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Project Report

Title: Simulating Photonic Devices using Finite-Difference Time-Domain Method.

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Certificate

This is to certify that the project titled ‘Simulating Photonic Devices using Finite-Difference Time-Domain Method’ submitted by Shivi Gupta (2030078) as a part of Summer Undergraduate Research and Graduate Excellence 2020 offered by Indian Institute of Technology, Kanpur, is a bonafide record of the work done by her under my guidance and supervision.

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Acknowledgements

I would like to thank IIT Kanpur for giving me this opportunity, to be able to explore a field I've always wanted to. Specially for conducting this program in an online mode. Though we missed out on the offline experience, this was unique in its own way and was still a great opportunity for learning.

I'm also extremely grateful to my mentor, Dr. Shilpi Gupta for suggesting this program in the first place, and for being encouraging whole throughout. Doing a project completely in the online mode had its own challenges, like not being able to meet in person and only doing simulation-based experiments. Ma'am helped in keeping my interest alive and kept helping me in every step of the project.

I'm also thankful to my family, for being ever-motivating and always caring for my well-being in these tough times. And my friends for not letting me feel low even without their physical presence.

Shivi Gupta

Abstract

Photonic Integrated Circuits (PICs) are circuits based on the propagation of photons or light on a chip. They have important applications in optical computing, high-speed communication and information processing. These circuits are usually at nanoscales. The individual components of a PIC are called photonic devices. These devices and integrated circuits can be simulated and studied using the finite element method, which is a numerical approximation of solving for Physical quantities.

Lumerical FDTD uses the finite-difference time-domain method, which is a numerical solver for Maxwell's equations. It involves meshing, that is, it divides the simulation region into cells and solves for Electric and Magnetic fields for the edges of the cells, thus enabling us to solve for propagation of light through complex devices.

This project involves studying and using these solvers to set up optical simulations and using these to calculate band structure diagrams, reflectance and transmittance plots and comparing them with theoretical plots. Starting with simple reflection and transmission through a medium change (air to glass), I simulated next reflection and transmission through a thin glass film. And finally, I carried out a study of 1-dimensional photonic crystals (which are alternating layers of media with different indices) using simulations.

Though simulations take long times to run and require large memories, they are an effective way to study about properties of photonic devices, since it's easy to study their properties with changes in dimensions, polarization and wavelength of propagating light, etc.

Contents

List of Figures

Introduction

Photonics is the Science of light. It deals with generating, propagating and detecting light using nanoscale devices. For example, waveguides and fibres are devices which confine light into a small cross section and are used in propagation. Grating couplers are devices used to couple light into a waveguide or fibre on a chip. Using these devices, photonic integrated circuits can be designed, which can have many applications. Since transmission of light over long distances is very fast, photonics can find use in many fields, such as high-speed communication, information processing, quantum computing, even health care.

Finite-difference time-domain method is a finite element method, which can be used to simulate and study photonic devices, modelling propagation of light through them. Simulating is an excellent method to study these since it can give quick results with variation in dimensions, wavelengths, etc. A drawback of simulations can be numerical and approximation errors since these work on interpolating data using finite number of points. Another drawback can be more time and memory requirements for bigger/complicated simulations.

In this project, I worked with Lumerical, which solves Maxwell's equation on finite grids as elaborated on, in the next section. I used this software for optical simulations, using which I plotted curves such as transmittance, reflectance and band structures, and compared them with theoretically plotted graphs.

Starting with simulating a medium change (from air to glass), I plotted reflectance (fraction of incident power reflected) and transmittance (fraction of incident power transmitted). I compared the simulation plots with plots calculated using Fresnel's coefficients.

In the next simulation, I plotted reflectance and transmittance through a thin layer of glass, with a thickness in nanometers.

Finally, I simulated a 1-D photonic crystal which consists of alternating layers of high and low refractive indices. I further simulated and studied defects in photonic crystals. For the theoretical plots, I used the transfer matrix method.
Photonic crystals give a bandgap in their reflectance and transmittance plots, which can have wide-ranged applications in PICs. They are even found in the environment, such as in wings of insects and in crystals. Introducing a defect gives a sharp peak in the bandgap which can be used to detect particular frequencies.

Following are the detailed analysis of the software and the optical simulations.

An Overview of the Software Used (Lumerical)

The finite element method is a widely used numerical method to solve many Physics and Engineering problems, for example, in modelling heat transfer, current flow and, as used here, electromagnetic properties of materials. It is based on discretizing and solving for the required quantities in those discrete regions to get an approximation for the correct numerical values. Finite-difference time-domain (FDTD) is one such method used to model the propagation of electromagnetic radiation through materials.

