Validation Report

Name of Report	A comparison of band diagrams calculated by the CRYSTALWAVE BandSolver with published data.
Performance Date	8th January 2004
Performed By	Lorenzo Bolla, Tom Davies
Product Name	BandSolver
Product Version & Compile Date	
References	"*Photonic Crystals: the road from theory to practice*", Steven G. Johnson, John D. Joannopoulos, Kluwer Academic Press, 2002 "*Block-iterative frequency-domain methods for Maxwell's equations in a planewave basis*", Steven G. Johnson, J. D. Joannopoulos*, Optics Express* **8**, no. 3, 173-190 (2001) http://ab-initio.mit.edu/mpb/doc/analysis-tutorial.html

A Comparison of band diagrams calculated by the CRYSTALWAVE Band Solver option with published data.

1. Report Summary

The aim of this study was to compare the band diagrams calculated by the CRYSTALWAVE Band Solver option with the results:

a) Obtained using the software MPB, developed by Steven G. Johnson at MIT, as published in [1] and [3].
b) Obtained using the software CRYSTALWAVE, developed by Photon Design.

1.1. Summary

The validation tests have been performed on both bi and tri dimensional photonic crystals structures. The first four tests are performed in 2D. Tests 5 and 6 are performed in 3D.

Test 1	Triangular lattice of rods in air	R = 0.2 ε_{sub} = 1.0 ε_{cyl} = 12.0	Ref. 3
Test 2	Square lattice of rods in air	R = 0.2 ε_{sub} = 1.0 ε_{cyl} = 12.0	Ref. 1
Test 3	Triangular lattice of holes in dielectric	R = 0.2 ε_{sub} = 12.0 ε_{cyl} = 1.0	Ref. 1
Test 4	Line defect in a triangular lattice of holes air	R = 0.35 ε_{sub} = 10.24 ε_{cyl} = 1.0	CrystalWave

Table 1: 2D structures

Test 5	Planar photonic waveguide (square lattice)	Ref. 1
Test 6	Planar photonic waveguide (triangular lattice)	Ref. 1

Table 2: 3D structures

For all the band diagrams, where not explicitly specified, on the x axis we have the wave vectors (that is, in the reciprocal lattice space) and on the y axis the normalised frequency, defined by:

$$F = {fc}/{a} = {\omega c}/{2\pi a}$$

Error% is defined as:

$$Error\% = \frac{F_{BandSolver} - F_{reference}}{F_{BandSolver}} \cdot 100$$

Where *a* is the lattice constant.

1.2. Validation Tests Results

1.2.1. Test 1

The structure considered in this test is a triangular lattice of dielectric rods in air.

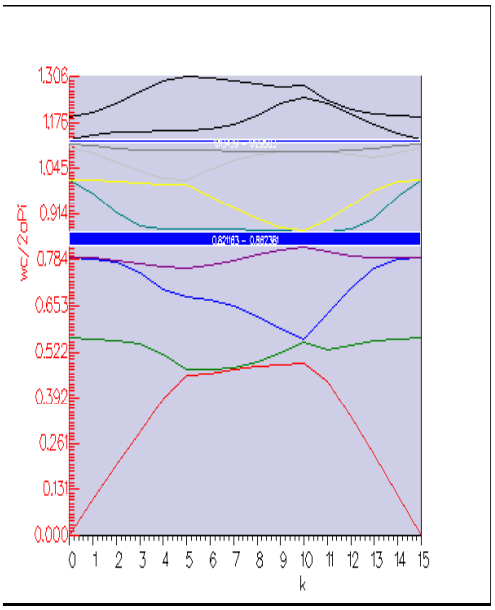
Lattice vectors: $R_1 = \left({\sqrt{3}}/{2}, -{1}/{2} \right), R_2 = \left({\sqrt{3}}/{2}, {1}/{2} \right)$

Radius of the cylinders: $R = 0.2a$

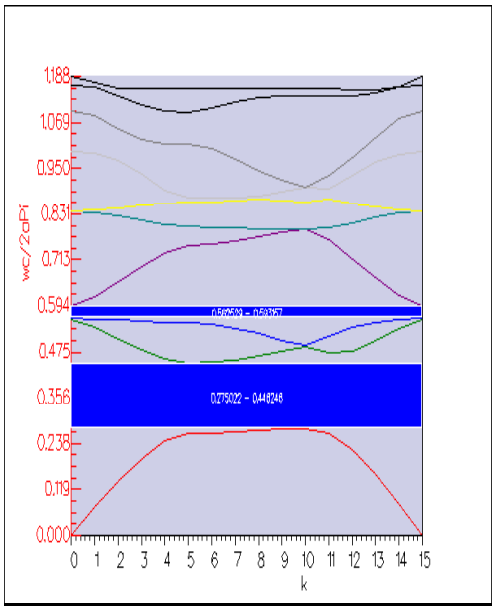
Refractive index of the cylinders: $\varepsilon_{cyl} = \sqrt{12}$

