# Trial for the simulation of 1-d microcavity structure using the FDTD method with python

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**Abstract**

We simulated the Microcavity structure by varying the Permittivity and attempted to simulate the progression of 550 nanometer light wavelength pulses in the given environment using the FDTD method. Additionally, we tried to draw the energy band structure of the given cavity, but failed to obtain the correct band structure.

**Introduction**

Microcavity is one of the photonic structures which has lots of studies have been done since the birth of the Quantum technologies. The basic structure of microcavity is made by 2 mirrors are parallel to each other and a photon (or electromagnetic pulse) incident between the gap of the mirrors, with specific angle, is reflected.[1] This structure is simple but has variety characteristics, and numerous studies follow for the physical applications. Here, we'll explain the basic structure and materials used in the simulation and FDTD method has been done with using python.

The simulated structure is composed of silver, Perovskite material, and DBR. The thickness of silver set as 55nm, and Perovskite material, $CsPbBr_3$,416nm,[2] and the DBR made upon $SiO_2$/$TiO_2$ in 4 layers with each layer is 40nm, 84nm.[3] We set those materials during the simulation using the known realistic permittivity for each material.

**Background**

The method for simulating the given conditions, is done by the Finite-Differentiation-Time-Domain (FDTD) method. In this Section, we'll briefly discuss about how FDTD method has been done for 1-dimensional structure in case of Electromagnetic field propagation.

FDTD method is based on the definition of differential, link between two different points and gain It's tangent value to use finite value instead of infinitesimal.

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[1] https://en.wikipedia.org/wiki/Optical_microcavity#cite_note-7

[2] **PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES**, Vol. 116 No. 41, October 8, 2019

[3] Boxuan Gao, John Puthenparampil George, Jeroen Beeckman, and Kristiaan Neyts, "Design, fabrication and characterization of a distributed Bragg reflector for reducing the étendue of a wavelength converting system," Opt. Express **28**, 12837-12846 (2020)

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

Here, $\Delta x$ is value that does not converge to 0, but small enough to approximately gain the tangent value of the given x point f of (x). To set each x points like vectors with index, then we can make grid to calculate the differential of function x. (Figure 1).

In the case of Electromagnetic wave (EM wave), the differential equation belongs to the Maxwell's curl equation. If we assume that EM wave propagates to one direction only, and there is no external current or charge (statistic current), we can calculate electronic wave and Magnetic wave as follows:

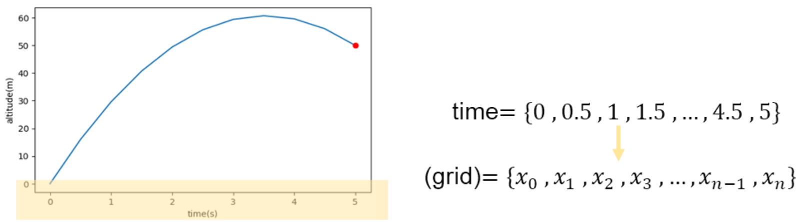


**Figure 1** Trajectory of throwing ball. If we set time as the domain of altitude, then we can make grid corresponds with time.

$$\nabla \times E = -\frac{\partial B}{\partial t}$$

$$\nabla \times B = \frac{\partial E}{\partial t}$$

Solving the curl equation LHS and RHS each, then the result is:

$$\frac{E_x(x + \Delta x, t) - E_x(x, t)}{\Delta x} - \frac{B_y(x + \Delta x, t)}{\Delta t} = \frac{B_y(x + \Delta x, t + \Delta t)}{\Delta t}$$

$$\frac{B_y(x + \Delta x, t) - B_y(x, t)}{\Delta x} - \frac{E_x(x + \Delta x, t)}{\Delta t} = \frac{E_x(x + \Delta x, t + \Delta t)}{\Delta t}$$

This result corresponds as using grid like below. The Red triangular point indicates Magnetic field, and blue circle corresponds for electronic field at certain time $t_i$.

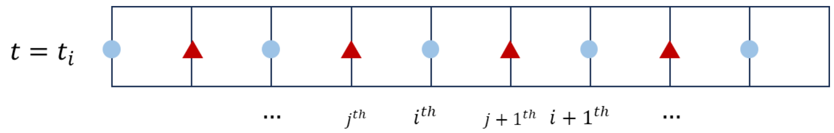


**Figure 2** grid as domain of given curl equation. The x inside the round bracket indicates spatial parameters, not the direction. The spatial parameters correspond to j , and i , for Magnetic field and electronic field.

