\]

\[
V_i = \sum_{n=-\infty}^{\infty} \left[ c_n^j J_n(k_n \rho) + g_n^j H_n^{(1)}(k_n \rho) \right] e^{i\mathbf{k} \cdot \mathbf{r}}
\]

where \((\rho, \phi) = \mathbf{r} - \mathbf{r}_j\). In the case of the 2D problem, we have \(k_n = k_n\) and \(k = k_n\) respectively denoting the exterior and interior wavenumbers, with the free space wavenumber given by \(k = 2\pi/\lambda\). The \(a^j\) coefficients (1) characterize the outward radiation from cylinder \(j\), while the \(b^j\) coefficients define the regular part of the field.
which comprises radiation that is incident on the cylinder from exterior sources, or from sources associated with all other cylinders. Correspondingly, in Eq. (2) the regular part of the field in the interior of the scatterers is characterized by coefficients \( c' \), while the coefficients \( q' \) represent the fictitious sources that we will use to tailor the external field. This is the first of the three main ideas underlying the FSS method.

For a single cylinder, the field continuity conditions at the cylinder boundary impose relations between the field coefficients that read

\[
\hat{b}' = \hat{R} a' + \hat{T} q', \quad c' = \hat{R}' a' + \hat{T}' q'. \quad (3)
\]

Only the first of these is of immediate use to us, indicating that the outgoing field \( b' \) is a reflection of the (standing wave) incident field \( a' \) and a transmission of the interior fictitious source \( q' \), with the matrices \( \hat{R} \) and \( \hat{T} \) fulfilling the role of Fresnel coefficients in the multipole basis. To make this particular cylinder vanish, thus creating a defect, we must choose the transmission of the fictitious source to be such that it cancels the reflected incident field. Thus, setting \( b' = 0 \), so that there is no outgoing radiation from the cylinder, we deduce the fictitious source

\[
q' = -\hat{T}^{-1} \hat{R} a'
\]

which makes the scatterer disappear in the presence of the incident field \( a' \). In a similar manner, instead of cancelling a single scatterer, we might wish to modify its characteristics, such as its radius, material properties etc., so that its properties are characterized by a different multipole reflection matrix \( \hat{R}_{\text{new}} \). This we do by setting \( b' = \hat{R}_{\text{new}} a' \), which leads to the following choice of the fictitious source:

\[
q' = -\hat{T}^{-1} (\hat{R} - \hat{R}_{\text{new}}) a'
\]

While the basic process is quite straightforward for a single scatterer, its use in the computation of a defect mode in an infinite structure is very difficult, if not impossible, due to the complexity of the field interactions. The solution of this problem is discussed in the following section, Sec. II.B.

\[\text{B. Source Superposition}\]

We now introduce the second of our key ideas, namely the formulation of the defect mode from a superposition of solutions of quasiperiodic field problems. We thus consider an array of cylinders containing embedded sources which are quasiperiodically phased, i.e., we set the source in cylinder \( j \) centred at \( r = r_j \) to be \( q' = q \exp(ik_0 \cdot r_j) \).

The defect mode is then formed from a superposition of the quasiperiodic field problems by integrating with respect to the Bloch vector \( k_0 \) over the first Brillouin zone (BZ) of the reciprocal lattice. The superposed solution then satisfies the wave equation and the boundary conditions, and is associated with a fictitious source distribution which, for cylinder \( j \) is

\[
q = \int_{BZ} \exp(ik_0 \cdot r_j) dk_0 = \begin{cases} q & \text{for } r_j = 0, \\ 0 & \text{for } r_j \neq 0. \end{cases} \quad (4)
\]

In this key step, the BZ integration eliminates the fictitious sources in all but the primary cylinder \( (j = 0) \). The sole remaining source at \( r = r_0 = 0 \) is thus available to modify the response field and, in doing so, to formulate the defect mode.

\[\text{C. Diffraction Grating Model}\]

While the principle of the approach is well founded, the need for a two-dimensional integration over the BZ, for the 2D geometries that we are considering, imposes a heavy computational burden which, if not addressed, would compromise the anticipated advantages of the method over conventional techniques (such as supercell methods). This difficulty can be overcome, however, by reformulating the problem to require only a one-dimensional integration. This reformulation is the third key idea, requiring the structure to be modelled as a set of diffraction gratings having an embedded, quasiperiodically phased array of sources which are sandwiched between two semi-infinite photonic crystals. The properties of the surrounding semi-infinite crystals, which act as mirrors, are modelled with a (plane wave) Fresnel reflection matrix \( R_\infty \), which follows from a Bloch mode analysis of the bulk...
photonic crystal[18,19]. The use of $R_\infty$ is crucial in that it encapsulates the second BZ dimension, and, in doing so, eliminates one level of integration.