Refractive index of the substrate: $\varepsilon_{sub} = 1$

Reciprocal lattice points studied: Γ, M, K, Γ

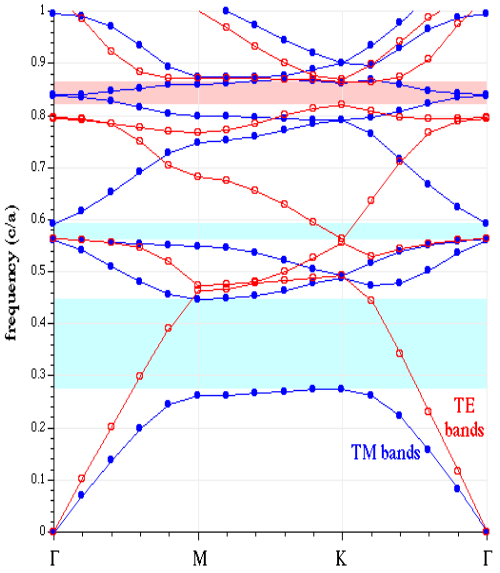


Test 1: TE band diagram

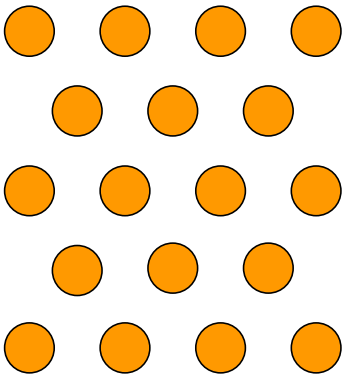


Test 1: TM band diagram

Figure 1



Test 1: Band diagram from Ref. 1



Test 1: triangular lattice

Figure 2

Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0
	M	0.461	0.460	-0.2
	K	0.490	0.490	0
2	Γ	0.560	0.565	0.9
	M	0.472	0.470	0.4
	K	0.556	0.550	1.1
3	Γ	0.789	0.790	-0.1
	M	0.680	0.68	0
	K	0.557	0.550	1.3

Table 3: TE polarization (using Band Solver with 64 plane waves)

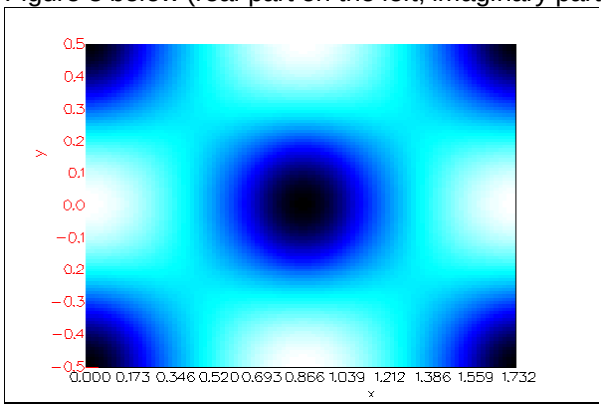
Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0
	M	0.262	0.260	+0.8
	K	0.274	0.275	-0.4
2	Γ	0.560	0.565	-0.9
	M	0.445	0.446	-0.2
	K	0.490	0.49	0
3	Γ	0.560	0.565	-0.9
	M	0.549	0.55	-0.2
	K	0.490	0.49	0

Table 4: TM polarization (using Band Solver with 64 plane waves)

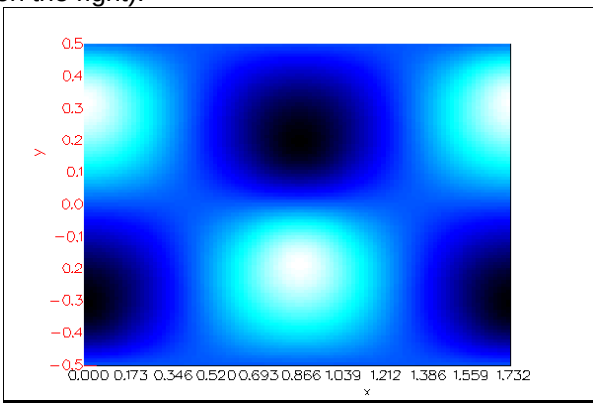
Note: Some of the values of the normalized frequency for the MPB diagram have been calculated graphically, if exact values were not available: therefore, the accuracy is not very high (no more than 0.01).

The comparison shows good agreement; all results are within 1%

As an example, the Bloch mode for the TM case at the reciprocal lattice point K, first band is shown in Figure 3 below (real part on the left, imaginary part on the right).



Test 1: Bloch mode @M point, first band (real)



Test 1: Bloch mode @M point, first band (imag)

Figure 3

1.2.2. Test 2

The structure considered in this test is a square lattice of dielectric rods in air.

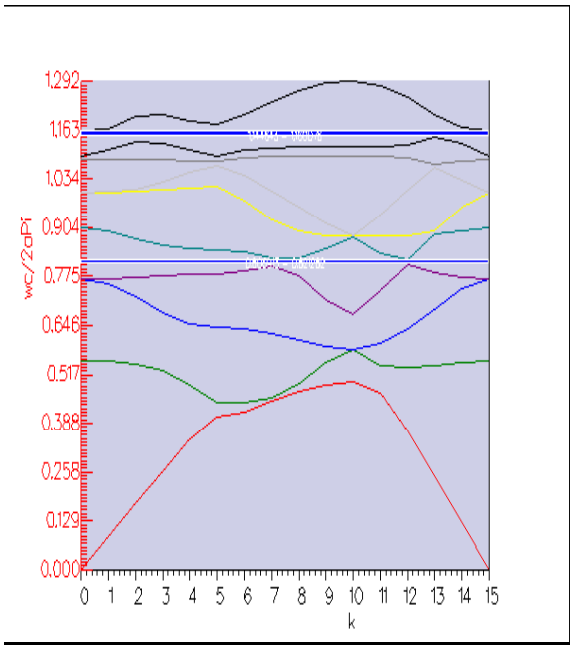
Lattice vectors: $R_1 = (1,0), R_2 = (0,1)$

Radius of the cylinders: $R = 0.2a$

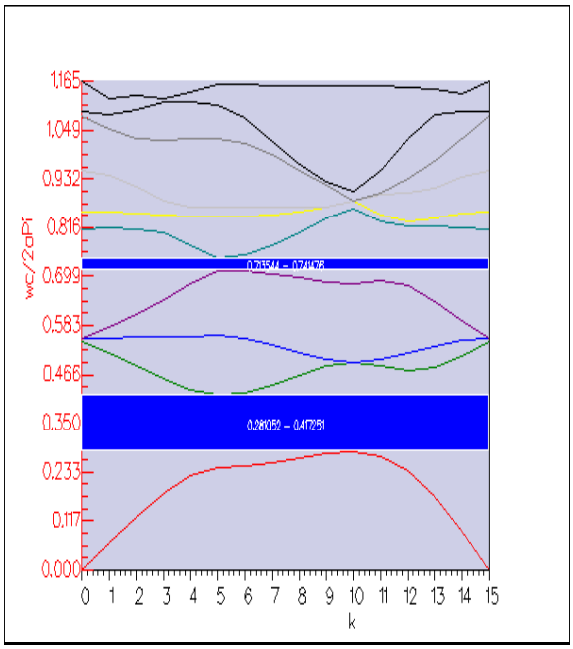
Refractive index of the cylinders: $\varepsilon_{cyl} = \sqrt{12}$

