APPLICATION OF FINITE ELEMENT METHODS TO PHOTONIC CRYSTAL MODELLING.

#### **B2: FINITE ELEMENT**

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#### ABSTRACT

Photonic Crystals (PCs) are materials with periodically modulated dielectric constant, through which certain frequencies of electromagnetic radiation cannot propagate; the luminary analogues of semiconductors [1].

The modes admitted by photonic crystals can be investigated effectively using the finite element method with the assistance of the Bloch-Floquet theorem, by considering a unit cell of the material and imposing periodic boundary conditions. Along with the Dirichlet and metric matrices, a third type of elemental matrix emerges.

The types of results that are of interest to photonic crystal manufacturers are introduced and presented; in this context, the benefits of using subspace iteration techniques to solve the eigensystems are discussed.

# INTRODUCTION

PCs offer enormous potential in the development of highly efficient narrow band (tuneable) lasers, integrated optical computing and high-speed optical communication networks, particularly in the production of purely optical circuits for Dense Wavelength Division Multiplexing [2].

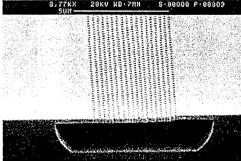


Figure l Bridge waveguide structure (pitch=300nm) courtesy of Martin Charlton, Southampton Microelectronics Research Group.

Success in the fabrication of such materials with band gaps in optical frequencies has been limited mainly to ones where the periodicity is restricted to two dimensions. The in-plane propagation modes of such materials can be investigated effectively using two-dimensional Lagrangian finite elements [3], providing a considerable reduction in complexity with respect to the three-dimensional curl-conforming treatment that would otherwise be necessary.

#### 2D SCALAR SPECTRAL PROBLEM

When the PC structure is invariant in one dimension Maxwell's equations can be split into two scalar spectral problems dealing with the transverse electric polarisation (TE mode) and the transverse magnetic polarisation (TM mode) respectively:

TE Mode: 
$$-\nabla \cdot \frac{1}{\varepsilon(\mathbf{x})} \nabla \psi = \lambda \psi$$
 (1)

TM Mode: 
$$\frac{1}{\varepsilon(\mathbf{x})} \nabla^2 \psi = \lambda \psi, \qquad (2)$$

where  $\varepsilon(\mathbf{x})$  is the material dielectric constant at spatial position  $\mathbf{x}$ ,  $\lambda$  is the frequency and  $\psi$  is the scalar field intensity.

### MODELLING PERIODIC STRUCTURES

The periodic structure of the PC allows the application of the Floquet-Bloch theory in which a crystal of infinite extent can be modelled using a unit cell with periodic boundary conditions [4]. The eigenmodes then have the form:

$$\psi = e^{i\mathbf{k}\cdot\mathbf{x}}u(\mathbf{x}), \qquad (3)$$

where k is the Bloch-quasimomentum vector and u(x) is the value of the eigenfunctions at spatial position x. The resulting change in the gradient operator:

$$\nabla \rightarrow \nabla + i\mathbf{k}$$
, (4)

gives rise to an eigensystem of the form:

$$(S + \mathbf{k} \cdot \mathbf{P} + \mathbf{k}^2 T) \psi = \lambda T \psi, \tag{5}$$

or,

$$A(\mathbf{k})\psi = \lambda B\psi \tag{6}$$

where S and T are the familiar Dirichlet and metric matrices and P is a vector of matrices assembled from elemental matrices that are defined in terms of the basis functions,  $\alpha_i$  as:

$$\mathbf{P}_{ij}^{e} = \int \alpha_{i} \nabla \alpha_{j} - \alpha_{j} \nabla \alpha_{i} \ d\Omega \tag{7}$$

The optical characteristics of a crystal can be

represented as a dispersion relation or density of states diagram. This is a histogram of the density of eigenstates against the normalised frequency. This is a useful data representation as it clearly shows any bandgaps (frequency regions where the frequency density drops to zero). Such a gap can be seen in Figure 2 for a normalised frequency,  $\omega a/2\pi c$  of 0.44 and 0.48.

We have found good agreement between twodimensional simulations and experimental investigation of photonic crystal structures that have been fabricated to date.

Both dispersion relations and density of states diagrams are produced by repeatedly solving the eigenvalue problem at a number of points in k-space taken from the first reduced Brillouin zone.

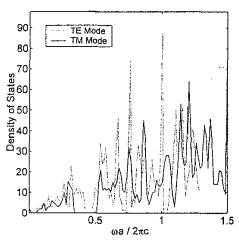


Figure 2 Density of states diagram for a triangular lattice of air rods in a substrate with a dielectric constant of 12.25, filling fraction = 80%. The TE and TM modes are represented by the dashed and solid lines respectively. A complete band gap is observed between the normalised frequencies,  $\alpha \alpha/2\pi c = 0.44$  and 0.48.

Using sub-space iterative techniques [5] to solve the eigensystem allows several problem specific optimisations to be made. Most importantly, eigensystems corresponding to similar k-vectors differ only slightly, hence using the previous solution as a starting point for the subsequent sub-space search significantly reduces the number of iterations required to converge. In addition, sub-space iteration does not compute the full eigenvalue spectrum allowing one to concentrate on the eigenvalues of interest; in the case of photonic crystals typically a relatively small number of the lowest ones.

It is interesting to investigate how the crystal geometry affects its optical properties, for example, in a triangular lattice of air rods in GaAs how does the rod radius affect the position and size of the band gaps. Plotting a gap map displays the relationship between crystal

structure and the resulting band gaps.

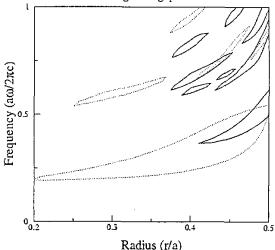


Figure 3 Gap-map for a triangular lattice plotting the band-gap frequency ranges for both the TE and TM modes against the rod radius. The data is computed for air rods in GaAs. A complete band gap appears for rod radius to lattice constant ratio of 0.42.

## CONCLUSIONS

Two-dimensional FEM analysis of two-dimensional photonic crystals offers satisfactory agreement with experimental results whilst providing substantial savings in terms of memory and computational costs with respect to fully three dimensional vector FEM implementations.

This allows a wide range of crystal structures to be simulated efficiently thus avoiding the necessity of expensive silicon fabrication during the crystal design phase.

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