In FDTD, the region for which Electromagnetic propagation is to be modelled, is divided into smaller cells. This is called meshing. Then, using Maxwell's equations, Electric and Magnetic fields are calculated for the edges of each cell for different time instances. One such cell (called as Yee cell) is shown in Figure 1: Representation of a finite 3D Yee cell
Picture taken from https://support.lumerical.com/hc/en-us/articles/360034914633-Finite-Difference-Time-Domain-FDTD-solver-introductionFigure 1, they can in general be 1D, 2D or 3D. Further, Fourier transforms can be taken to obtain results in the frequency domain.

FDTD is a commonly used method for Photonics simulations, since it can model effects of scattering, diffraction, reflection etc up to numerical accuracy.

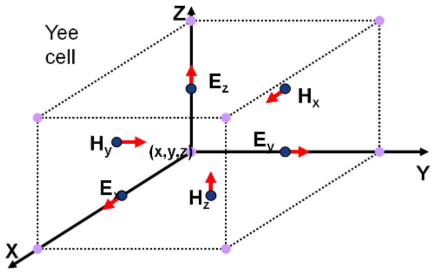

Figure 1: Representation of a finite 3D Yee cell
Picture taken from https://support.lumerical.com/hc/en-us/articles/360034914633-Finite-Difference-Time-Domain-FDTD-solver-introduction

One software which employs this FDTD method is Lumerical. It involves many packages, the ones used in the project are the following:

1. Lumerical FDTD: 3D Electromagnetic Simulator

This tool is used to simulate light propagation in general 2D and 3D devices. Simulation involves defining a simulation region (meshing), placing simulation objects and collecting and post-processing results. Some examples of simulation objects-

- Sources: Used to inject the EM fields into the simulation region. They can be of different types such as plane wave sources, Electric and Magnetic dipole sources, etc.

- Materials: Lumerical contains database of material constants (permittivity, permeability, index as functions of frequency) for commonly used materials such as glass, gold, etc. These can be used to simulate devices containing these materials.
- Monitors: Used to detect propagating light. There are further many kinds of monitors, such as power monitors and movie monitors.

Other than this, Lumerical contains its own scripting language, which can be used to vary properties of the simulation such as some dimension or source frequency.

2. Lumerical MODE: Waveguide Simulator

This tool is particularly used for simulating devices with confined modes such as waveguides. It also contains simulation objects and uses the Finite Difference Eigenmode (FDE) solver to calculate modes for a waveguide using a cross-section.

There are many more packages and nuances of the software not talked about here which are also very helpful in simulating photonic devices and integrated circuits.

Theoretical Calculations for Reflectance and Transmittance

Following the analysis done in Peatross and Ware[1], Fresnel's coefficients are given by

$$r_s \equiv \frac{E_r^{(s)}}{E_i^{(s)}} = \frac{n_i \cos\theta_i - n_t \cos\theta_t}{n_i \cos\theta_i + n_t \cos\theta_t}$$

$$t_s \equiv \frac{E_t^{(s)}}{E_i^{(s)}} = \frac{2 n_i \cos\theta_i}{n_i \cos\theta_i + n_t \cos\theta_t}$$

$$r_p \equiv \frac{E_r^{(p)}}{E_i^{(p)}} = \frac{n_i \cos\theta_t - n_t \cos\theta_i}{n_i \cos\theta_t + n_t \cos\theta_i}$$

$$t_p \equiv \frac{E_t^{(p)}}{E_i^{(p)}} = \frac{2 n_i \cos\theta_i}{n_i \cos\theta_t + n_t \cos\theta_i}$$

Where n_i and n_t are refractive indices of the first medium and second medium respectively, and θ_i and θ_t are angle of incidence and angle of refraction respectively. The subscript and superscript (s) stands for s-polarised and (p) for p-polarised component of incident light. Subscripts *i*, *t* and *r* stand for incident, reflected and transmitted components respectively.

Further, reflectance(*R*) and transmittance(*T*) are obtained from the Fresnel's coefficients by

$$R_s \equiv \frac{P_r^{(s)}}{P_i^{(s)}} = |r_s|^2 \text{ and } R_p \equiv \frac{P_r^{(p)}}{P_i^{(p)}} = |r_p|^2$$

$$T_s \equiv \frac{P_t^{(s)}}{P_i^{(s)}} = 1\text{-}R_s \text{ and } T_p \equiv \frac{P_t^{(p)}}{P_i^{(p)}} = 1\text{-}R_p$$

These are the equations used in plotting the theoretical results.

For the multilayer stack (photonic crystals), the theoretical results are plotted with the help of matrix transfer method, again based on the equations derived in Peatross and Ware[1].

Devices Simulated

1. Reflection and refraction through glass

Using FDTD, a simple simulation was set up to track reflection and transmission from air to glass. Reflectance and transmittance plots were generated using the simulation, plotted alongside theoretically calculated plots. The theoretical calculations were done using Fresnel's coefficients using the index fits from Lumerical's material database.

This was done for s-polarized and p-polarized light, both for normal incidence (with varying frequency) and incidence at an angle (for a particular frequency).