Refractive index of the substrate: $\varepsilon_{sub} = 1$

Reciprocal lattice points studied: Γ, X, M, Γ

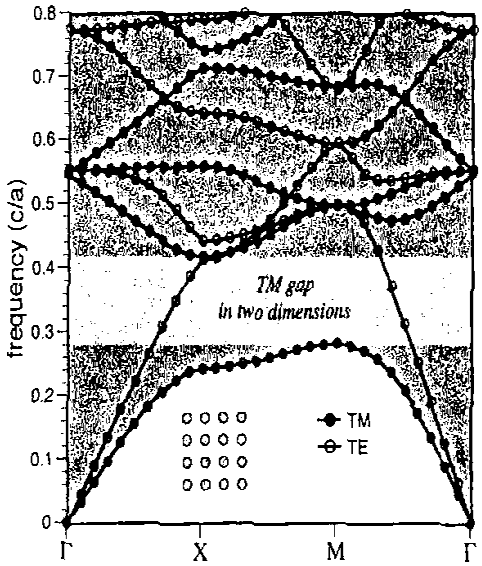


Test 2: TE band diagram

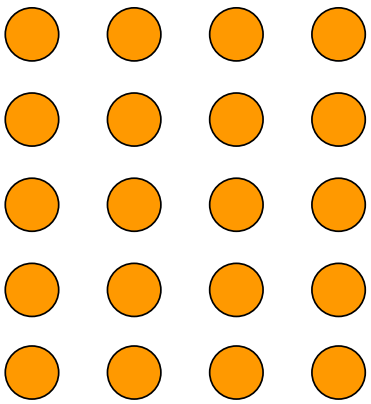


Test 2: TM band diagram

Figure 4



Test 2: Band diagram from Ref. 1



Test 2: square lattice

Figure 5

Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0.0
	X	0.408	0.42	-3.0
	M	0.496	0.50	-0.8
2	Γ	0.552	0.55	0.4
	X	0.441	0.44	0.2
	M	0.588	0.59	-0.3
3	Γ	0.768	0.77	-0.3
	X	0.640	0.64	0.0
	M	0.588	0.59	-0.3

Table 5: TE polarisation (using Band Solver with 64 plane waves)

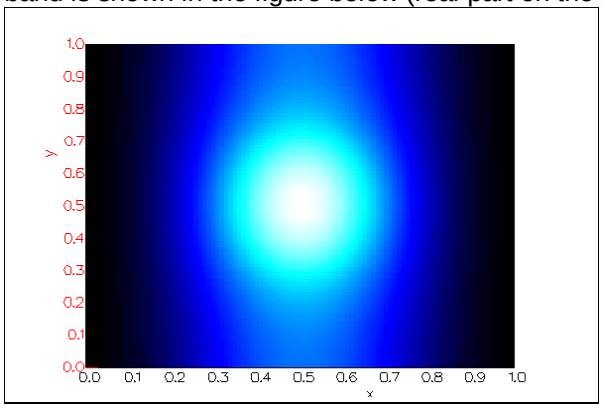
Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0.0
	X	0.242	0.240	0.8
	M	0.281	0.280	0.4
2	Γ	0.546	0.550	-0.7
	X	0.417	0.420	-0.7
	M	0.496	0.500	-0.8
3	Γ	0.551	0.550	0.2
	X	0.556	0.555	0.2
	M	0.496	0.500	-0.8

Table 6: TM polarisation (using Band Solver with 64 plane waves)

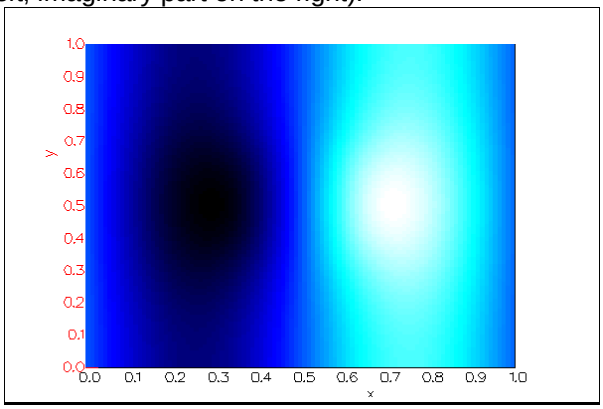
Note: The values of the normalized frequency for the MPB diagram have been calculated graphically: therefore, the accuracy is not very high (no more than 0.01).

The comparison shows an agreement within 1.0%.

As an example, the profile of the Bloch mode for the TM case at the reciprocal lattice point X, first band is shown in the figure below (real part on the left, imaginary part on the right).



Test 2: Bloch mode @X point, first band (real)



Test 2: Bloch mode @X point, first band (imag)

Figure 6

1.2.3. Test 3

The structure considered in this test is a triangular lattice of holes in a dielectric substrate.