In what now follows, we set up the formulation for a single grating layer and then extend this to handle compound defects (i.e., multiple cylinder defects in a single layer) in Sec. II.E, and multiple layers of either simple or compound defects in Sec. II.F. We begin with the multipole representation of the diffraction properties of the grating which are expressed by the Rayleigh field identity

$$a = S b + J^- f^-_1 + J^+ f^+_2.$$  \hspace{2cm} (5)

While Eq. (5) may be derived rigorously[17] using Green’s function methods, it may also be justified using a physical argument in which we observe that the regular part of the field, i.e., that part of the field not sourced at the primary cylinder, is due to outgoing radiation from all other cylinders of the grating ($S b$) and also to external sources which, in our case, are due to the incoming plane waves, $f^-_1$ and $f^+_2$, incident on the primary grating layer, respectively from above and below. The grating acts as a phased array and so the multipole contributions due to this line of antennas are characterized by the Toeplitz matrix of lattice sums $S = [S_{l,m}]$ in which

$$S_l = \sum_{s=0}^{\infty} H_{1}^{(3)}(k_e \mid s \mid d) e^{-i \arg(s)} e^{i \alpha_s s_d}$$ \hspace{2cm} (6)

denotes the lattice sum of order $l$ (see, for example, Botten et al [16]).

In Eq. (5), the quantities $f^\pm = [f^+_j, f^-_j]$ are vectors of coefficients in the plane wave expansions of the field in the region between the cylinder gratings.

$$V_j(x, y) = \sum_{p=-\infty}^{\infty} \frac{\chi_p^{-1/2}}{k_p} e^{-i \chi_p (y-y_j)} \left[ f^+_j e^{-i \chi_p (y-y_j)} + f^-_j e^{i \chi_p (y-y_j)} \right] e^{i a_x x},$$ \hspace{2cm} (7)

with the phase origins chosen appropriately at $y = y_j$ in the middle of each layer that separates adjacent gratings. In Eq. (7),

$$\alpha_p = \alpha_0 + \frac{2 \pi p}{d}$$ and $$\chi_p = \sqrt{k_e^2 - \alpha_p^2},$$ \hspace{2cm} (8)

are respectively proportional to the direction sines and cosines of the grating orders, and follow from the diffraction grating equation. The matrices $J^\pm$ which appear in Eq. (5) are used to change the representation of the field from the plane wave basis to the multipole basis.

In a similar manner to that used to derive Eq. (5), we can form expressions for the outgoing fields on either side of the single grating layer, i.e.,

$$f^+_I = f^+_2 + K^- b, \quad f^-_O = f^-_1 + K^- b$$ \hspace{2cm} (9)

respectively, for the outgoing plane waves immediately above and below the grating. These are expressed in terms of the incoming fields and the field scattered by the grating $K^- b$. The matrices $K^\pm$ play an analogous role to the $J^\pm$ matrices, but perform a change of basis from the multipole to the plane wave representation.

Combining Eqs (9) together with the multipole boundary conditions (3) and the Rayleigh identity (5), we arrive at expressions for the plane wave fields that are outgoing from the central grating:

$$f^+_I = R f^-_O + T' f^+_O + Q^- q, \hspace{2cm} (10)$$

$$f^-_O = T f^-_I + R' f^+_I + Q^- q,$$ \hspace{2cm} (11)

in which $R$ and $T$ denote the (plane wave) reflection and transmission scattering matrices of the grating for incidence from above, $R'$ and $T'$ are the corresponding scattering matrices for incidence from below, and $Q^\pm$ are operators which compute the upward and downward plane wave fields (at the mid-points of the layers) due to the embedded fictitious source $q$ in the grating layer. Here,

$$R = K^+ G \tilde{R} J^-,$$ \hspace{2cm} (12)

$$R' = K^- \tilde{G} R J^+,$$ \hspace{2cm} (13)

$$T = P + K^- \tilde{G} R J^-,$$ \hspace{2cm} (14)

$$T' = P + K^+ \tilde{G} R J^+,$$ \hspace{2cm} (15)

where $Q^\pm = K^\pm G \tilde{T}$, $G = (1 - \tilde{R} S)^{-1}$ and $P = \text{diag}(\exp(i \chi_p h))$. Here, $G$ denotes the multipole scattering operator and is singular at
points in the Brillouin zone that correspond to modes of the bulk crystal, while \( P \) characterizes the propagation of an (incident) plane wave field across a single grating layer of thickness.