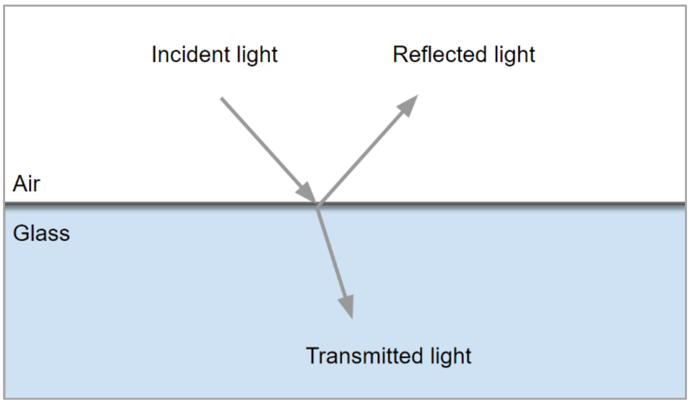

Figure 2: Representational diagram of the simulation

1. Normal incidence

The wavelength of incident light was varied from 400nm to 700nm.

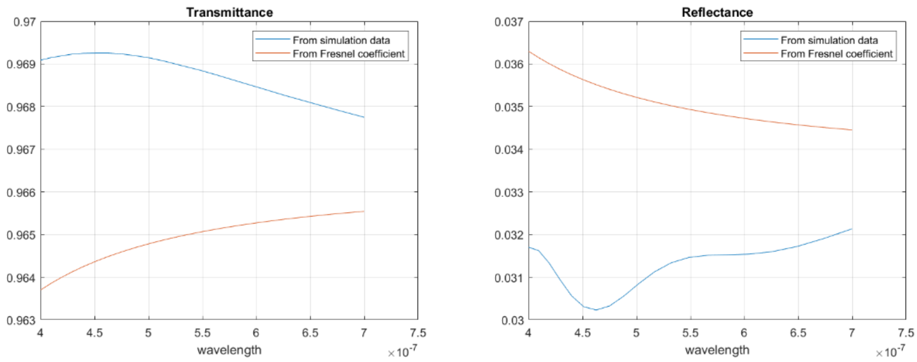

Figure 3: Transmittance and Reflectance plots for normal incidence

The numerical errors between the two curves are small, of the order of 10^{-3}.

2. Incidence at an angle

Wavelength of the light was kept constant at 532nm.

a) For s-polarized light

Keeping the incident light s-polarized, incident angle was varied from 0 to 90°.

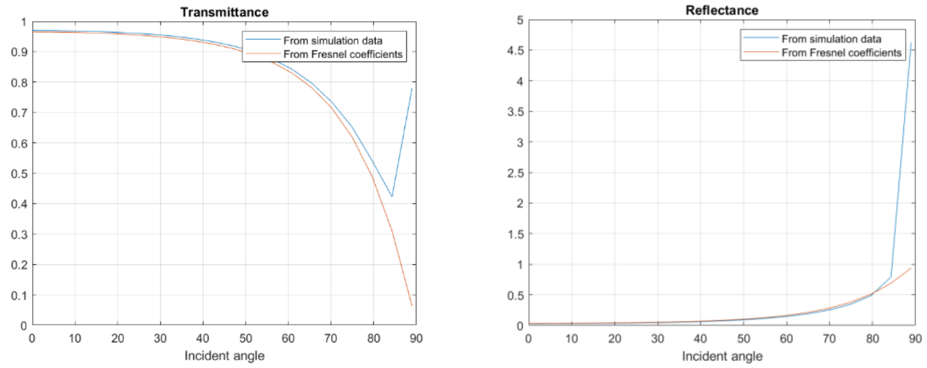

Figure 4: Transmittance and reflectance plots for s-polarized light

b) For p-polarized light

Keeping the incident light s-polarized, incident angle was varied from 0 to 90°.

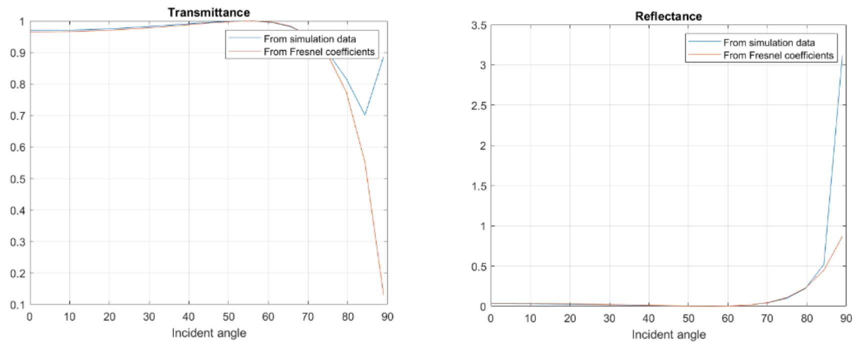

Figure 5: Transmittance and reflectance plots for p-polarized light

Errors between the two plots (theoretical and simulation) in Figure 4 and Figure 5 increase because of increase in numerical error at oblique angles.