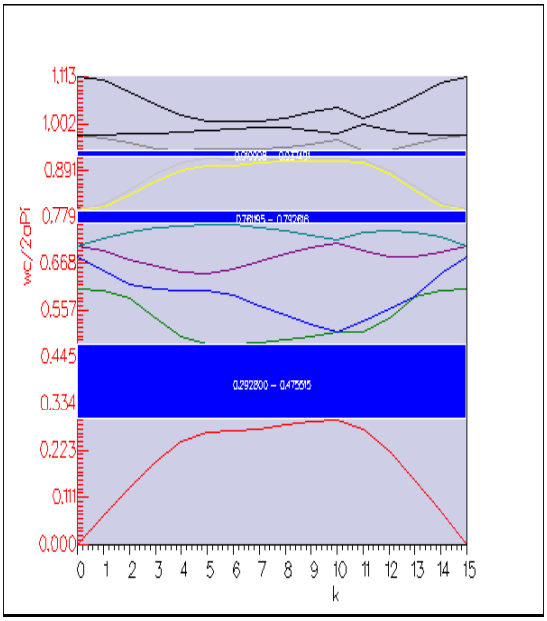
Lattice vectors: $R_1 = \left(\sqrt{3}/2, -1/2\right), R_2 = \left(\sqrt{3}/2, 1/2\right)$

Radius of the cylinders: $R = 0.45a$

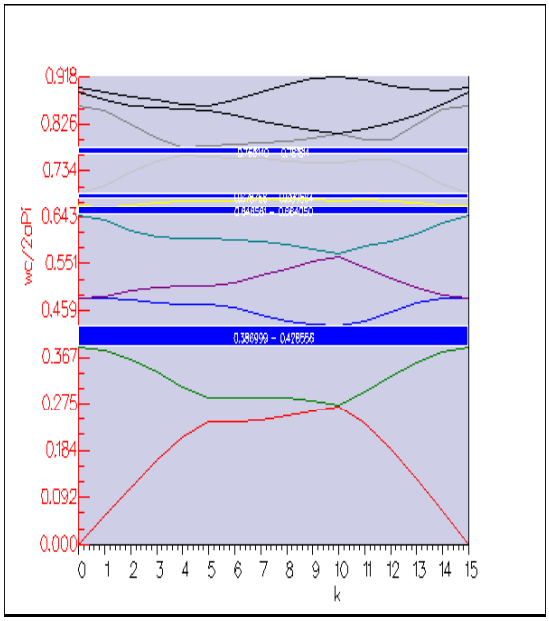
Refractive index of the cylinders: $\varepsilon_{sub} = 1$

Refractive index of the substrate: $\varepsilon_{dil} = \sqrt{12}$

Reciprocal lattice points studied: Γ, M, K, Γ

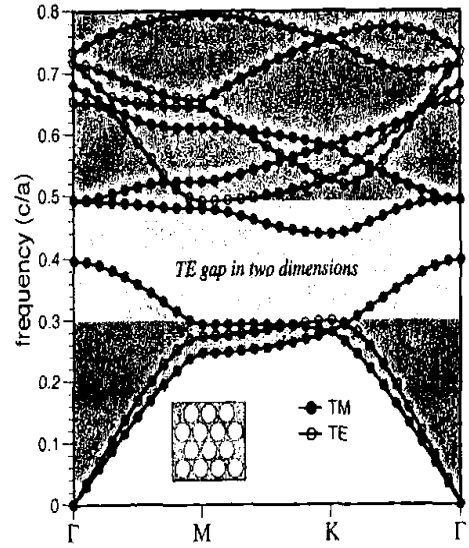


Test 3: TE band diagram

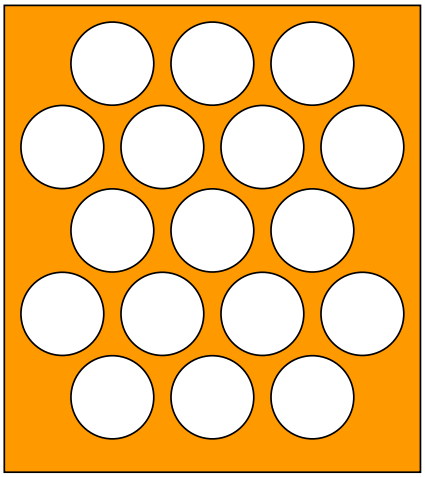


Test 3: TM band diagram

Figure 7



Test 3: Band diagram from Ref. 1



Test 3: triangular lattice

Figure 8

Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0.0
	M	0.275	0.28	-1.8
	K	0.300	0.29	3.3
2	Γ	0.656	0.64	2.4
	M	0.491	0.48	2.2
	K	0.525	0.52	1.0
3	Γ	0.713	0.71	0.4
	M	0.648	0.64	1.2
	K	0.526	0.54	2.7

Table 7: TE polarisation (with 64 plane waves in Band Solver)

Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0
	M	0.246	0.25	-1.6
	K	0.280	0.28	0.0
2	Γ	0.399	0.40	-0.25
	M	0.294	0.29	1.4
	K	0.280	0.28	0.0
3	Γ	0.492	0.49	0.41
	M	0.479	0.48	-0.2
	K	0.439	0.44	-0.2

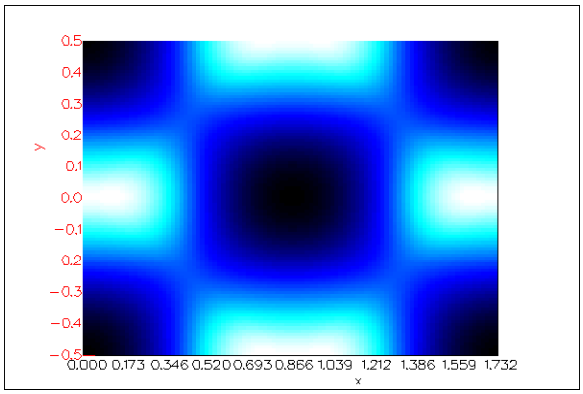
Table 8: TM polarisation (with 64 plane waves in Band Solver)

Note: The values of the normalized frequency for the MPB diagram have been calculated graphically: therefore, the accuracy is not very high (no more than 0.01).

