Validation Report

Name of Report	Calculation of band diagrams for 1D non-linear photonic crystals using the FDTD method.
Performance Date	16th May 2006
Performed By	Wolfram Pernice
Product Name	OmniSim, CrystalWave
Product Version & Compile Date	
References	"*Finite-difference time-domain analysis of band structures in one-dimensional Kerr-nonlinear photonic crystals"*, I.S. Maksymov, L.F. Marsal , J. Pallares, Optics Communications, 239 (2004) 213–222

Calculation of band diagrams for 1D non-linear photonic crystals using a complex FDTD band-solver

Report Summary

The aim of this study was to validate the implementation of third-order non-linearity in the FDTD engine used by OmniSim and CrystalWave. The implementation is compared to band diagrams presented in reference 1. Calculations are performed using a simple complex FDTD solver that uses the same calculation procedure for non-linear fields as the FDTD engine developed by Photon Design.

1. Description of calculation method

a) Linear photonic band-gaps:

In order to calculate the band structure of 1D photonic crystals a complex FDTD algorithm is used. Electric and magnetic fields are staggered in space and time according to the positions of the traditional Yee-algorithm. Though the geometrical structure under consideration is only one-dimensional, the FDTD algorithm used solves Maxwell's equations on a two-dimensional grid. We therefore note that in principle the algorithm is capable of calculating more complex photonic crystal band-gaps. Band-diagrams are computed for TE-like excitation only, that is we consider the field vectore (Ex, Ey, Hz).
The structure is excited by an electric dipole located at a non-symmetry point within the unit cell. Excitation is applied only to Ey fields in order to get a non-directional field distribution within the grid. Hz Field values are stored at 100 random points at positions randomly chosen for every calculation. The dipole source is driven as a narrow Gaussian pulse in the time-domain to yield a broad frequency window. Periodic boundary conditions are used at all sides of the computational window. That means that we need to apply Bloch boundary conditions at both electric and magnetic field steps. Due to the

staggering of fields on the grid, boundary conditions for the electric fields are applied at the left side of the computational domain and for magnetic fields at the right side of the computational region.
The boundary conditions determine the k-point in the frequency band diagram. After running the calculation for a chosen number of time-steps, we take the Fourier transform of the sum of the sampled field values. The frequency spectrum shows distinct peaks at frequencies which are dependent on the k-vector used in the boundary conditions. An example of a spectrum calculated using the described method is shown in Figure 1.