2. Reflection and refraction through a thin glass film

Again using FDTD, a simulation was set up to model propagation of light through a thin layer of glass. As before, simulation data was plotted along with theoretical plots calculated using Fresnel's coefficients. This was done for s-polarized and p-polarized light, for both normal incidence as well as incidence at an angle. The width of the thin glass layer was taken to be 200nm.

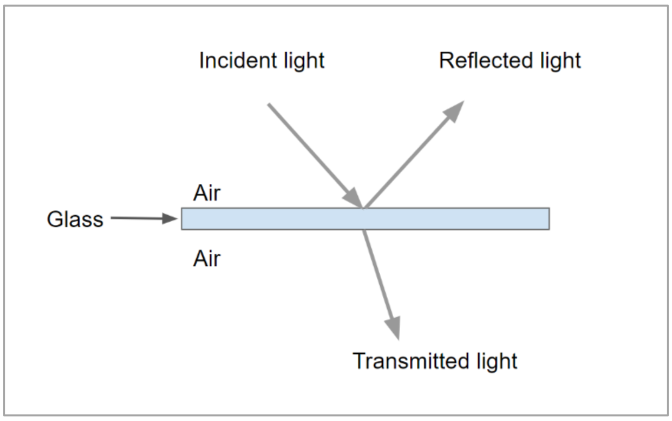

Figure 6: Representational diagram of the simulation

1. Normal incidence

The wavelength of incident light was again, varied from 400nm to 700nm.

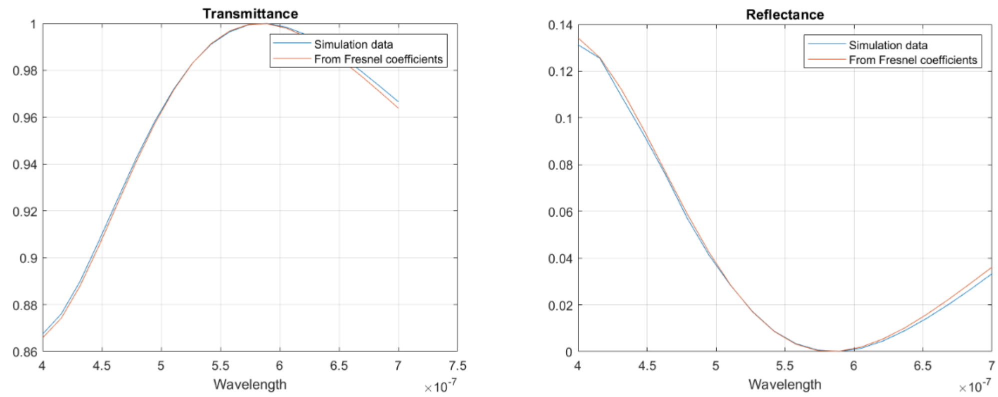

Figure 7: Transmittance and Reflectance plots for normal incidence

There is a peak in transmittance at 589.5nm (2*(thickness of film)*(refractive index)) because of constructive interference. Path difference between the waves transmitted are integral multiples of wavelength at the maxima point.

2. Incidence at an angle

Wavelength of the light was kept constant at 532nm.

a) For s-polarized light

Keeping the incident light s-polarized, incident angle was varied from 0 to 90°.

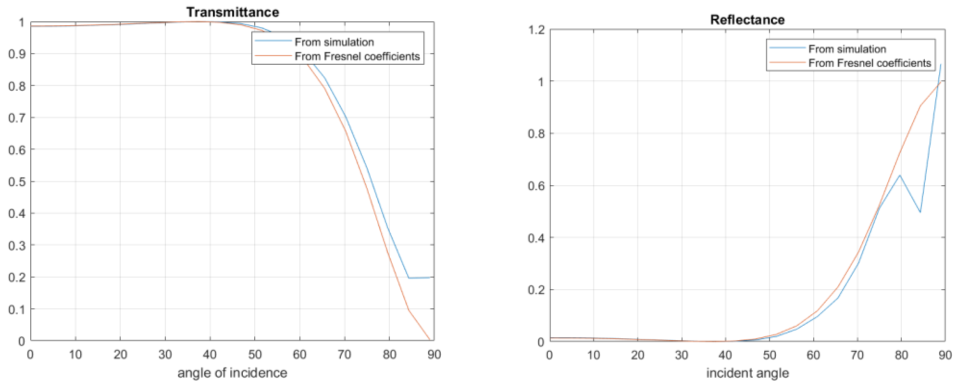

Figure 8: Transmittance and reflectance plots for s-polarized light

a) For p-polarized light

Keeping the incident light s-polarized, incident angle was varied from 0 to 90°.