These equations are available only in 1-D space. The time dependence can be represented below steps. If grid of certain time is decided, then we can update the grid to corresponding time value. By repeating the procedure, the time-dependent differential equation can be solved.

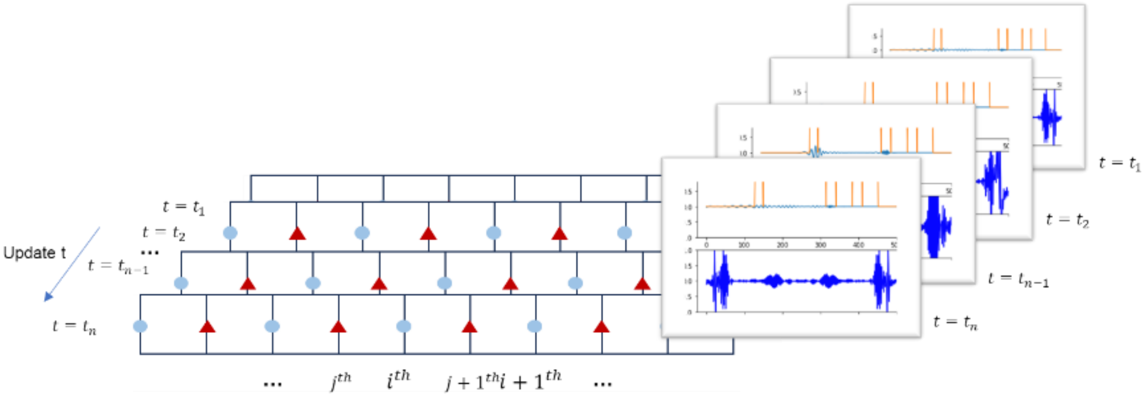


**Figure 3** . Time-update procedure scheme.

**Simulation Procedure**

The Original simulation code originates to the youtube channel.[4] The code was re-composed for the simulation environment. Main code used as follows:

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.constants as ct

#physical parameters

eps0 = ct.epsilon_0 #permitivity of vacuum
mu0 = ct.mu_0       #permeability of vacuum
c0 = ct.speed_of_light
imp0 = np.sqrt(mu0/eps0) #impedance at vacuum


#Building meshgrid for FDTD

jmax = 500       #spatial meshgrid
jsource = 2      #indicate spatial points where EM pulse begins
nmax = 4000      #count value for time. No units.

Ex = np.zeros(jmax)
Hz = np.zeros(jmax)

Ex_prev = np.zeros(jmax) # blank array for updating time-varying Ex
Hz_prev = np.zeros(jmax) # blank array for updating time-varying Hz
```

[4] https://www.youtube.com/watch?v=S-6Z8N-30AU

```
#Grid accuracy,
lambda_min = 500e-9
dx = lambda_min/20 # value of between the each point of grid point set as
2.5e-9
dt = dx / c0


#Material design

eps=np.full(500,eps0)
eps[128:149]=4.243*eps0
eps[150:315]=4.4873*eps0
eps[316:341]=36*eps0
eps[342:384]=84*eps0
eps[385:410]=36*eps0
eps[411:452]=84*eps0
eps_m = eps material_prof = eps_m > eps0


response = np.zeros(nmax) #Blank array to get response of material through
time


#Define EM Pulse (Gaussian wave packet, monotonic laser-green color)

def Source_Function(t):
        lambda_0 = 550e-9
        w0 = 2*np.pi*c0/lambda_0
        tau = 30
        t0 = tau*3
        return np.exp(-(t-t0)**2/tau**2)*np.sin(w0*t*dt)

#FDTD calculation - main loop

for n in range(nmax):
        #update magnetic field boundaries (Bor boundary conditions)
        Hz[jmax-1] = Hz_prev[jmax-2]
        for j in range(jmax-1):
                Hz[j] = Hz_prev[j] + dt/(dx*mu0) * (Ex[j+1] - Ex[j]) Hz_prev[j]
        = Hz[j]
        #Magenetic field source
        Hz[jsource-1] -= Source_Function(n)/imp0
```

```
            Hz_prev[jsource - 1] = Hz[jsource -1]
    #update magnetic field boundaries
    Ex[0] = Ex_prev[1]
    #Update electric field source
    for j in range(1,jmax):
            Ex[j] = Ex_prev[j] + dt/(dx*eps_m[j]) * (Hz[j] - Hz[j-1])
            Ex_prev[j] = Ex[j]
    #Electric field source
    Ex[jsource] += Source_Function(n+1)/imp0
    Ex_prev[jsource] = Ex[jsource]

   response[n]=Ex[250]
            if n%10 == 0: plt.subplot(2,1,1)
            plt.plot(Ex)
            plt.plot(material_prof)
            plt.ylim([-1,1])

            plt.subplot(2,1,2)
            plt.plot(fft_Ex,color='b')
            plt.ylim([-1,1])
            plt.show()
            plt.close()