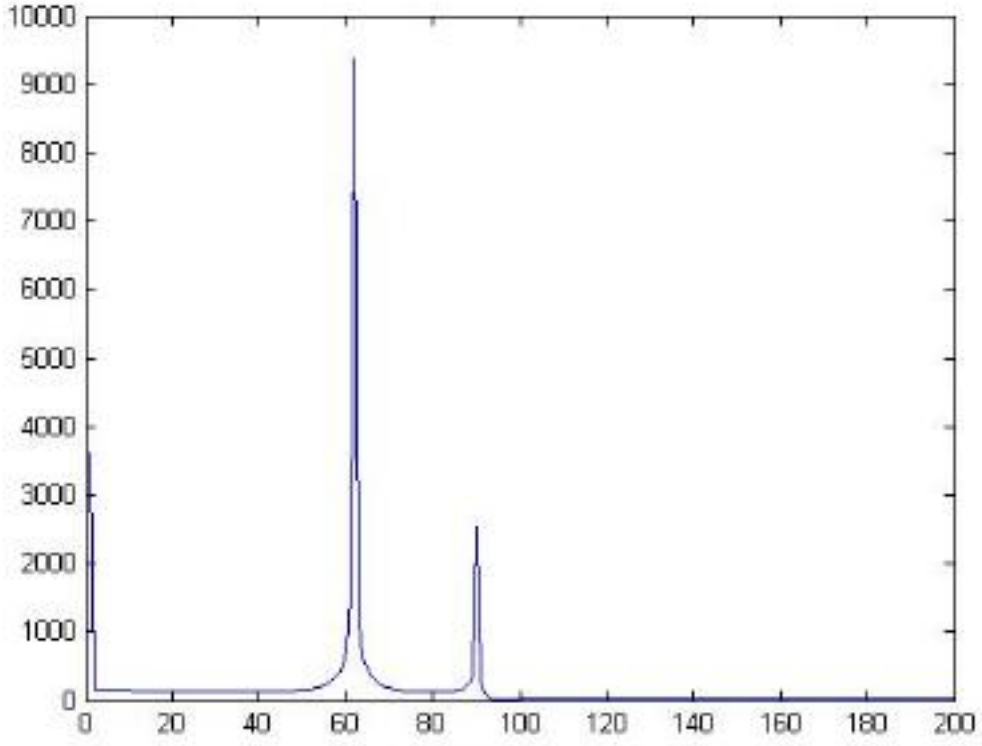

Figure 1. The frequency spectrum of a one-dimensional GaAs photonic crystal at the Gamma point. Axis units are arbitrary.

The spectrum was calculated for the Gamma point in k-space. Therefore the boundary conditions are equivalent to circular boundary conditions rendering the algorithm purely real. The two distinct peaks correspond to the first and second band of the photonic crystal.
The simulation time determines the sharpness of the peaks. For photonic structures with closely spaced Bands longer calculation times are required as single peaks might merge together and would not be detectable by an automized calculation procedure. Note that the heights of the peaks are not relevant in to the calculation of the band structure.

b) Non-Linear photonic band-gaps:

The calculation procedure for non-linear photonic crystals proceeds the same way as for linear photonic crystals. As we are using a non-linear algorithm, we do not only require electric and magnetic fields but also the electric displacement fields. In order to facilitate the algorithm we compute the displacement fields throughout the photonic structure and calculate the electric fields from the displacement fields according to Maxwell's equations. This is obviously not a memory efficient calculation procedure. However, because we are working on only one unit cell, memory is not an issue.
The updating equations in the time domain are given as

$$\frac{\partial}{\partial t}\vec{D} = \nabla \times \vec{H}, \qquad \frac{\partial}{\partial t}\vec{H} = \nabla \times \vec{E}$$

$$\vec{D} = (\varepsilon + \chi_3 \left|\vec{E}\right|^2)\vec{E}$$

In FDTD fashion the displacement fields are calculated from the previous displacement fields and magnetic fields. Using the newly obtained displacement fields the electric fields can then be calculated by applying a Newton iteration scheme in order to solver the non-linear equation for the electric fields. Subsequently the magnetic fields are then computed with the electric fields from the previous half time-step.

2. Validation example for a linear photonic crystal

Initially the implementation of the FDTD band-solver is compared to results calculated using Photon Design's band-solver tool. For the structure under investigation a one dimensional photonic crystal consisting of GaAs slabs in air is chosen.

Test Structure	1D photonic crystal	L = 1.0 Filling factor: 0.2 ε_{sub} = 1.0 ε_{cyl} = 13.0	Ref. 1

Table 1: 1D 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:

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

The structure considered in this test is one-dimensional photonic crystal consisting of alternating layers of air and GaAs of dielectric permittivity 13.

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

Thickness of the GaAs layer: $R = 0.2a$

Refractive index of the GaAs: $n_{GaAs} = \sqrt{13}$

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

Reciprocal lattice points studied: Γ, K, Γ

The results from the FDTD band-solver are compared to results calculated using the Photon Design band solver. A sample band-diagram is shown in Figure 2. The calculated diagram agrees closely with the BandSolver tool, if the resolution in the y direction is sufficiently good. The resolution for the FDTD band solver was set to be 30 grid points in both x and y direction. This is most likely not high enough to reach convergence to the expected band-diagrams. The error, however, is reasonably small in order to show the validity of the approach. When using calculation with roughly 50 points in each direction, better accuracy is observed. Using more grid points slows down the calculation considerably because the FDTD was implemented in Matlab and therefore runs as interpreted commands rather than in a compiled executable.