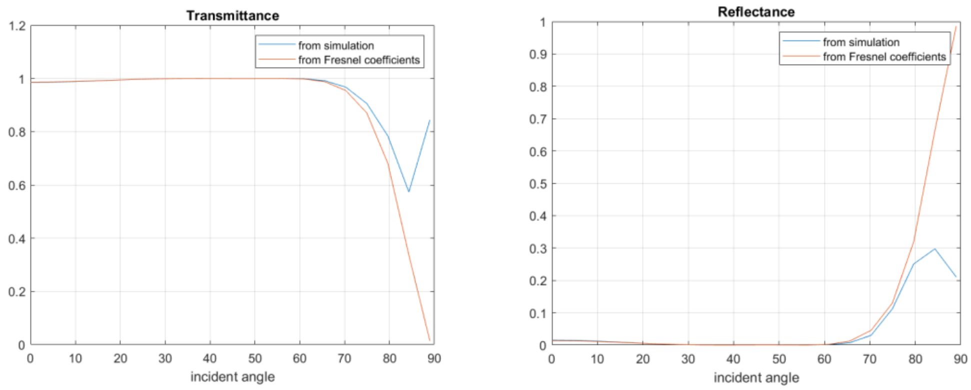

Figure 9: Transmittance and reflectance plots for s-polarized light

3. 1-Dimensional Photonic crystal

A 1-dimensional photonic crystal consists of thin layers alternating in thickness and material. A photonic crystal consisting of many layers acts as a bandpass filter for a range of frequencies because of constructive interference between the different light rays getting reflected and transmitted from the many layers.

Here, the photonic crystal simulated consists of alternating layers of TiO_2 (with a thickness of 80nm) and SiO_2 (with a thickness of 110nm) assuming non-dispersive indices for both. The theoretical plots are generated using transfer matrix method.

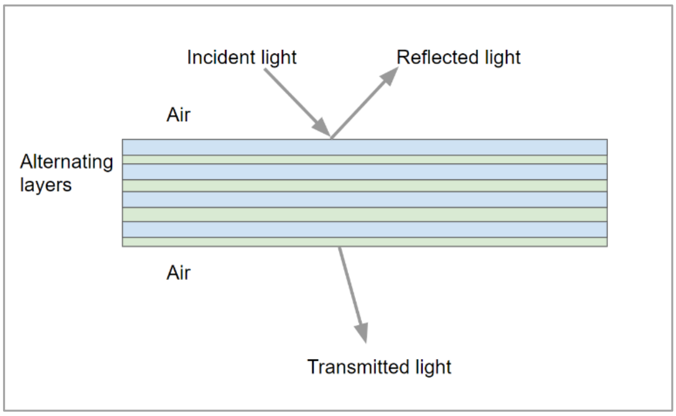

Figure 10: Representational diagram of the simulation

1. Single films of TiO_2 and SiO_2

Plotting the transmittance and reflectance for thin films of each, TiO_2 with thickness 80nm and SiO_2 with thickness 110nm to compare them with the photonic crystal plots. Both plots are for normal incidence of light.

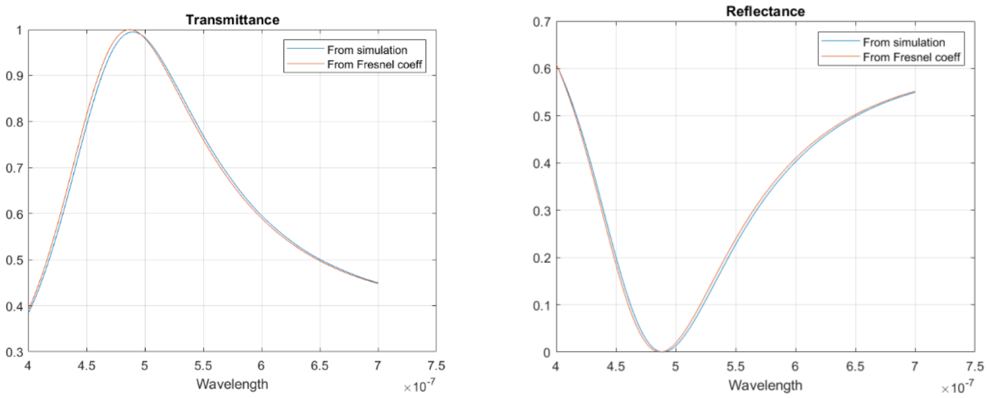

Figure 11: Transmittance and reflectance for the TiO_2 layer

Transmittance

Reflectance

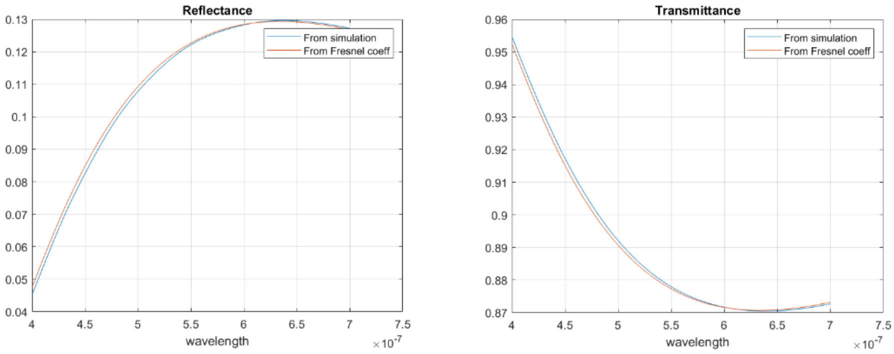

Figure 12: Transmittance and reflectance for the SiO_2 layer

2. Plots for finite photonic crystals

Following plots are for normal incidence.

