Appendix A

Plane wave method

The plane wave method (PWM) for the calculation of the band structure of PCs is presented in this appendix.

First, the general formalism of this method in briefly introduced. The expansion of the inverse dielectric function has been used for all calculations instead the expansion of the dielectric function itself, since better convergence is obtained in this way [55]. The case of a one dimensional periodic arrangement is discussed for illustrative purposes and to introduce the notation used thereafter. Successively, the formalism of the PWM for two dimensional models periodic along orthogonal directions is presented. For rectangular elements aligned with these orthogonal directions, the use of plane wave basis functions collinear with the lattice vectors is straightforward and yields accurate results, as in the case of lamellar gratings discussed in section 1.5.2. The two-dimensional PWM has been employed in the study of rectangular and centred rectangular structures discussed in chapter 2 and consequently, the formalism is treated in relation to the applications.

A.1 Plane wave method

To find the solution of equation 2.1 for a distribution of index of refraction periodic in three dimensions , *i.e.* $\varepsilon(\vec{r}+\vec{R}) = \varepsilon(\vec{r})$ with $\vec{R} = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$, $\{\vec{a}_j\}_j$ the set of lattice vectors and $\{l_j\}_j$ sets of integers, one *Fourier*-expands the inverse dielectric function

$$\frac{1}{\varepsilon(\vec{r})} = \sum_{\vec{G}} \eta_{\vec{G}} e^{i\vec{G}\vec{r}}, \qquad \eta_{\vec{G}} = \frac{1}{\mu(\Omega)} \int_\Omega \frac{1}{\varepsilon(\vec{r})} e^{-i\vec{G}\vec{r}} d\vec{r},$$

with $\vec{G} = l_1\vec{b}_1 + l_2\vec{b}_2 + l_3\vec{b}_3$ and $\left\{\vec{b}_j \middle| \vec{a}_i\vec{b}_j = 2\pi\delta_{ij}\right\}$ the set of basis vectors of the reciprocal lattice, Ω the primitive cell and $\mu(\Omega)$ its volume.

As for the last example in section 2.1, *Bloch* theorem is applied to the solutions

$$\vec{H}_{\vec{k}}(\vec{r},\omega) = \vec{u}_{\vec{k}}(\vec{r},\omega) e^{i\vec{k}\vec{r}}, \qquad \vec{u}_{\vec{k}}(\vec{r}+\vec{R},\omega) = \vec{u}_{\vec{k}}(\vec{r},\omega).$$

Since the functions $\vec{u}_{\vec{k}}$ are periodic they can equally be *Fourier*-expanded

$$\vec{u}_{\vec{k}}(\vec{r},\omega) = \sum_{\vec{G}'} \vec{u}_{\vec{k},\vec{G}'} e^{i\vec{G}'\vec{r}}, \qquad \vec{u}_{\vec{k},\vec{G}'} = \frac{1}{\mu(\Omega)} \int_\Omega \vec{u}_{\vec{k}}(\vec{r},\omega) e^{-i\vec{G}'\vec{r}} d\vec{r}.$$

Substituting the two expansions in equation (2.1) one obtains

$$\sum_{\vec{G}'} \sum_{\vec{G}''} \eta_{(\vec{G}'-\vec{G}'')} \left(\left(\left(\vec{G}'' + \vec{k}\right) \cdot \vec{u}_{\vec{k},\vec{G}'} \right) \left(\vec{G}' + \vec{k}\right) - \left(\left(\vec{G}'' + \vec{k}\right) \cdot \left(\vec{G}' + \vec{k}\right) \right) \vec{u}_{\vec{k},\vec{G}'} \right) \times$$
$$\times e^{i\left(\vec{G}''+\vec{k}\right)\vec{r}} + \frac{\omega^2}{\mathrm{c}^2} \sum_{\vec{G}''} \vec{u}_{\vec{k},\vec{G}''} e^{i\vec{G}''\vec{r}} = 0,$$

where $\vec{G}'' = \vec{G} + \vec{G}'$, which is valid for all locations $\vec{r}$ and therefore reduces to

$$\sum_{\vec{G}'} \eta_{(\vec{G}'-\vec{G}'')} \left(\left(\left(\vec{G}'' + \vec{k}\right) \cdot \vec{u}_{\vec{k},\vec{G}'} \right) \left(G'_j + k_j\right) - \left(\left(\vec{G}'' + \vec{k}\right) \cdot \left(\vec{G}' + \vec{k}\right) \right) \right) u_{\vec{k},\vec{G}',j} +$$
$$+ \frac{\omega^2}{\mathrm{c}^2} u_{\vec{k},\vec{G}'',j} = 0, \qquad \text{(A.1)}$$

with $j = 1, 2, 3$.