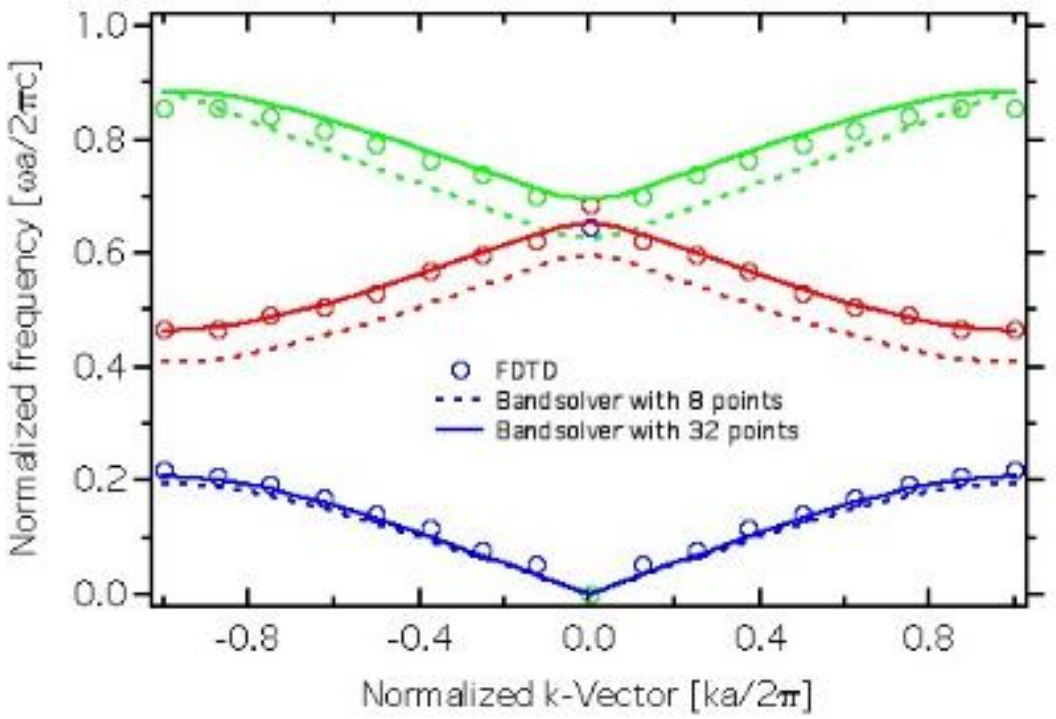

Figure 2.: Band diagram calculated using the FDTD bandsolver tool. For comparison band diagrams for two different resolutions of Photon Design's BandSolver tool are included.

3. Validation results for a nonlinear photonic crystal

The relevant validation was carried out for the non-linear photonic crystal desribed by Maksymov et al. in reference [1]. The geometric dimensions are the same as in the previous linear example. Again a photonic crystal with filling factor 0.2 and dielectric constant of 13 for the GaAs in air is used. The third order non-linear constant is set to be 0.01. As pointed out by Maksymov, the magnitude of the constant can be scaled with the amplitude of the driving dipole source, because the third-order non-linear effect is dependent on the magnitude of the electric fields but scales linearly with the magnitude of the third-order susceptibility.

In difference to the linear photonic crystal a frequency shift of the bands are expected for increasing intensity of the electric fields. The effect is less noticeable for lower bands than for higher order bands. In our case we expect a red-shift in the frequency bands which is dependent on the amplitude of the amplitude of the driving source. We therefore conducted two experiments for two different excitor amplitudes, the second amplitude having a value 5 times the first one.

In Figure 3 we show the results for the first test case. For comparison, the calculated bands for the linear photonic crystal given by the dashed lines are also included. The graph shows the bands calculated using the FDTD implementation from included in OmniSim and CrystalWave as well as the bands calculated using the method described by Maksimov. Very good agreement between the two methods is observed for all three bands. The expected red-shift is apparent for the second and third band which leads to a slightly enlarged band-gab between the second and third band.

In Figure 4 we show a calculation done for the same structure, but with 5 times higher amplitude of the driving excitor. Again, excellent agreement between Maksimov's and our results is observed. The band-gap between the second and third band widens and the red-shift for those two bands is significantly larger.