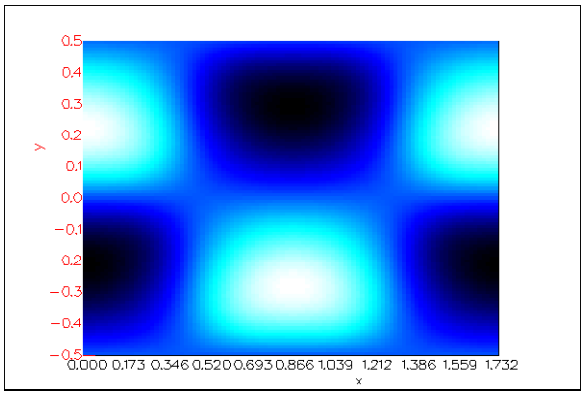
The comparison shows an agreement within 3.3%.

The comparison is not as good as in the two previous tests. This is probably due to the fact that we have used a greater number of plane waves as a basis set (64), compared to MPB (32). Also, the geometry of this problem is more challenging than in the previous examples: the radius of the cylinders is very large ($R = 0.45a$) and two adjacent cylinders almost touch. If the refractive index is not discretised well, then this results in a geometry that is substantially different, where the cylinders actually overlap.

As an example, the profile of the Bloch mode for the TM case at the reciprocal lattice point M, first band (real part on the left, imaginary part on the right).



Test 3: Bloch mode @M point, first band (real)



Test 3: Bloch mode @M point, first band (imag)

Figure 9

1.2.4. Test 4

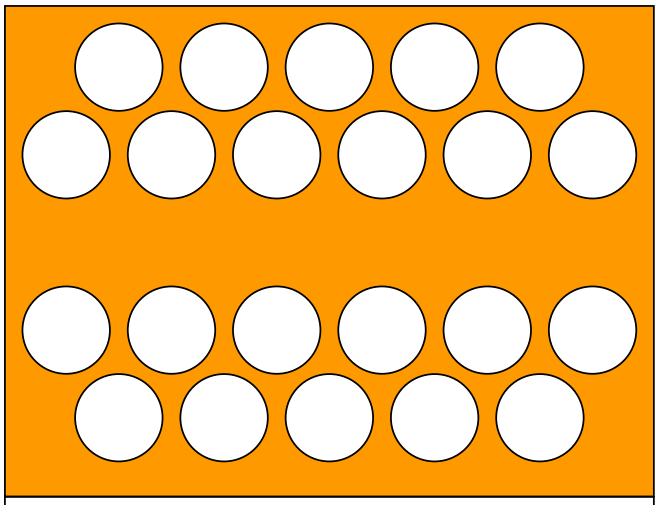
The structure considered in this test is a line defect in a triangular lattice of holes in a dielectric substrate.

Lattice vectors: $R_1 = \left(\sqrt{3}/2, -1/2\right), R_2 = \left(\sqrt{3}/2, 1/2\right)$

Radius of the cylinders: $R = 0.309a$

Refractive index of the cylinders: $\varepsilon_{cyl} = 1$

Refractive index of the substrate: $\varepsilon_{sub} = 10.24$



Test 4: line defect in triangular lattice

Figure 10

First the complete band diagram of the lattice (without defect) is computed. The comparison between the results obtained with the Band Solver option and CRYSTALWAVE is in Table 9.

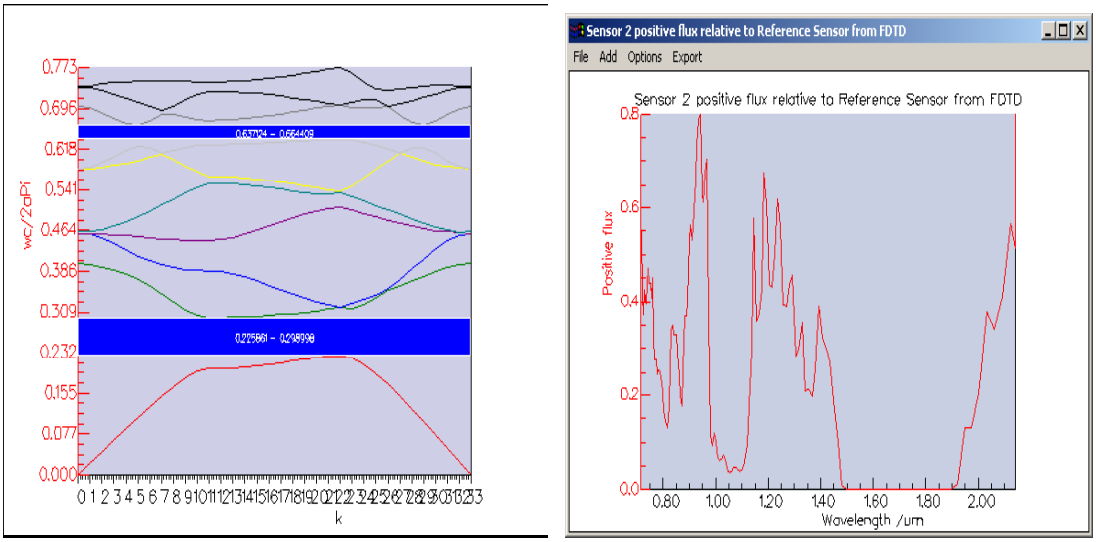
	First bandgap – low frequency	First bandgap – high frequency
BandSolver	0.226	0.301
CRYSTALWAVE	0.221	0.281

Table 9: band gaps computed by BandSolver and by CRYSTALWAVE

Note: The values in Table 9 are normalised to the lattice constant (0.4204 for CRYSTALWAVE, 1 for the Band Solver).

The comparison shows an agreement within 7%.

Note that the bandgap given by CRYSTALWAVE is valid for a smaller range of directions than the one calculated by the Band Solver. This is because it has been calculated analysing the power transmitted by the system for a set of plane waves with different frequency but the same direction.



Test 4: TE complete band diagram. Left: BandSolver. Right: CrystalWave.