A matrix representation of the last expression will be given in section A.2 for the simpler one-dimensional case.

A.2 Plane wave method in one dimension

For a one-dimensional system, symmetric with respect to discrete translation in one direction, say $\hat{z}$, and invariant with respect to continuous translation in all directions perpendicular to $\hat{z}$, it is sufficient to consider the following reciprocal lattice vectors in the treatment of section A.1:

$$\vec{G'} = \left(0, 0, l'\frac{2\pi}{a}\right)^T, \qquad \vec{G''} = \left(0, 0, l''\frac{2\pi}{a}\right)^T.$$

The lattice constant is a and l', l'' are integer numbers. To be able to compute numerically the expansions, a limit N is set such that $-N \leq l', l'' \leq N$.

To find the *Fourier* coefficients, the inverse dielectric constant is first rewritten as follows:

$$\frac{1}{\varepsilon(z)} = \frac{1}{\varepsilon_1} + g(z),$$

$$g(z) = \begin{cases} 0 & , \quad |z| > fa - R, \\ \dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 \varepsilon_2} & , \quad |z| \leq fa - R. \end{cases}$$

The function $g(z)$ describes a stepwise distribution of two materials with respective dielectric constants ε_1 and ε_2, and a filling fraction f of the first material in the period a. The pattern is repeated at each lattice "vector" $R = l'a$. The *Fourier* expansion of this function is

$$\frac{1}{\varepsilon(z)} = \sum_G \eta_G e^{iGz}, \qquad G = l\frac{2\pi}{a},$$

$$\eta_G = \frac{1}{a}\int_{z_0}^{z_0+a} \frac{1}{\varepsilon(z)} e^{-iGz} dz$$

$$= \begin{cases} \dfrac{1}{\varepsilon_1} + f\dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1\varepsilon_2} & , \quad l = 0 \\ f\dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1\varepsilon_2}\dfrac{\sin(f\pi l)}{f\pi l} & , \quad l \neq 0 \end{cases}$$

TE polarisation

With TE polarisations the magnetic field oscillates in the plane of incidence, which is chosen to be xz and therefore one sets

$$\vec{k} = (k_x, 0, k_z)^T, \qquad \vec{u}_{\vec{k},l} = \left(u_{\vec{k},l,x}, 0, u_{\vec{k},l,z}\right)^T.$$

One can now substitute these expressions in the system of equations A.1 and the following $2(2N+1)$-dimensional eigenvalue problem is obtained:

$$M \begin{pmatrix} u_{\vec{k},-N,x} \\ u_{\vec{k},-N,z} \\ u_{\vec{k},-N+1,x} \\ \vdots \\ u_{\vec{k},N-1,z} \\ u_{\vec{k},N,x} \\ u_{\vec{k},N,z} \end{pmatrix} = -\frac{\omega^2}{\mathrm{c}^2} \begin{pmatrix} u_{\vec{k},-N,x} \\ u_{\vec{k},-N,z} \\ u_{\vec{k},-N+1,x} \\ \vdots \\ u_{\vec{k},N-1,z} \\ u_{\vec{k},N,x} \\ u_{\vec{k},N,z} \end{pmatrix},$$

$$M = \begin{pmatrix} M_{-N,-N} & M_{-N,-N+1} & \cdots \\ \vdots & \ddots & \\ & & M_{N,N} \end{pmatrix},$$

$$M_{l,l'} = \begin{pmatrix} -\eta_{l-l'}\left(l\frac{2\pi}{a} + k_z\right)\left(l'\frac{2\pi}{a} + k_z\right) & -\eta_{l-l'}\left(l\frac{2\pi}{a} + k_z\right)k_x \\ -\eta_{l-l'}k_x\left(l'\frac{2\pi}{a} + k_z\right) & -\eta_{l-l'}k_x^2 \end{pmatrix}.$$