Direct comparison with the OmniSim and CrystalWave products is not possible for all k-points as Bloch periodic boundary conditions are not yet part or the implementation and would also mean significant changes to the algorithm. However, as mentioned before, the calculated fields will remain purely real for the gamma point and the boundary condition for this case is equivalent to the periodic boundary conditions that are part of the products. We therefore compare the frequency spectrum

obtained by using the following OmniSim layout to the calculation of the gamma point with the complex FDTD bandsolver.

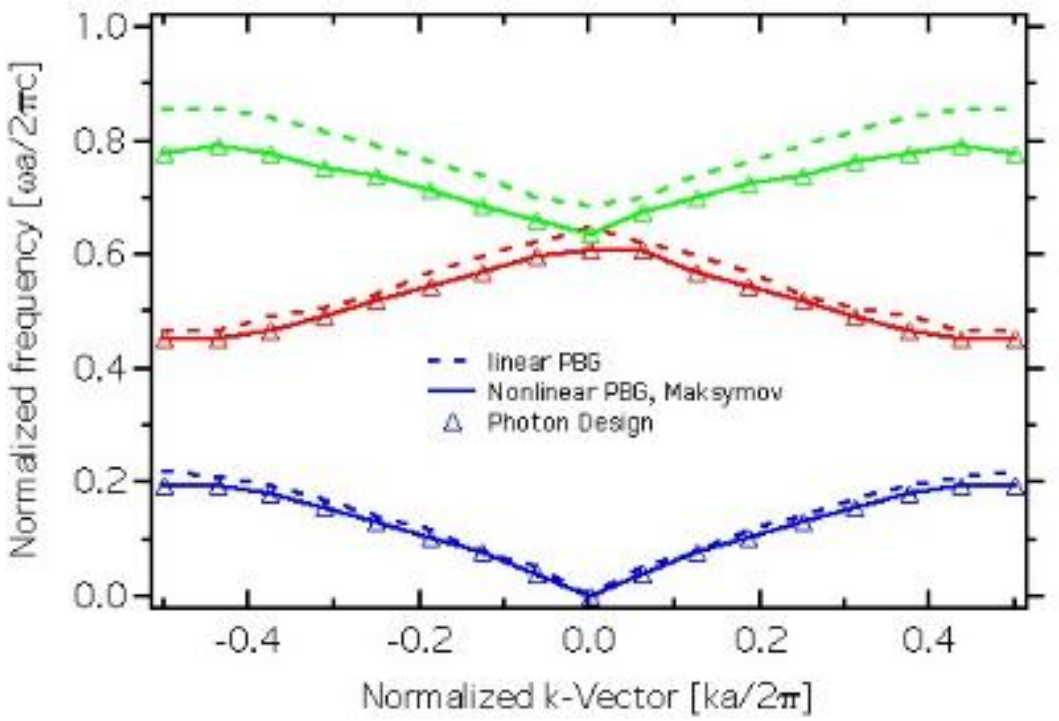

Figure 3.: Non-linear band-diagram calculated for a dipole source with normalized power 1.