    #main loop end

    resp_fft=np.fft.fft(response)
    amp = abs(resp_fft)*(2/len(resp_fft))
    freq = np.fft.fftfreq((len(resp_fft)),nmax)

    #array for data
    array_1 = []
    index1 = np.where(amp >= 0.001)

    for k in index1:
            array_1.append(amp[k])


    plt.subplot(2,1,1)
    plt.plot(response)
    plt.xlabel("time (a.u)")
```

```
plt.ylabel("E (a.u)")

plt.subplot(2,1,2)
plt.plot(freq,amp)
plt.xlim(0.6e-5,1.6e-5)
plt.xlabel("frequency")
plt.ylabel("Amplitute")
plt.show()
plt.close()
```

*-These codes were stopped until getting FFT data processing. Additional codes were attached to Appendix. B*

**Result**

We can get two kinds of results from the simulation. First, the simulation of EM wave propagation and corresponding Fourier transform in the 1-D microcavity structure through time.

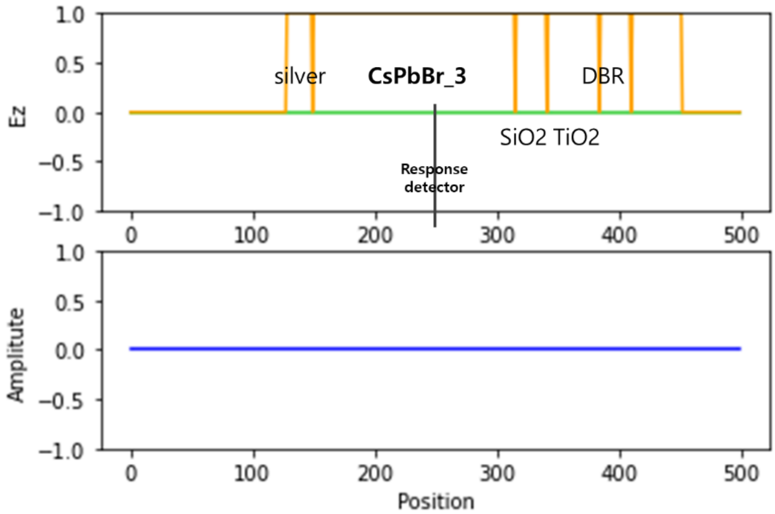


Figure 4 a. Explanation of plot image. Orange line indicates the materials with permittivity. At the DBR part, the thicker layer corresponds with TiO2, and the thinner one is SiO2. Green line indicates electronic wave packet, and blue line with the subplot below indicates Fourier transformation of wave propagation. Location of Response detector used to gain energy band of given structure. The source of permittivity of materials is belonging to here[5].

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[5] https://refractiveindex.info/

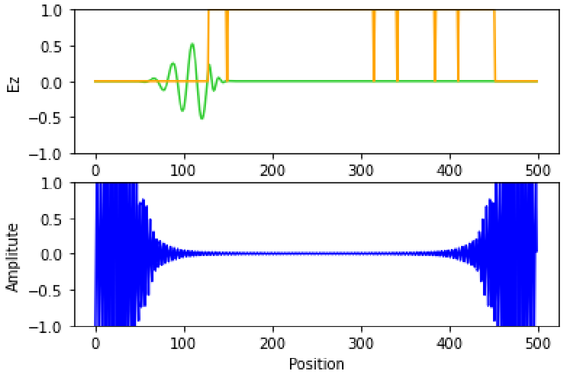


Figure 4 b. time=400, corresponding plot

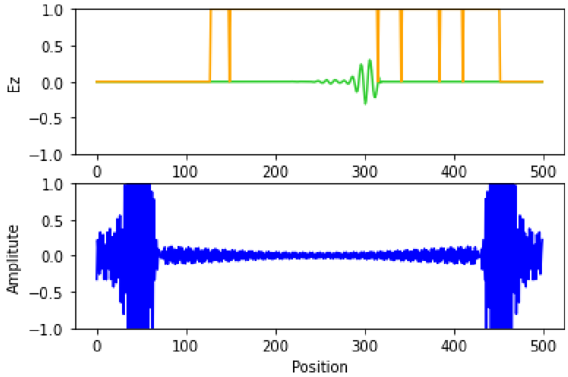


Figure 4 c. time = 800, corresponding plot

When plotting continuously with a shorter time interval, we could see that the waves change with time. We can observe the symmetric shape while wave packet reflected after colliding with DBR. (Figure 5.) The reason of those shapes can be assumed that two different signals transformed together, one is for reflected wave, and other one is about transmitted wave at SiO2 layer.

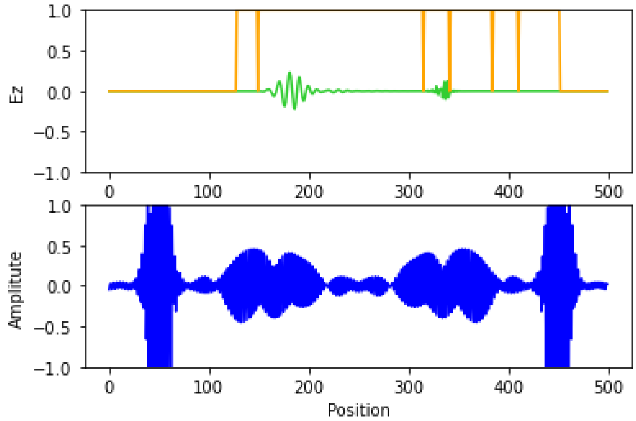


Figure 5. symmetric signal of Fourier transform