In turn, the grating source coefficients \( b \) may be expressed in terms of the incoming driving fields, \( f_{i} \) and \( f_{j}^{+} \) and the internal source \( q \):

\[
b = \tilde{Y}^{-} f_{i} + \tilde{Y}^{+} f_{j}^{+} + \tilde{q},
\]

where \( \tilde{Y}^{\pm} = G \tilde{R} J^{\pm} \) and \( \tilde{q} = G \tilde{T} q \). We “close the loop” by recognizing that the incoming fields required in Eq. (16) are related to the outgoing fields (10, 11) through Fresnel matrices that encapsulate the properties of the semi-infinite mirrors surrounding the grating layer. That is,

\[
f_{i}^{-} = \tilde{R}_{\infty} f_{i}^{+}, \quad f_{j}^{+} = \tilde{R}_{\infty} f_{j}^{-},
\]

in which the matrices \( \tilde{R}_{\infty} \) and \( \tilde{R}_{\infty}^{-} \) are derived from an analysis of the Bloch modes of the bulk photonic crystal[18]. By combining Eqs (10-17), we see that \( b \) can be expressed directly in terms of the fictitious source, and so we derive the simple linear relationship

\[
b = Z q
\]

between the outgoing source coefficients \( b \) and the fictitious source \( q \).

D. Formulation of the Mode of a Simple Defect

Using the fundamental equation (18), in which \( Z = Z(k,\alpha_{0}) \), we express the outgoing multipole field (\( b \)) in terms of the fictitious source (\( q \)) and are now in a position to construct a defect mode. If we set \( b = 0 \) and solve for the roots of \( \det Z(k,\alpha_{0}) = 0 \), we compute the dispersion curve of a waveguide. This is because the cylinders of the grating are quasiperiodically phased (i.e., \( b^{i} = b \exp(i k_{0} \cdot r_{j}) \)) and so by causing any one of them to vanish will cause the entire row of cylinders to vanish, thus forming a simple W1 waveguide.

The calculation of the defect mode of an actual cavity, however, requires a superposition of quasiperiodic solutions and thus, for a simple defect comprising the removal of just a single scatterer, we are led to the solution of

\[
\langle Z(k) \rangle q = 0
\]

in which

\[
\langle Z(k) \rangle = \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} Z(k,\alpha_{0}) d\alpha_{0}
\]

is computed by averaging \( Z(k,\alpha_{0}) \) over the one-dimensional Brillouin Zone.

We conclude the section with some remarks concerning the method’s implementation. We firstly reiterate that the step that underpins the high efficiency of the method is the conversion of the 2D superposition process to one which requires only a one-dimensional integral. Without the use of the grating model, the computational complexity required for the superposition integral over the 2D Brillouin Zone would rival that of conventional supercell methods for finding modes, leading either to long computation times or reduced accuracy. We now consider more closely the implementation of the method, accepting that, while the theory models a genuinely infinite structure, the process of computing the superposition integral numerically truncates an infinite process and approximates it by a finite sum.

The process of computing \( \langle Z(k) \rangle \) by numerical integration involves the calculation of

\[
\langle Z(k) \rangle = \sum_{j=0}^{N} w_{j} Z(k,2\pi\xi_{j}/d)
\]

in which the weights \( \{w_{j}\} \) and the abscissae \( \{\xi_{j}\} \) are chosen according to some integration rule. We typically use Gaussian quadrature because it is well suited to the behaviour of the integrand. However, let us contemplate the implications of choosing instead the trapezoidal rule, which is widely used for computing integrals of periodic functions. The distribution of the sample points and the superposition of the fictitious sources that is implied by Eq. (21) effectively leaves a source in every \( N^{th} \) cylinder. Thus, although the theory models a genuinely infinite structure, an implementation that uses the trapezoidal rule effectively models a structure which
has defects in every \( N \)th cylinder. While the numerical implementation is thus analogous to a supercell model, there are major differences from the usual approaches which must deal with 2D supercells. In our case, the supercell is one-dimensional and thus can be arbitrarily large, allowing us to model accurately defect modes with extremely large spatial extent without compromising the computational efficiency.

E. General Formulation of the Mode for a Complex Defect

The approach that we have adopted for the modelling of a single scatterer defect generalizes readily to compute the mode of a complex defect. For the sake of conceptual simplicity, we will formulate this initially in the multipole basis using a superposition that involves a 2D Brillouin zone integration, and then proceed to develop the grating model which, while computationally superior, is conceptually more difficult as it entails the composition of the solution for compound defects in a sequence of gratings. This we outline in the present section and the following section, Sec. II.F.