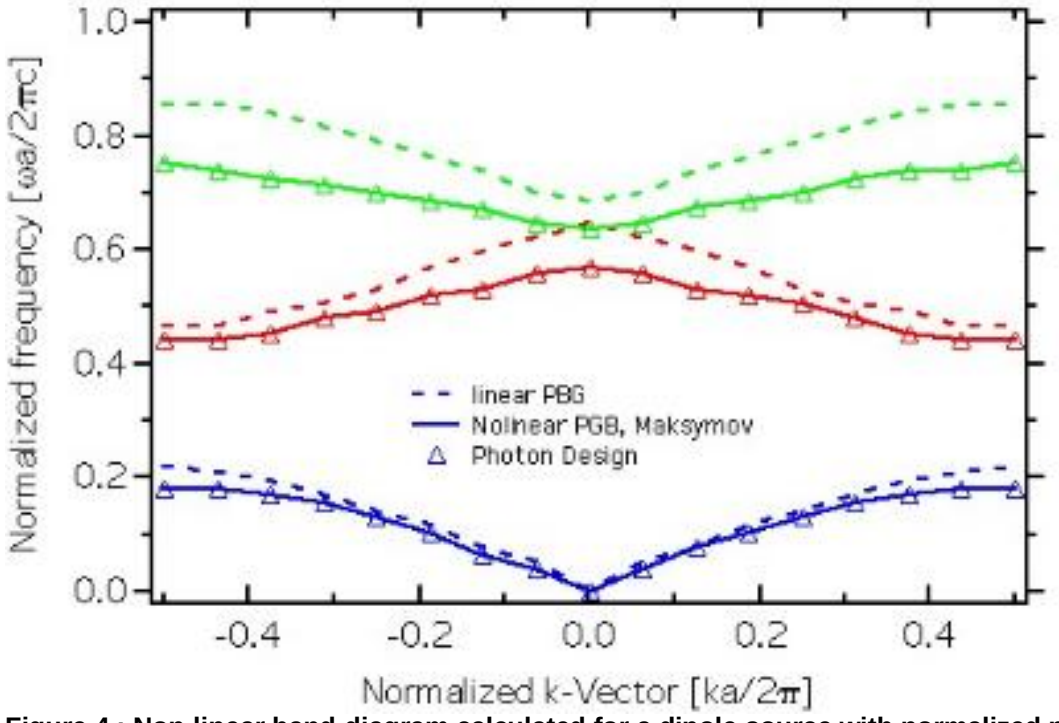

Figure 4.: Non-linear band-diagram calculated for a dipole source with normalized power 5.
adfa

The results are shown in Figure 5. The expected red-shift in the second and third band is clearly visible. With increasing excitor power, the bands move towards lower frequencies and the band-gap widens slightly.

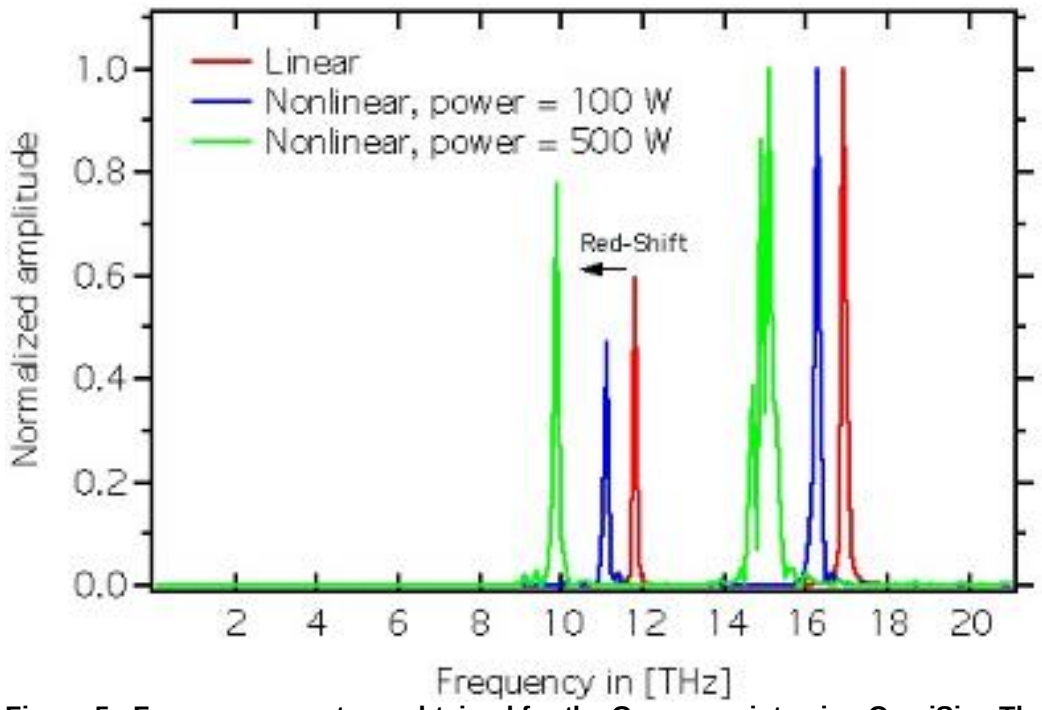

Figure 5.: Frequency spectrum obtained for the Gamma point using OmniSim. The spectra are calculated for the linear case, a non-linear photonic crystal with excitor powers of 100 Watts and 500 Watts.