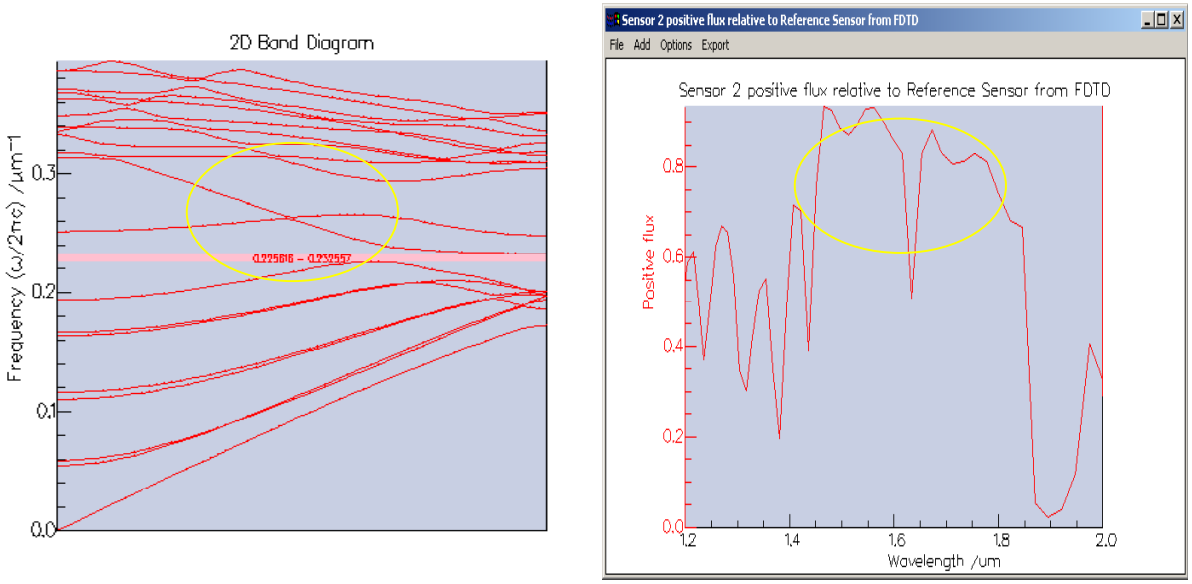
Figure 11

Then the band diagram of the line defect was computed.

Using the Band Solver, only plane waves with a propagation vector parallel to the channel's axis were used. Within the previously computed band gap, two modes (circled in Figure 12 below) can be seen. One of these modes is even (whose characteristic has negative slope), one odd (whose characteristic has positive slope).

Using CRYSTALWAVE, only the even mode is excited. Power is transmitted through the channel with unitary efficiency.

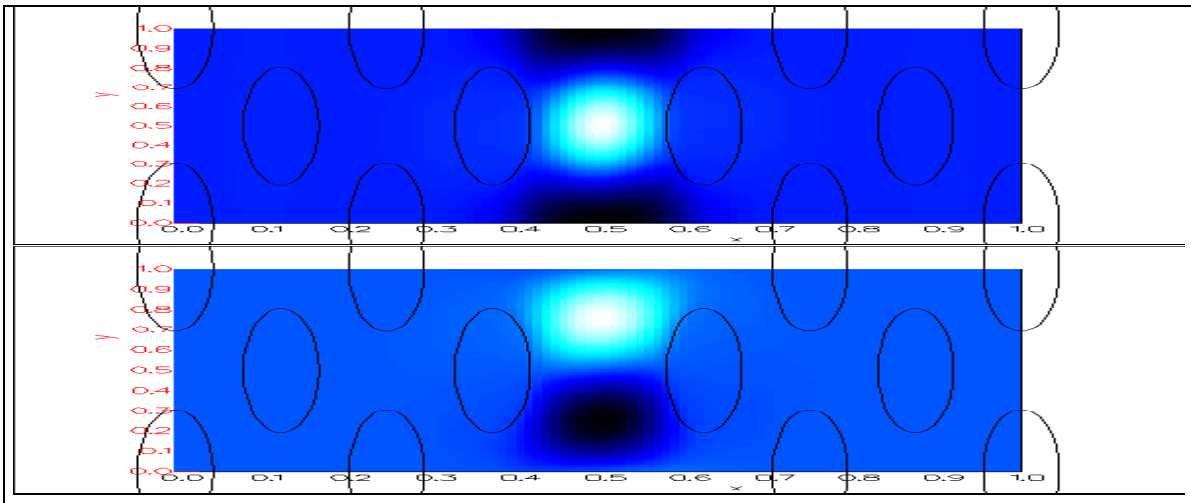
Note the trough in the centre of the bandgap: in the Band Solver's bandgap this correspond to the point where even and odd modes cross. At this point the characteristic is almost flat, which implies that the group velocity of the modes is almost zero. In a time-domain algorithm (in CRYSTALWAVE) this means that power at this frequency takes more time to exit the channel. Thus running the simulation for a longer period makes the trough smaller.



Test 4: TE line defect band diagram. Left: BandSolver. Right: CrystalWave.

Figure 12

As an example, the Figure 13 below shows the even mode guided by the line defect, at the wavelength 1.55 (Note: the axis are normalised to the lattice vectors).



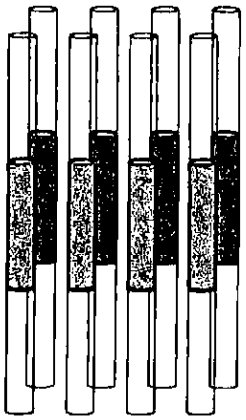
Test 4: bloch mode at lambda = 1.55, @k-point #7. (real and imag part)

Figure 13

1.2.5. Test 5

The structure considered in this test is a planar photonic crystal waveguide, made of a square lattice of dielectric rods in air with $\varepsilon_{cyl} = 1$, lattice constant *a*, radius $R = 0.2a$ and height $H = 0.2a$, with low index ($\varepsilon_{low} = 2$) rods extending infinitely above and below. See Figure 14 below.
Reciprocal lattice points studied: Γ, X, M, Γ.

