Simulating the band gap of a PPhC mirror using MEEP

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Geometry of the proposed mirror

The proposed PPhC mirror consists of a square lattice of gold, on which a square lattice of SiO2 of thickness 130 nm is placed. Further a square lattice of hBN of thickness 20 nm is placed on top of the SiO2 lattice, Further, gold cylinders of radius 64 nm and height 66 nm are punched through the SiO2 lattice periodically with the distance between the centres of adjacent cylinders being 272 nm. The x and y axis form the square lattice, with z axis being oriented along the height of the mirror.

Theory

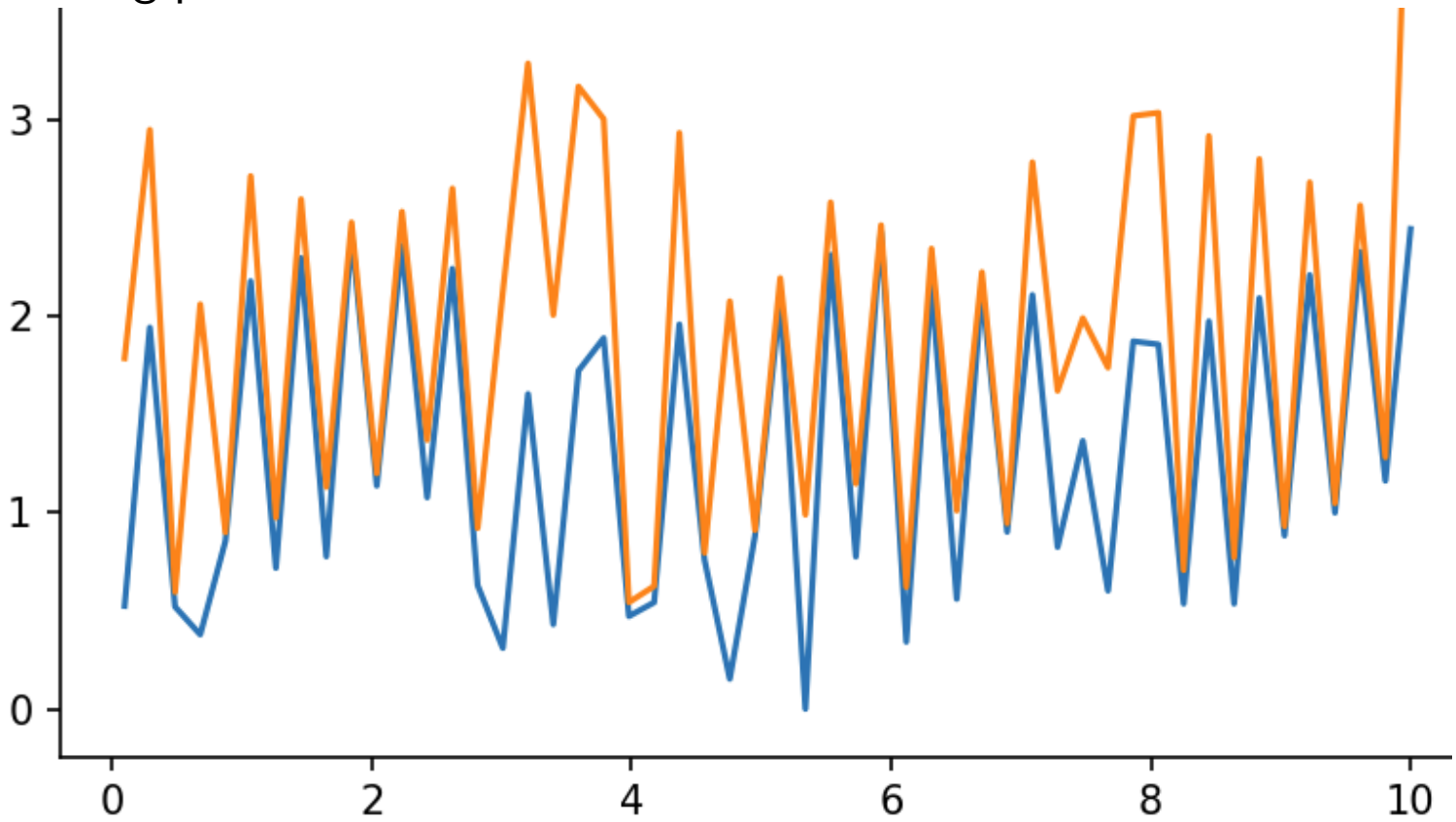
Let there be a space in which the permittivity varies as $\epsilon(r)$. We can show from the Maxwell equations that:

$$\boldsymbol{\nabla} \times (\frac{1}{\epsilon(r)} \boldsymbol{\nabla} \times H(r)) = (\frac{\omega}{c})^2 H(r)$$

Where H(r, t) is the macroscopic magnetic field and varies with time as $H(r,t) = H(r)e^{-iwt}$ MEEP solves this so called master equation numerically. We put a source of varying frequency at the center of our lattice and calculate different values of frequencies. We take H(r) as $H(r) = A\sin(k.r + \phi)$. We vary the value of $mod(k)$ which is indicative of wavelength, and calculate different solutions to ω. We plot the lowest 2 solutions against k.

Plot and code

For a simulation of 50 data points between 0 and 10 units along k-axis, we get the following plot:



The y axis is scaled in eV.

Possible errors

I haven't taken into account multiple factors, which could be leading to errors in my results:
1. I have imposed a default boundary condition (found in another template for calculating a band gap of a different lattice online) for this code, I was not able to cover enough theory within the stipulated time.
2. I only simulated for a lattice of 4 cylinders (which I did to reduce the computation time, which was quite large). Since ideally this number would be much larger, this could lead to errors.
3. I have not scaled the k - axis properly. In reality, we would take the direction of the wave vector determined by points of high symmetry in the lattice. However, I was not able to cover enough theory in the stipulated time to determine these points, and have taken the wave vector to be oriented along x-axis.

Resources used

1. MEEP tutorial: Band Diagram, Resonant Modes, and Transmission of a Waveguide Cavity
2. Joannopoulos, John D., Johnson, Steven G., Winn, Joshua N. and Meade, Robert D.. Photonic Crystals: Molding the Flow of Light (Second Edition). 2 : Princeton University Press, 2008.
3. MEEP documentation and tutorials