TM polarisation

With TM polarisations the magnetic field is normal to the plane of incidence and therefore one sets

$$\vec{k} = (k_x, 0, k_z)^T, \qquad \vec{u}_{\vec{k},l} = \left(0, u_{\vec{k},l,y}, 0\right)^T.$$

In this case, from equation (A.1) a $(2N+1)$-dimensional problem is obtained

$$M \begin{pmatrix} u_{\vec{k},-N,y} \\ \vdots \\ u_{\vec{k},N,y} \end{pmatrix} = -\frac{\omega^2}{\mathrm{c}^2} \begin{pmatrix} u_{\vec{k},-N,y} \\ \vdots \\ u_{\vec{k},N,y} \end{pmatrix},$$

$$M = \begin{pmatrix} \ddots & \vdots & \\ \cdots & -\eta_{l-l'} k_x^2 \left(l\frac{2\pi}{a} + k_y\right)\left(l'\frac{2\pi}{a} + k_y\right) & \cdots \\ & \vdots & \ddots \end{pmatrix}.$$

A.3 Plane wave method in two dimensions

For a periodic arrangement of orthogonal elements aligned with and placed in an orthogonal lattice, it is straightforward to formulate the system of equations A.1 using a basis of orthogonal plane waves.

For a two-dimensional system, symmetric with respect to discrete translations in two orthogonal direction, say $\hat{x}$ and $\hat{z}$, and invariant with respect to continuous translation in $\hat{y}$ direction, it is sufficient to consider the following reciprocal lattice vectors in the treatment of section A.1:

$$\vec{G}_x = \begin{pmatrix} l_x \frac{2\pi}{a_x} \\ 0 \\ 0 \end{pmatrix}, \quad \vec{G}'_x = \begin{pmatrix} l'_x \frac{2\pi}{a_x} \\ 0 \\ 0 \end{pmatrix}, \quad \vec{G}_z = \begin{pmatrix} 0 \\ 0 \\ l_z \frac{2\pi}{a_z} \end{pmatrix}, \quad \vec{G}'_z = \begin{pmatrix} 0 \\ 0 \\ l'_z \frac{2\pi}{a_z} \end{pmatrix}.$$

The lattice constants are a_x and a_z, and l_x, l'_x, l_z, l'_z are integer numbers. To be able to compute numerically the expansions, a limit N is set, such that $-N \leq l_x, l'_x, l_z, l'_z \leq N$.

The derivation of the terms of the *Fourier* expansion of the inverse dielectric function η_{l_x,l_z} is discussed below for the cases of a rectangular lattice of rectangular elements and a centred rectangular lattice of rectangular elements.

Once the terms of the *Fourier* expansion of the inverse dielectric function are found, the system of equations A.1 can be expressed in matrix form.

With TE polarisations the magnetic field oscillates in the plane of incidence, which is chosen to be xz and therefore one sets

$$\vec{k} = (k_x, 0, k_z)^T, \qquad \vec{u}_{\vec{k},l_x,l_z} = \left(u_{\vec{k},l_x,l_z,x}, 0, u_{\vec{k},l_x,l_z,z}\right)^T.$$

One can now substitute these expressions in the system of equations A.1 and the following $2(2N+1)^2$-dimensional eigenvalue problem is obtained:

$$M\begin{pmatrix} u_{\vec{k},-N,-N,x} \\ u_{\vec{k},-N,-N,z} \\ u_{\vec{k},-N+1,-N,x} \\ \vdots \\ u_{\vec{k},N-1,N,z} \\ u_{\vec{k},N,N,x} \\ u_{\vec{k},N,N,z} \end{pmatrix} = -\frac{\omega^2}{\mathrm{c}^2}\begin{pmatrix} u_{\vec{k},-N,-N,x} \\ u_{\vec{k},-N,-N,z} \\ u_{\vec{k},-N+1,-N,x} \\ \vdots \\ u_{\vec{k},N-1,N,z} \\ u_{\vec{k},N,N,x} \\ u_{\vec{k},N,N,z} \end{pmatrix},$$

$$M = \begin{pmatrix} M_{-2N(N+1),-2N(N+1)} & M_{-2N(N+1),-2N(N+1)+1} & \cdots \\ \vdots & \ddots & \\ & & M_{2N(N+1),2N(N+1)} \end{pmatrix},$$