(a) rod slab



Test 5: planar photonic crystal

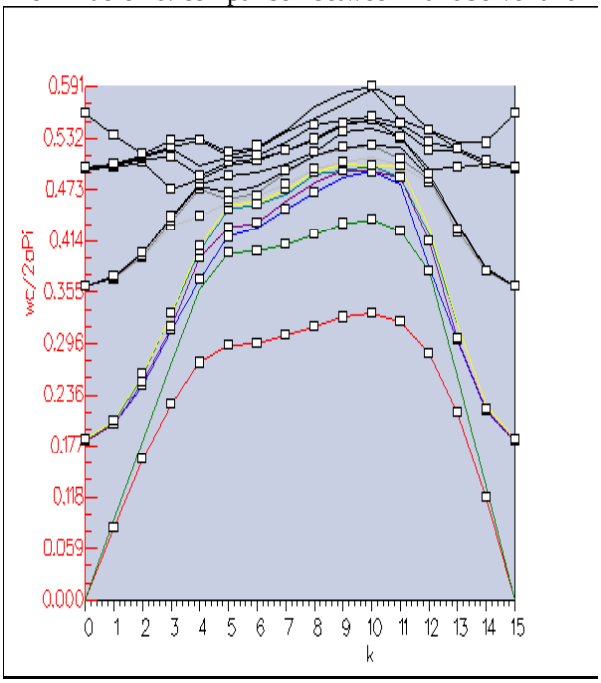
Figure 14

Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0
	X	0.296	0.30	-1.3
	M	0.326	0.33	-1.2
2	Γ	0	N/A	N/A
	X	0.397	0.40	-0.8
	M	0.425	0.43	-1.1

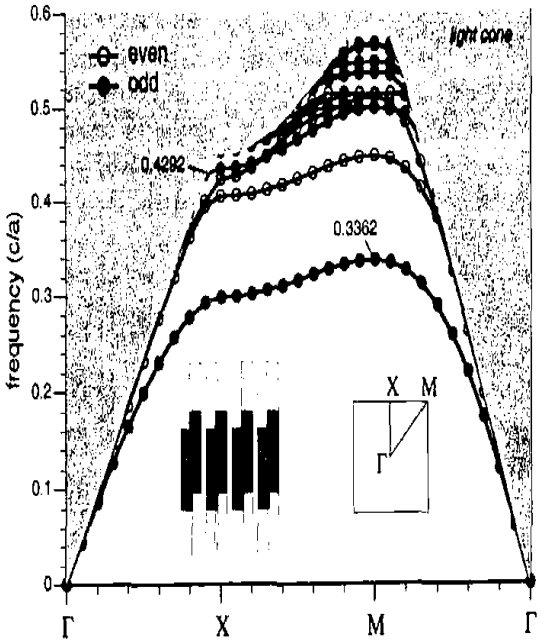
3	Γ	0.177	N/A	N/A
	X	0.414	0.42	-1.4
	M	0.473	0.48	-1.5

Table 10: comparison between BandSolver and MPB

From Table 10: comparison between BandSolver and MPB, we can see an agreement within 1.5%.



Test 5: band diagram

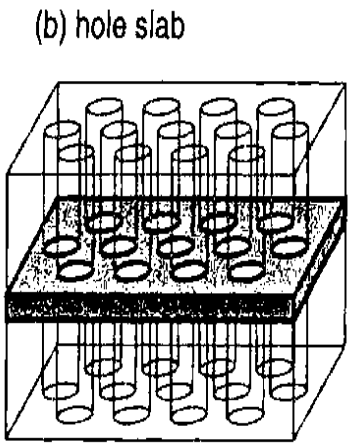


Test 5: band diagram from Ref. 1

Figure 15

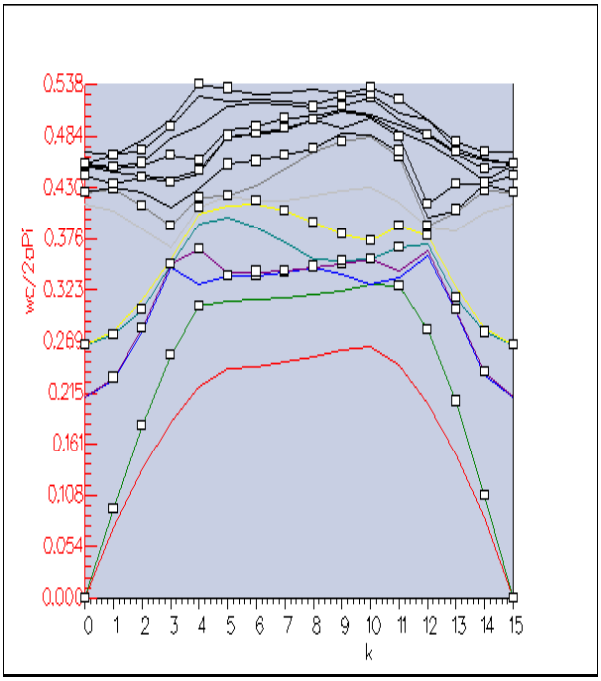
1.2.6. Test 6

The structure considered in this test is a planar photonic crystal waveguide, made of a triangular lattice of low index ($\varepsilon_{cil} = 1$) in a slab of high index ($\varepsilon_{cil} = 1$), lattice constant *a*, radius $\varepsilon_{cil} = 1$ and height $h = a$ (low index rods extending infinitely above and below the slab). See Figure 16 below. Reciprocal lattice points studied: Γ, M, K, Γ.