Second, we can calculate Energy band using the change of electronic wave at spatial grid point 250, for given material structure. However, it should be noted that this might not be an exact result.

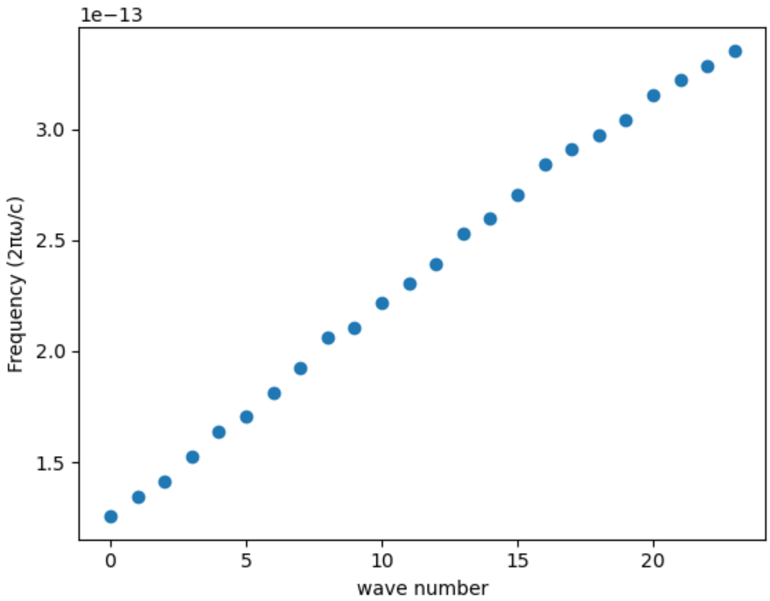

Figure 6 Energy band of simulated result

**Discussion**

First, we should consider whether the total simulation procedure is valid to describe physical system. In real microcavity system, the pulse between two mirrors, silver and DBR, must be coherent and resonant. However, in the simulated case, resonance between the two materials were not achieved, even the time passed. To solve this problem, trial for modifying the spatial weight corresponding to the resonator (CsPbBr_3) was existed, yet expected result wasn't found. The reason might come from implementing permittivity corresponding with silver. Due to its low relative permittivity, silver makes waves that can easily transmit and have low reflectance. However, to make a successful resonator structure, two flat mirrors are required, and, in this simulation, silver couldn't play the role of mirrors. The reason deduced that, because in the real physical system, mirror isn't just composed by silver only but some other material coated with silver, so the surface that contact with target material (in this case, CsPbBr_3) can role a high reflectance mirror.

Secondly, to get Energy band, according to the textbook[6], To obtain the energy band, the response of matter is required, but in this simulation structure it was difficult to determine which spatial point to get response. This is because of the difficulty to get one dimension data within Python, while the data obtained by the changes of the entire electromagnetic wave over time separated both the time dimension and the space dimension. Lastly, there is some inevitable problem in this simulation, that we don't know about the information of amplitude of the pulse source. This couldn't affect to final result, but it might carefully considered if we do further research using the simulation.

[6] I. A. Sukhoivanov and I. V. Guryev, in Photonic Crystals: Physics and Practical Modeling, ed. W. T. Rhodes (Heidelberg, Springer, 2009), p. 167.