We consider a 2D lattice with embedded sources \( q \exp(i k_0 \cdot r_j) \) at the centre of each cylinder. Since the field problem is quasiperiodic, the field in the vicinity of each cylinder can be expanded in the multipole series (1) in which

\[
\begin{align*}
a_j &= a \exp(i k_0 \cdot r_j) \quad \text{and} \\
b_j &= b \exp(i k_0 \cdot r_j)
\end{align*}
\]

where \( a \) and \( b \) are vectors of multipole coefficients for the central (reference) cylinder.

The Rayleigh field identity then follows by observing that the regular part of the field in the vicinity of the reference cylinder is given by the sum of the outgoing waves sourced by each cylinder in the phased array. Thus,

\[
a = S^A b, \quad \text{where} \quad S^A = [S^A_{lm}] = [S^A_{l-m}],
\]

where

\[
S^A_n = \sum_{j \neq 0} H_n^{(1)}(k | r_j |) e^{i \text{arg}(r_j)} e^{i k_0 r_j} \quad (23)
\]

denotes the array lattice sum of order \( n \), in which the summation \( j \) is over all but the central cylinder in the array. Then, combining Eq. (22) with the boundary conditions (3), we deduce that

\[
b = Z q, \quad \text{where} \quad Z(k, k_0) = (I - R S^A)^{-1} T. \quad (24)
\]

Let us now construct the mode of a complex defect formed by removing the cylinders at a finite number of lattice points \( r_m \) where \( s_m \in S \), with \( S \) denoting the set of cylinders to be removed. We now introduce the compound fictitious source

\[
q = \sum_{m} q_m e^{-i k_0 r_m} \quad (25)
\]

and write down expressions for the fictitious source in each cylinder \( j \), \( q_j' = q_j \exp(i k_0 \cdot r_j) \), and the corresponding outgoing field coefficients for each cylinder, \( b_j' = b_j \exp(i k_0 \cdot r_j) \). These are:

\[
q_j' = \sum_{m} e^{-i k_0(r_j-r_m)} q_m, \quad (26)
\]

\[
b_j' = \sum_{m} Z(k, k_0) e^{i k_0(r_j-r_m)} q_m. \quad (27)
\]

Then, integrating over the 2D Brillouin zone, it is clear that the averaged fictitious source at cylinder \( j \) \( \langle q_j' \rangle = 0 \) except for those \( j \in S \) for which \( \langle q_j' \rangle = \langle q_m' \rangle = q_m \). These sources are then available to tailor the outgoing field, thereby producing a defect mode by effectively removing all cylinders \( j \in S \). To do so, we set

\[
0 = \langle b_j' \rangle = \sum_{m} \bar{Z}_{lm} q_m \quad \forall s_j \in S \quad (28)
\]

where

\[
\bar{Z}_{lm} = \langle Z(k, k_0) e^{i k_0(r_j-r_m)} \rangle, \quad (29)
\]

and derive a system of equations \( \bar{Z}(k) q = 0 \) from which we compute the frequency of the defect mode from the solution of \( \text{det} \bar{Z}(k) = 0 \), and also the mode structure from the null space of \( \bar{Z}(k) \).

Note that in calculating \( \bar{Z}_{lm} \), the integrand involves the scattering operator \( M^{-1} \) where \( M = I - R S^A \). Since the poles of \( M^{-1} \) (i.e., the
values of $k_0$ for which $\det M = 0$ correspond to the Bloch modes of the bulk photonic crystal, it follows that unless we operate in a complete band gap the Brillouin zone integration required is in the superposition process will be undefined, corresponding to the absence of a defect mode.

For the sake of computational efficiency, however, we must return to our grating formulation, replacing the 2D Brillouin zone integration by a 1D integration. In the case of the compound defect, we will initially consider sources embedded in a single grating, and then proceed to extend the treatment in Sec. II.F by considering sources in multiple layers. For a single layer, Eq. (28) continues to hold, with the definition of $\mathbf{Z}_{lm}$ now given by

$$\mathbf{Z}_{lm} = \left( \mathbf{Z}(k, \alpha_0) e^{i \alpha_0 (s_l - s_n)} \right)^l,$$  \hspace{1cm} (30)

where the $s_l$ are integers denoting the cylinders in the grating that are to be annihilated or altered.

F. Extension to Multiple Grating Layers

The final stage in the theoretical development is the extension of the FSS method to handle complex defects involving compound sources in multiple layers. The interaction of the fields and sources is now more complicated and we thus need to adopt a systematic approach that generalizes our earlier treatment.

We consider a defect spanning $n$ grating layers, enumerated by $l = 1, 2, ..., n$ from top to bottom, each with a phased array of fictitious sources $q_l$.