a) 5 alternating layers (10 for each material)

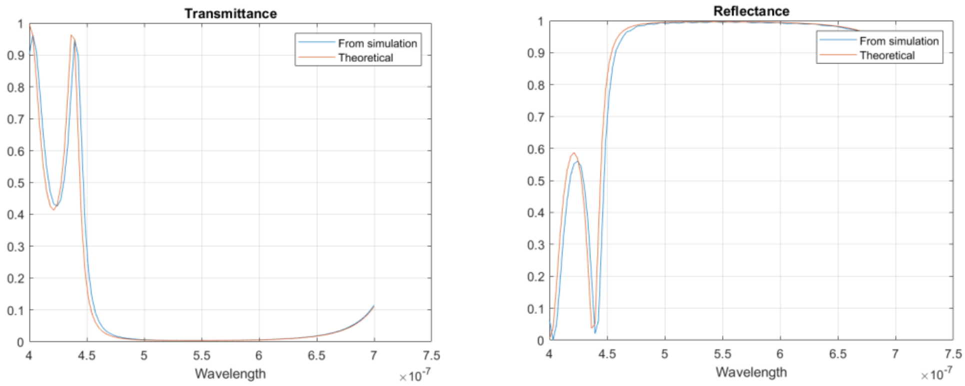

Figure 13: Transmittance and reflectance plots for a 10-layer photonic crystal

b) 10 alternating layers (20 for each material)

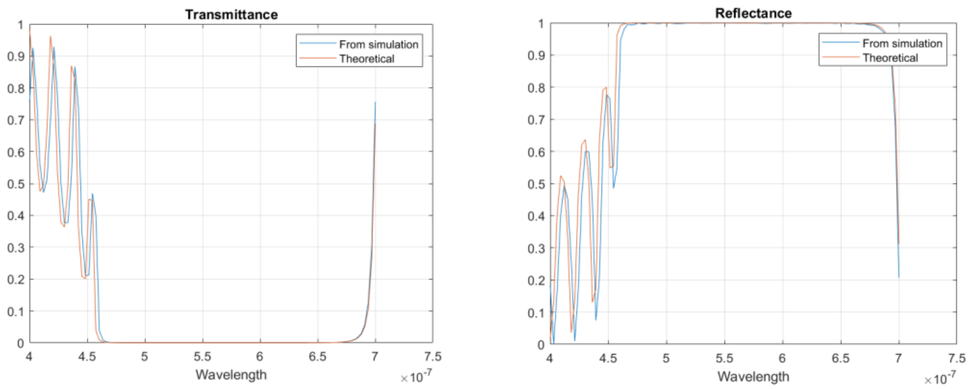

Figure 14: Transmittance and reflectance plots for a 20-layer photonic crystal

The plots show the emergence of a pass-band. A photonic crystal does not allow a band of frequencies to get transmitted through. This happens because of constructive interference in the reflecting direction and destructive interference in the transmitting direction. Thus, it can be used as a bandpass filters in optical circuits. As the number of layers keep on increasing, the flat region of the curve gets bigger. For a better bandpass filter, a photonic crystal with more number of layers should be preferred.

c) Bandstructure diagram

Plotting the bandstructure using the simulation involved placing randomly arranged dipole sources in the photonic crystal and collecting data after elapsing a small amount of simulation time. The dipole sources inject electric and magnetic fields in a range of frequencies. Because of the geometry of the device, only some frequencies retain and the rest die down because of destructive interference. This is used in plotting the bandstructure diagram.