From Figure 5 it is apparent, that the spectra for the non-linear case do not show clearly distinct peaks. With increasing excitor power the spectral width of the resonance peaks increases and neighbouring maxima occurr. This is also reported by Maksimov. The widening of the resonance peaks makes it however difficult to obtain an automized bandsolving tool, as the experimenter needs to select the right resonance peaks by hand.

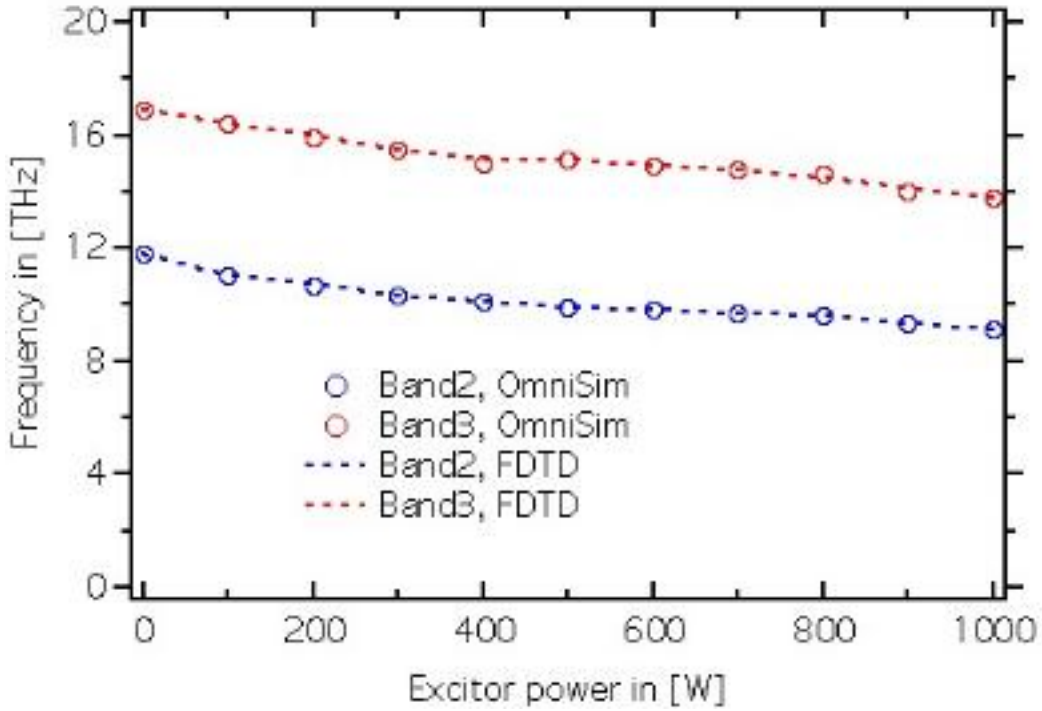

Figure 6.: Red shifts computed using OmniSim and the FDTD bandsolver for various dipole excitor powers.

In Figure 6 we compare the red-shifts calculated using the FDTD bandsolving tool and OmniSim. As they are using the same method to compute the bands, the obtained results are in very good agreement. Slight differences occur due to different ways of evaluating the spectra and in different resolutions.

4. Conclusions

In this report we investigated the validity of the implementation for third-order non-linear materials, corresponding to materials showing a Kerr effect or intensity dependent change of refractive index. The validation was performed by calculating photonic band-gaps for a non-linear one-dimensional photonic crystal. Close agreement was observed between our method and the procedure described in reference [1]. Direct comparison between OmniSim and the FDTD bandsolving tool is possible for computing spectra at the gamma point. For these calculations both methods give very similar answers.

5. References

[1] "*Finite-difference time-domain analysis of band structures in one-dimensional Kerr-nonlinear photonic crystals*", I.S. Maksymov, L.F. Marsal , J. Pallares, Optics Communications, 239 (2004) 213–222