We identify upward and downward propagating plane waves ($f^\pm_l$) at each of the interfaces $l = 1, 2, ..., n + 1$ between the gratings, with interfaces $l = 1$ and $l = n + 1$ respectively being immediately above and below the uppermost and lowermost gratings that have embedded sources (see Fig. 1). At these interfaces we apply the mirror conditions

$$f^+_l = R_l f^+_l, \hspace{1cm} f^-_{n+1} = R_{n+1} f^-_n.$$  \hspace{1cm} (31)

With this nomenclature, we commence the derivation by generalizing Eq. (16) for each layer $l$:

$$b_l = \tilde{Y}^- f^-_l + \tilde{Y}^+ f^+_l + \tilde{q}_l.$$  \hspace{1cm} (32)

That is, the outgoing, multipole field $b_l$ from layer $l$ is generated by incoming plane wave fields from above ($f^-_l$) and below ($f^+_l$), and by the embedded fictitious source $q_l$, which is associated with the term $\tilde{q}_l = G \tilde{T} q_l$.

We now develop representations of the upward and downward going plane wave fields ($f^\pm_l$) between each layer. These may be thought of as being generated by the outside driving fields $f^-_l$ and $f^+_l$, respectively from above and below the set of grating layers that contain sources, and from the sources embedded in each of the layers. We thus write:

$$f^-_l = T_{l,l-1} f^-_{l-1} + R_{l,l-1}^i f^+_l + \sum_{m=1}^{l-1} Q_{[l,l-1],m} q_m.$$  \hspace{1cm} (33)

In deriving this, we observe that the downward propagating waves ($f^-_l$) at the interface immediately above grating $l$ must be generated by sources above it. Accordingly, there are contributions from the exterior field $f^-_{l-1}$ which is transmitted from above through the layers $m = 1, ..., l - 1$, from the upward field $f^+_l$ which is reflected back by the layers $m = 1, ..., l - 1$, and also from plane wave contributions, represented by $Q_{[l,l-1],m} q_m$, which are generated by the fictitious sources in each of the layers $m = 1, ..., l - 1$. The contributions of the fictitious sources may be analyzed one layer at a time, with the operator $Q_{[l,l-1],m}$ characterizing downward propagating plane waves from a layer $m$ within the block of layers $[1, l - 1]$, accounting for the multiple scattering amongst these layers. Expressions for the operators $Q_{[l,l],m}$, $R_{l,l}$, $R_{l,l}^i$, $T_{l,l}$ and $T_{l,l}^i$ are derived in the Appendix.

Proceeding in a similar manner, we also write down an analogous expression for $f^+_l$:

$$f^+_l = T_{l,n+1} f^+_l + R_{l,n} f^-_l + \sum_{m=l}^{n} Q_{[l,n],m} q_m.$$  \hspace{1cm} (34)
and then solve Eqs (33) and (34) to arrive at the representation of the interior plane wave fields \( f_i^+ \) that are required in Eq. (32):

\[
f_i^+ = \left( I - R_{l,i-1} R_{l+1,i} \right)^{-1} \left( T_{l,i-1} f_i^- + R_{l,i-1} T_{l+1,i} f_{i+1}^+ \right) + \sum_{m=1}^{l-1} Q_{l,j-1,m} q_m + R_{l,i-1} \sum_{m=l}^{n} Q_{l,j,m} q_m ,
\]

\[
f_{i+1}^+ = \left( I - R_{l,i} R_{l+1,i} \right)^{-1} \left( R_{l,i} T_{l,i-1} f_i^- + T_{l,i} f_{i+1}^+ \right) + R_{l,i} \sum_{m=1}^{l} Q_{l,j-1,m} q_m + \sum_{m=l}^{n} Q_{l,j,m} q_m .
\]

Eqs (36-37) involve the exterior driving (incoming) fields \( f_i^- \) and \( f_{i+1}^+ \) which are computed using the mirror condition (31) and explicit expressions for the outgoing waves \( f_i^+ \) and \( f_{i+1}^+ \):

\[
f_i^+ = R_{l,i} f_i^- + T_{l,i} f_{i+1}^+ + \sum_{m=1}^{n} q_{l,[j,m]} q_m ,
\]

\[
f_{i+1}^+ = T_{l,i} f_i^- + R_{l,i} f_{i+1}^+ + \sum_{m=1}^{n} q_{l,[j,m]} q_m .
\]

Solving Eqs (31), (37) and (38) we deduce that the incoming exterior fields are given by

\[
\begin{pmatrix}
  f_i^- \\
  f_{i+1}^+
\end{pmatrix}
= \begin{pmatrix}
  I - R_{l,i} R_{l+1,i} & -R_{l,i} T_{l,i} \\
  -R_{l,i} T_{l,i} & I - R_{l,i} R_{l+1,i}
\end{pmatrix}
\begin{pmatrix}
  q_i \\
  q_{i+1}
\end{pmatrix}
\]

\[
\times \begin{pmatrix}
  R_{l,i} & 0 \\
  0 & R_{l,i}
\end{pmatrix}
\begin{pmatrix}
  Q_{l,[j,1]} & \cdots & Q_{l,[j,n]} \\
  Q_{l,[j,1]} & \cdots & Q_{l,[j,n]}
\end{pmatrix}
\begin{pmatrix}
  q_j \\
  \vdots \\
  q_n
\end{pmatrix} .
\]