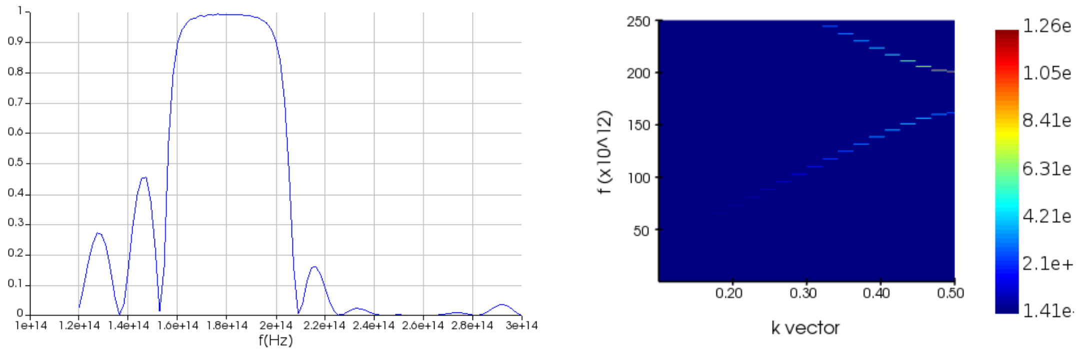

Figure 15: Reflectance plot and the corresponding bandstructure diagram

In a bandstructure diagram, frequency for the corresponding wave vector is plotted. As can be seen in Figure 15, there is a range of frequencies for which the k vector does not exist. Which means that range cannot propagate through the crystal. This range corresponds to the same pass-bands in the reflectance/transmittance plots as can be seen in the figure.

d) Comparing normal, s and p polarized incidence

Following is the plot containing reflectance for normal incidence, p-polarised and s-polarised incident light.

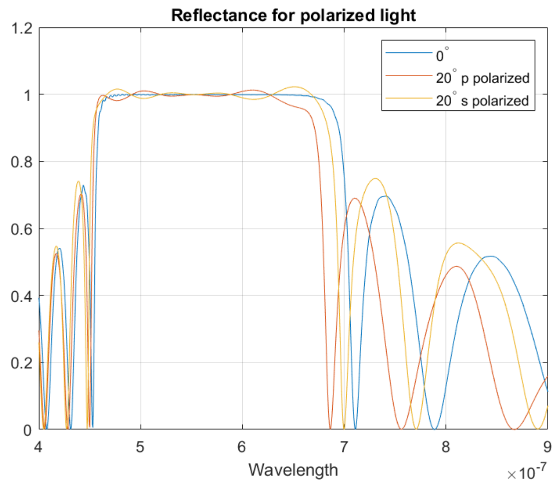

Figure 16: Reflectance plots for polarized incident light

4. Defect in a photonic crystal

Defect in a 1-dimensional photonic crystal refers to a defect in thickness in one of the intermediate layers. Here, the defect layer is taken to be the middle layer. This has useful properties as well, since defects give rise to a sharp peak in the pass-band of the original photonic crystal.

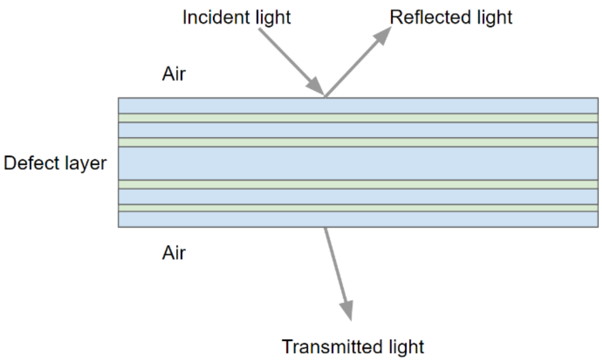

Figure 17: Representational diagram of the simulation

a) Changing number of layers

Following are the transmittance plots for 8 (total) layers each side and 10 (total) layers each side of the defect layer.

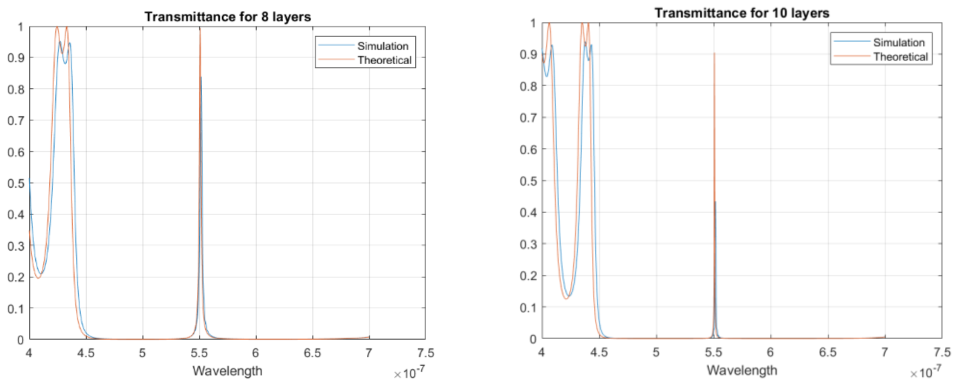

Figure 18: Transmittance plots for change in number of layers

As is visible in the figure, the Q-factor of the peak increases, i. e. the peak becomes sharper with increase in number of layers of the photonic crystal.

b) Changing material of the defect layer

Following is the plot for the two different defect layers, keeping number of layers same in both the cases.