$$M_{(2N+1)l_x+l_z,(2N+1)l'_x+l'_z} =$$

$$= \eta_{l_x-l'_x,l_z-l'_z}\begin{pmatrix} -\left(l'_z\frac{2\pi}{a_z}+k_z\right)\left(l_z\frac{2\pi}{a_z}+k_z\right) & \left(l'_z\frac{2\pi}{a_z}+k_z\right)\left(l_x\frac{2\pi}{a_x}+k_x\right) \\ \left(l'_x\frac{2\pi}{a_x}+k_x\right)\left(l_z\frac{2\pi}{a_z}+k_z\right) & -\left(l'_x\frac{2\pi}{a_x}+k_x\right)\left(l_x\frac{2\pi}{a_x}+k_x\right) \end{pmatrix}.$$

With TM polarisations the magnetic field is normal to the plane of incidence and therefore one sets

$$\vec{k} = (k_x, 0, k_z)^T, \qquad \vec{u}_{\vec{k},l_x,l_z} = \left(0, u_{\vec{k},l_x,l_z,y}, 0\right)^T.$$

In this case, from equation (A.1) a $(2N+1)^2$-dimensional problem is obtained

$$M\begin{pmatrix} u_{\vec{k},-N,-N,y} \\ u_{\vec{k},-N+1,-N,y} \\ \vdots \\ u_{\vec{k},N-1,N,y} \\ u_{\vec{k},N,N,y} \end{pmatrix} = -\frac{\omega^2}{\mathrm{c}^2}\begin{pmatrix} u_{\vec{k},-N,-N,y} \\ u_{\vec{k},-N+1,-N,y} \\ \vdots \\ u_{\vec{k},N-1,N,y} \\ u_{\vec{k},N,N,y} \end{pmatrix},$$

$$M_{(2N+1)l_x+l_z,(2N+1)l'_x+l'_z} =$$

$$= -\eta_{l_x-l'_x,l_z-l'_z}\left(\left(l'_x\frac{2\pi}{a_x}+k_x\right)\left(l_x\frac{2\pi}{a_x}+k_x\right)+\left(l'_z\frac{2\pi}{a_z}+k_z\right)\left(l_z\frac{2\pi}{a_z}+k_z\right)\right).$$

A.3.1 The rectangular lattice

To find the *Fourier* coefficients, the inverse dielectric constant is first rewritten as follows:

$$\frac{1}{\varepsilon(x,z)} = \frac{1}{\varepsilon_1} + g_x(x)g_z(z),$$

$$g_x(x) = \begin{cases} 0 & , \quad |x| > f_x a_x - l_x a_x, \\ \dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 \varepsilon_2} & , \quad |x| \leq f_x a_x - l_x a_x. \end{cases}$$

$$g_z(z) = \begin{cases} 0 & , \quad |z| > f_z a_z - l_z a_z, \\ \dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 \varepsilon_2} & , \quad |z| \leq f_z a_z - l_z a_z. \end{cases}$$

The functions $g_x(x), g_z(z)$ are top-hat functions. The dielectric function corresponds to a rectangular element of dielectric constant ε_2 in each unit cell with a background dielectric constants ε_1. The linear filling fractions of the rectangular element are f_x, f_z in x, z direction, respectively. The unit cell is repeated in a rectangular lattice with lattice constants a_x, a_z, which is indicated above by the integers l_x, l_z.

The *Fourier* coefficients of the inverse dielectric function are given by:

$$\eta_{l_x,l_z} = \begin{cases} \dfrac{1}{\varepsilon_1} + f_x f_z \dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 \varepsilon_2} & , \quad l_x \text{and} l_z = 0 \\ f_x f_z \dfrac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 \varepsilon_2} \dfrac{\sin(f_x \pi l_x)}{f_x \pi l_x} \dfrac{\sin(f_z \pi l_z)}{f_z \pi l_z} & , \quad l_x \text{or} l_z \neq 0. \end{cases}$$

Reconstruction of the dielectric function using the coefficients in the *Fourier* expansion yields the result shown in figure A.1. The filling fractions were $f_x = 0.6$ and $f_z = 0.5$.