Finally, combining Eqs (32) and (39), we show that the source coefficients \( b_l \) depend linearly on the fictitious sources \( \{ q_m \} \) in each grating \( l \). Thus,

\[
b_l = \sum_{m=1}^{n} Z_{l,m} q_m \quad \forall l = 1, 2, \ldots, n,
\]

or, in partitioned matrix notation,

\[
b = Z q,
\]

in which \( b \) and \( q \) are partitioned vectors \( b = [b_l] \) and \( q = [q_m] \), and \( Z \) denotes the block partitioned matrix \( Z = [Z_{l,m}] \).

Modes may be extracted by solving the homogeneous system \( Z q = 0 \), as before. In the most general case, with complex defects requiring a compound source in each row, each element of the partitioned vectors \( b \) and \( q \) itself becomes a partitioned vector. Thus, in general, an element of \( q \) would be identified by \( q_{lj} \), in which \( l \) refers to the grating row and \( j \) to the fictitious source associated with the cylinder to be modified. Similarly, the matrix \( Z_{lj} \) itself becomes a partitioned matrix which is indexed as \( Z_{lj, mk} \), with the subscript \( lj \) referring to cylinder \( j \) in row \( l \), and the subscript \( mk \) referring to the source in cylinder \( k \) of row \( m \).

G. Extension of the Implementation to 3D Problems

The formulation that we have outlined thus far is for the in-plane (i.e., \( z \)-independent) solution for either \( E_z \) or \( H_z \) polarization, in which only a single \( z \) field component (either \( E_z \) or \( H_z \)) is non-zero. In a fully 3D problem, as occurs in the modelling of a photonic crystal fibre, the fields have an axial dependence of the form of \( \exp(i\beta z) \) and fields must be expressed in terms of the axial components (\( E_z \) or \( H_z \)) of the electric and magnetic fields. These two components are not independent and are coupled through the field continuity conditions on the cylinder boundaries. Accordingly, the problem transforms from one which is scalar in nature to one which is vectorial. Nevertheless, the overall structure of the formulation is unchanged.

A first key change to the implementation is that the multipole vectors \( a \) and \( b \) must incorporate representations of both \( E_z \) and \( H_z \) and so become partitioned vectors, e.g., \( b = [b^E, b^H] \), in which the two vector components are vectors of multipole coefficients for \( E_z \) and \( H_z \) respectively. Next, the Toeplitz matrix of multipole coefficients is replaced by a block diagonal matrix \( \{ S, S \} \). This is because the Rayleigh
identity $a = Sb$ is satisfied separately by each of the electric and magnetic field quantities, with no cross coupling involved. On the other hand, the multipole boundary condition matrices $\hat{R}$ and $\hat{T}$ must be modified to accommodate the vector nature of the problem and are replaced by block diagonal matrices of the form
\[
\begin{bmatrix}
\hat{R}^{EE} & \hat{R}^{EH} \\
\hat{R}^{HE} & \hat{R}^{HH}
\end{bmatrix},
\]
(42)
in which each partition is a diagonal matrix, and with the off-diagonal blocks characterizing the cross-coupling of the fields that occurs at the cylinder interfaces. The interior and exterior wave numbers in the multipole expansions take a revised form $k_j = \sqrt{k^2 - n_j^2 - \beta^2}$, reflecting the fields’ $\exp(i\beta z)$ dependence.

Note that the plane wave aspects of the solution are structurally similar to those outlined in the preceding sections, needing only to be modified by the inclusion of TE and TM resolutes that describe the vector nature of the field. A more complete discussion of the point is given in our earlier paper, Wilcox et al[14].

III. VERIFICATION AND APPLICATION OF THE THEORY

We now demonstrate the accuracy and utility of the generalized FSS method for computing defect modes. The method was validated by testing it against alternative techniques, including the commercial software RSoft BandSOLVE, for computing waveguide modes and field modes in photonic crystal fibres. In all cases, the method generates high accuracy results in a very efficient manner.