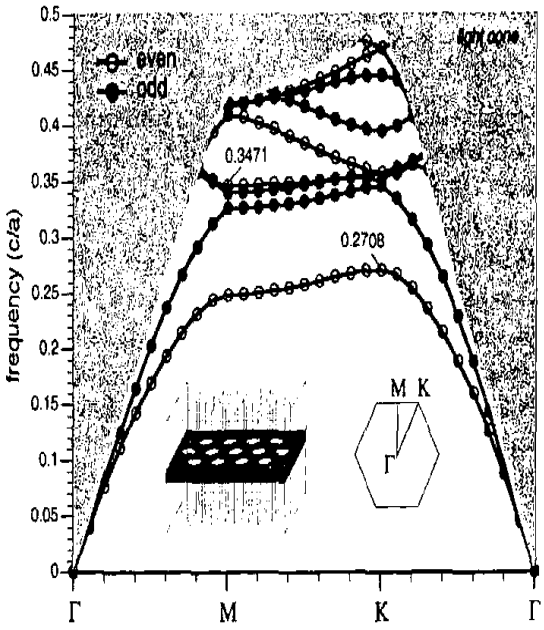


Test 6: planar photonic crystal

Figure 16



Test 6: band diagram



Test 6: band diagram from Ref. 1

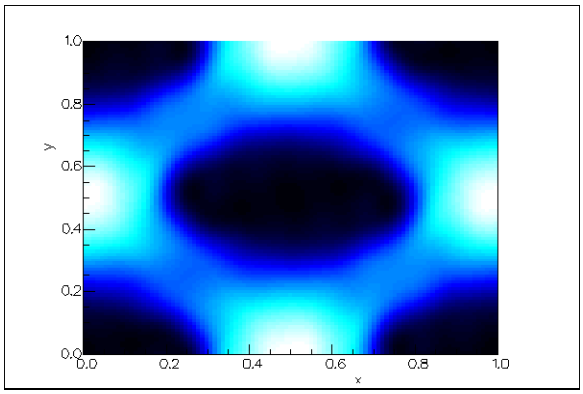
Figure 17

Band	Reciprocal lattice point	F (BandSolver)	F (MPB)	Error %
1	Γ	0	0	0
	M	0.237	0.24	-1.3
	K	0.268	0.27	-0.7
2	Γ	0	0	0
	M	0.312	0.32	-2.6
	K	0.328	0.34	-3.7
3	Γ	0.215	n/a	n/a
	M	0.328	0.34	-3.7
	K	0.328	0.34	-3.7

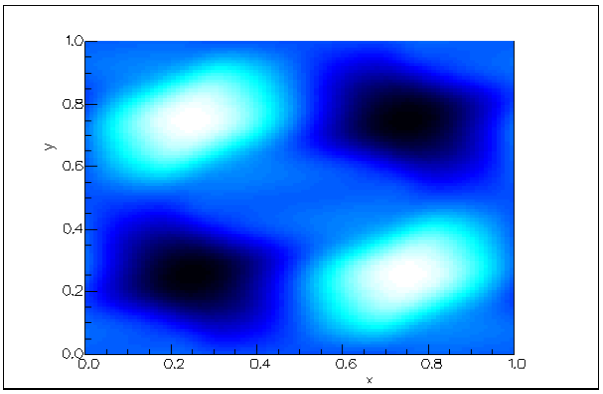
Table 11: comparison between BandSolver and MPB.

The comparison shows an agreement within 3.7%.

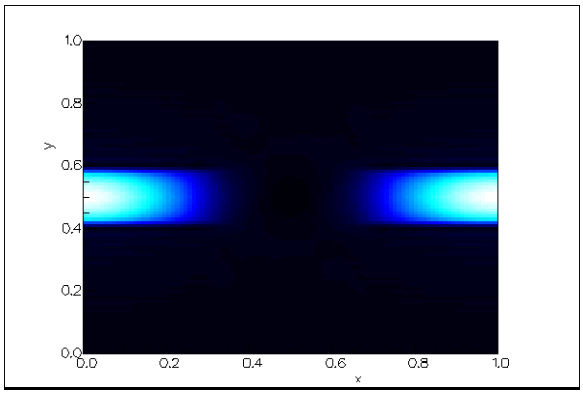
As an example, the profile of the real part of the Bloch mode at the reciprocal lattice point M, first band is shown in the figure below. The fields are plotted on a horizontal section passing through the high index slab and on a vertical section passing through the centre of the unit cell.
Note: values on the axis of the following graphs are normalized to the lattice vectors.



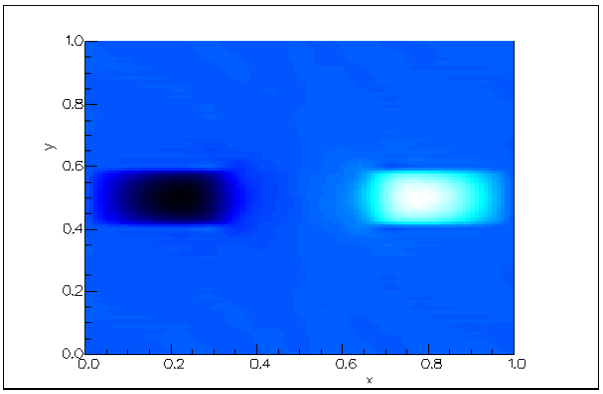
Horizontal section, x component



Horizontal section, y component



Vertical section, x component



Vertical section, y component

Test 6: Bloch mode (real part) @M, first band.

Figure 18

2. References

[1] "*Photonic Crystals: the road from theory to practice*", Steven G. Johnson, John D. Joannopoulos, Kluwer Academic Press, 2002

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[3] http://ab-initio.mit.edu/mpb/doc/analysis-tutorial.html

[4] "Large-bandwidth planar photonic crystal waveguides", Thomas Sondergaard, Andri Lavrinenko, Optics Communications 203 (2002), 263-270

[5] "Theoretical analysis of finite-height semiconductor-on-insulator-based planar photonic crystal waveguides", Thomas Sondergaard et al., J. of Lightwave Technology, 20(8), August 2002