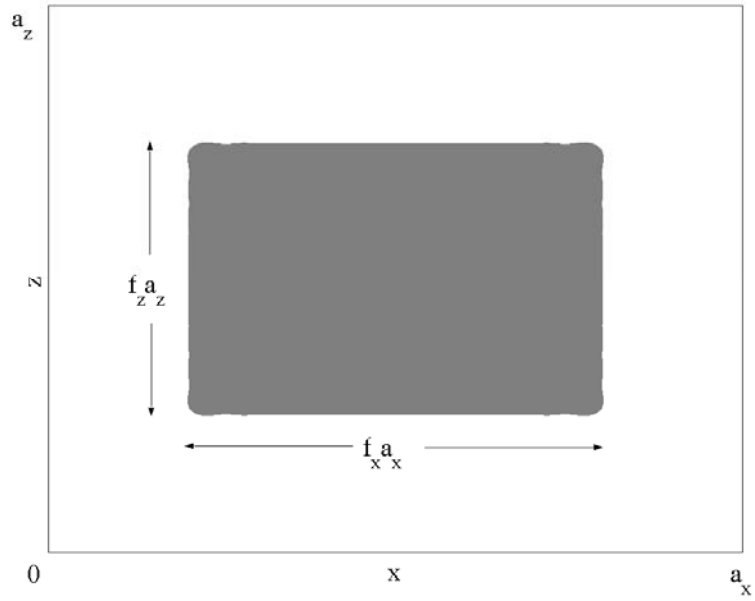

Figure A.1: Reconstruction of the dielectric function of the rectangular lattice.

A.3.2 The centred rectangular lattice

The centred rectangular lattice has two elements (atoms) per rectangular cell. The second element is shifted by half a lattice constant along each lattice vector with respect to the first one.

The *Fourier* coefficients of the inverse dielectric function are obtained via integration of the function over the rectangular cell. For non-overlapping elements however, the superposition of the coefficients of each element in the rectangular cell also gives the correct result, when considering the phase shift between expansion terms of different elements in the reciprocal space. For the sake of brevity this method is presented here. The coefficients are as follows:

$$\eta'_{l_x,l_z} = \eta_{l_x,l_z} \cos(l_x\pi + l_z\pi) - \delta_{l_x,l_z} \frac{1}{\varepsilon_2},$$

where η_{l_x,l_z} are the coefficients of the rectangular lattice presented above and δ_{l_x,l_z} is *Kronecker*'s symbol. The cos-factor expresses the phase shift between

the different elements mentioned above and the last term subtracts the excess background inverse dielectric function resulting from the superposition.

Reconstruction of the dielectric function using the coefficients in the *Fourier* expansion yields the result shown in figure A.2. The filling fractions were $f_x = 0.3$ and $f_z = 0.5$.

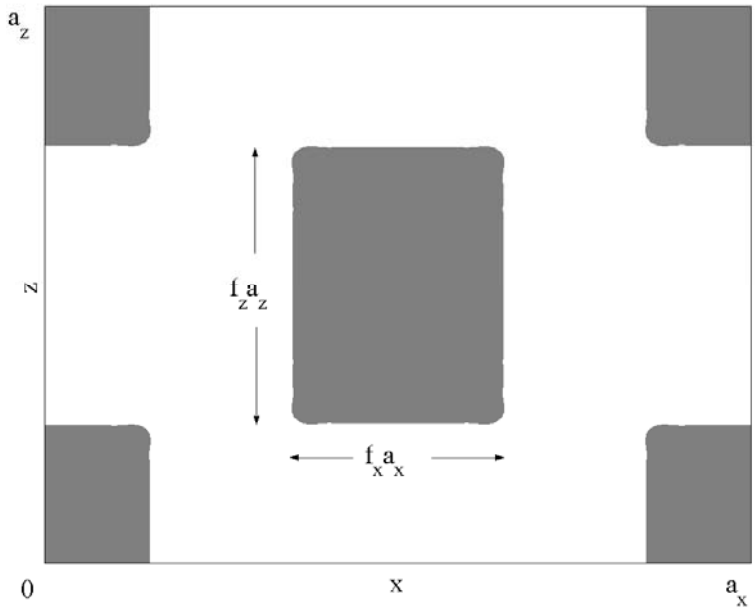

Figure A.2: Reconstruction of the dielectric function of the rectangular centred lattice.