Our first example is the calculation of a waveguide mode which numerically validates the fictitious source concept that underpins the entire method. The structure that we consider is a W3 waveguide in a hexagonal lattice of dense cylinders, of normalized radius $a/d = 0.2$ and refractive index $n_i = 3$ in a background of refractive index $n_e = 1$. The structure, with three layers removed, is shown in Fig. 2(a) and a field plot of the $E_y$ (TM) polarized mode for a normalized frequency of $d/\lambda = 0.32$ is shown in Fig. 2(b).

\[\text{(a)}\]
\[\text{(b)}\]

Fig. 2. (a) The W3 waveguide that we consider. (b) The field of the fundamental mode at a normalized frequency of $d/\lambda = 0.32$ with normalized propagation constant $a_0d = 1.67541$.

\[\text{(a)}\]
\[\text{(b)}\]

Fig. 3. (a) Dispersion curve of the W3 PC waveguide of Fig. 2(a). (b) Near the cut-off of the second mode.

Fig. 3(a) shows the dispersion curve for the waveguide modes, while Fig. 3(b) shows an enlarged view of the dispersion curve near the cutoff of the second mode. The red curve was computed with the FSS method, while the blue dots were generated using a Bloch mode (super-cell) method for photonic crystals in which the scattering matrices are computed by a finite element technique[20], a completely different method. Clearly the agreement is excellent.
Our next example is the calculation of cavity modes in a complex structure. The basic geometry is the same as for Fig. 2, deriving from a square lattice of cylinders of normalized radius $a / d = 0.2$ and refractive index $n_i = 3$ in a background of refractive index $n_e = 1$. From this, we remove four cylinders, two in each of two adjacent rows, to construct a square defect. For $E_\parallel$ polarization, this structure has two degenerate modes with a resonant frequency $d / \lambda = 0.396354377$ that are shown in Figs 4(a) and 4(b).

An alternative approach is to regard the structure as a triangular lattice and remove four cylinders that span three rows, as in Fig. 5. While this, of course, must yield the same degenerate pair of modes, the computational scheme is entirely different and, as such, the comparison of these results with those of Fig. 4 is a genuine test of the method’s robustness and accuracy. We now find the resonant frequency to be $d / \lambda = 0.396354309$, which is the same as previously to seven significant figures. The two orthogonal modes computed by the FSS method are shown in Figs 5(a) and (b), and by taking appropriate linear combinations, we recover, in panels 5(c) and (d), the plots of Figs 4(a) and (b).

It is also interesting to compare these results for what is a well confined mode with those obtained using a multipole formulation for a finite square cluster[16] of 144 cylinders (i.e., in a $12 \times 12$ array) from which the central four cylinder have been removed as in Fig. 4(a). Using this calculation, we estimate that the defect mode frequency is $d / \lambda = 0.39635856 + 7.94 \times 10^{-6}$, where the imaginary part of the frequency is associated with losses caused by the finite confinement.

The preceding results, while validating the method, do not demonstrate its unique strength in handling the truly difficult cases in which methods that assume a finite structure, either explicitly or implicitly, fail. In Fig. 6 we show a poorly...
confined defect mode near the edge of the band gap which, because of its highly extended nature, makes it impossible for standard (supercell) methods to achieve the same accuracy. In this example, we consider the same square lattice as in previous examples but this time reduce the refractive index of the central cylinder to be $n_{\text{defect}} = 2.7$. Using truncated multipole expansions that include harmonics up to order $N_j = 6$, and with plane wave expansions including diffraction orders -3,-2,...,3 [14], a Gaussian integration with $N = 40$ points allows our prototype FSS method, written in Mathematica and using MathLink to access a Fortran routine to compute the scattering matrices, to find the defect mode of Fig. 6, for a normalized frequency of $d/\lambda = 0.32083778154$, in less than 3 minutes on a standard 3.0 GHz Pentium 4 system running Microsoft Windows XP. Convergence tests demonstrated that the result is accurate to the 11 significant figures shown. While the mode can be located by a supercell method, such as the commercial RSoft BandSOLVE software in comparable time, it is not possible for it to achieve nearly the same accuracy. See our earlier paper (Wilcox et al[14]) for a more comprehensive discussion of these matters.

Finally, we present a fully three-dimensional example for the mode of a photonic crystal fibre having a large core which is formed by removing three holes arranged in a triangular pattern (Fig. 7(a)). The bulk structure comprises a hexagonal lattice of air holes of radius $a/d = 0.12$ in a background of refractive index $n_e = 1.45$. Figs 7(b) and (c) respectively display field plots for the axial components of the electric and magnetic fields of the fundamental mode at a normalized frequency of $d/\lambda = 7.5188$, while Fig. 8 plots the dispersion curve of the fundamental mode of the PCF.