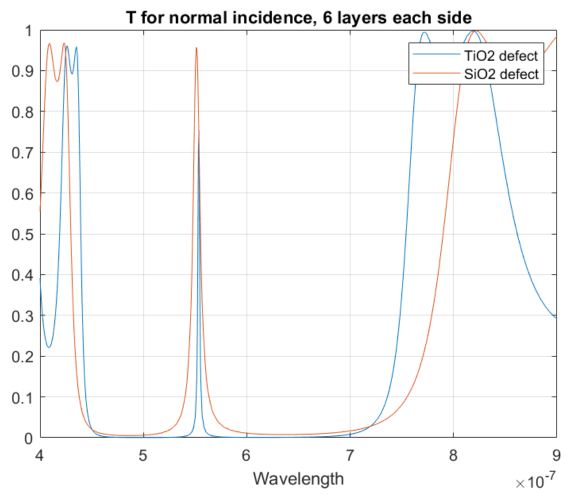

Figure 19: Transmittance plots for change in defect layer

This indicates that higher index defect layer gives a sharper peak at the centre.

c) Changing defect thickness

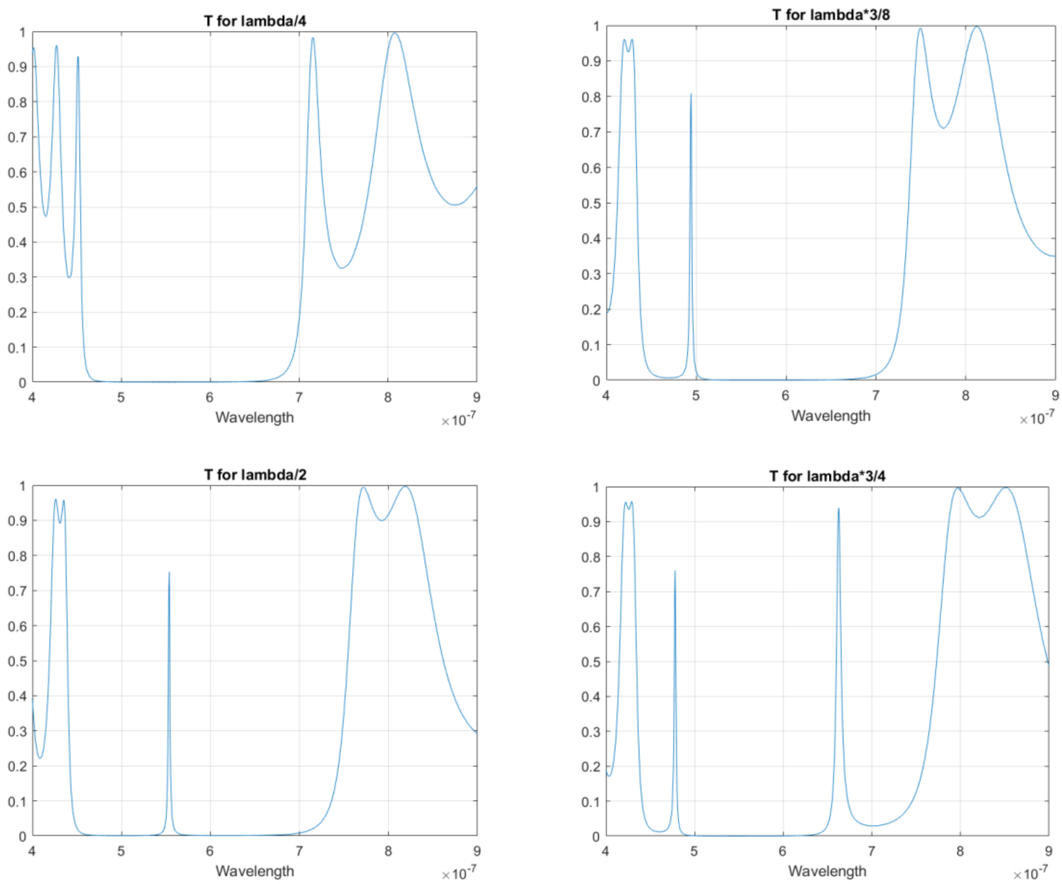

Figure 20: Transmittance plots with increasing defect thickness

As thickness of the defect is increased from λ/4 (original thickness) to λ/2, where λ is the wavelength of incident light, the peak keeps moving to the right. After λ/2 thickness, two peaks can be seen in the plot.

Conclusion

Simulating is a useful tool in studying optical devices. Results obtained from simulations match somewhat accurately with theoretical results. This accuracy can further be increased by using smaller meshes. But, since smaller meshes require more memory and take longer to run, there is a trade-off. Using appropriately sized meshes depending on the device specifications can give better results.

Optics, as a field is very wide and even the software used here has many more applications. For example, varFDTD is a solver which collapses a 3-dimensional simulation to a 2-dimensional one, thus making the simulations faster to run. Waveguide mode theory has a wide range of applications in propagation of light, and can also be simulated using these methods.

This project has thus, only briefly touched a big field which has innumerable real-world applications.

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