IV. DISCUSSION AND CONCLUSION

Though the FSS method was developed specifically to deal with modes near cut-off, the method was recently used in our group in a different context, namely in work on MOFs with high refractive index inclusions. These fibres, which guide light by the Anti-Resonant Reflective Optical Waveguide (ARROW) mechanism, may have many modes, some of which are “bound” (in that they decay evanescently in the microstructured cladding), and others that can propagate in this region. Though for a sufficiently thick cladding the former have much lower losses than the latter, in practice it may be difficult to classify a mode if the cladding is thin, even if the mode is not close to cut off. This is especially so when the external boundary of the microstructured cladding acts as a reflector, leading to a modest degree of confinement. In this instance, the use of the FSS allowed us to solve the problem for an infinite cladding, allowing us to classify the mode easily and unambiguously.

In conclusion, we have discussed a major extension of the Fictitious Source Superposition method so that it can deal with extended defects, rather than just simple point defects. In this extension of the theory the advantages of the original treatment remain: it allows for the modeling of structures with a genuinely infinite cladding, making the use of a supercell unnecessary. We achieve this by starting from a truly periodic, and hence infinite system, and inserting fictitious
sources in the inclusions in order to change the properties of a finite number of them. Though here the fictitious sources were used to *remove* some inclusions completely, it is equally possible to change the properties of these inclusions more generally, for example changing their refractive index, or radius.

APPENDIX

Recurrence Relations for Reflection and Transmission Scattering Matrices

The reflection and transmission scattering matrices of blocks of grating layers are computed by recurrence relations. We denote by \( R_{l,n} \) and \( R'_{l,n} \) the reflection scattering matrices of a block of layers \( l,l+1,...,n \) for incidence from above and below respectively, with a corresponding definition for the transmission matrices. We also introduce reflection matrices of each grating \( R_i \) and \( R'_i \) from above and below, and the corresponding transmission matrix forms \( T_i \) and \( T'_i \).

For the uniform structure that we consider here, we have \( R_{l,n} = R \), \( R'_{l,n} = R' \), \( T_i = T \) and \( T'_i = T' \) for all \( l \).

For incidence from above, it is convenient to compute the reflection and transmission matrices of a block of layers by backward recursion:

\[
R_{l-1,n} = R + T'_i R_{l-1,n} (I - R'_i R_{l-1,n})^{-1} T_{l-1},
\]

\[
T_{l-1,n} = T_i (I - R'_i R_{l-1,n})^{-1} T_{l-1}.
\]

Correspondingly, for incidence from below, it is preferable to compute these by forward recursion:

\[
R'_{l,n} = R'_i + T_i R'_{l,n} (I - R_{l,n} R'_i)^{-1} T'_i,
\]

\[
T'_{l,n} = T_{l,n} (I - R_{l,n} R'_i)^{-1} T'_i.
\]

Fictitious Source Operator Relations

Here, we derive expressions for the operators \( Q^+_{l,n,p} \) and \( Q^-_{l,n,p} \) which respectively yield coefficients in the upward and downward going plane wave expansions immediately above and below the block of layers \( l,l+1,...,n \), caused by a grating containing embedded sources \( q_p \) at layer \( p \).

We do not consider any external excitation—the only source in the system is the layer of embedded fictitious sources \( q_p \).

We then follow the propagation of the fields according to the equations

\[
g^+_l = Q^+_{l,p} q_p + T^-_l g^+_p, \quad g^+_p = \mathbf{R}_{p+1,n} g^+_{p+1},
\]

\[
g^-_l = R'_l g^+_{p+1} + Q^-_{l,p} q_p, \quad g^-_{p+1} = Q^-_{l,n,p} q_p,
\]

and by solving these, we may infer \( Q^+_{l,n,p} \) from the definition \( g^+_l = Q^+_{l,n,p} q_p \) and \( Q^-_{l,n,p} \) from Eq. (48). Thus,

\[
Q^+_{l,n,p} = Q^+_{l,p} + T'_l R_{p+1,n} (I - R'_i R_{p+1,n})^{-1} Q^-_{l,p}, \quad Q^-_{l,n,p} = T_{p+1,n} (I - R_{l,p} R'_{p+1,n})^{-1} Q^+_{l,n,p},
\]

with

\[
Q^+_{l,n,p} = T'_l (I - R_{l,p} R'_{l+1,n})^{-1} Q^-_l,
\]

\[
Q^-_{l,n,p} = T_p (I - R_{l+1,p} R'_p)^{-1} R'_p Q^+_p,
\]

which may be derived with a similar analysis.

ACKNOWLEDGMENT

This work was produced with the assistance of the Australian Research Council under its Centres of Excellence Program. The authors thank Paul Steinvurzel, Dr Boris Kuhlmey and Dr Chris Poulton for useful discussions.

REFERENCES


