2019-10-14

NUMERICAL SIMULATION AND COMPARISON OF THE ELECTRIC AND MAGNETIC FIELD VARIATIONS IN FREE SPACE AND IN ZINC OXIDE NANOPARTICLES USING ONE DIMENSIONAL FDTD METHOD

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NUMERICAL SIMULATION AND COMPARISON OF THE ELECTRIC AND MAGNETIC FIELD VARIATIONS IN FREE SPACE AND IN ZINC OXIDE NANOPARTICLES USING ONE DIMENSIONAL FDTD METHOD

A THESIS SUBMITTED TO THE SCHOOL OF GRADUATE STUDIES OF BAHIR DAR UNIVERSITY IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE IN PHYSICS (QUANTUM OPTICS)

BY
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BAHIR DAR, ETHIOPIA
SEPTEMBER 2019

BAHIR DAR UNIVERSITY

COLLEGE OF SCIENCE

DEPARTMENT OF PHYSICS

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BAHIR DAR UNIVERSITY

COLLEGE OF SCIENCE

Date: September 2019

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Title: **Numerical simulation and comparison of the Electric and Magnetic field variations in free space and in ZnO nano particle using one dimensional FDTD method**

Department: **Physics**

Degree: **M.Sc.** Convocation: **September** Year: **2019**

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Signature of Author

This work is dedicated to my Family

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ACKNOWLEDGMENTS

First and foremost, I would like to express my deepest thanks to GOD and His mother Mary.

Secondly, I wish to express my special thanks to my kind hearted advisor Dr. Gajanan Honnavar for the successful completion of this thesis. Without his guidance, this thesis would not have been the same as presented.

Thanks a lot for everybody that has been involved in my thesis directly or indirectly. Finally, Thanks to my family for making all this possible and the financial support.

Nothing can describe my deepest love for my family.

ABSTRACT

In this study an incident plane electromagnetic wave in free space and in ZnO NPs is numerically simulated using 1D FDTD method. The simulation of the propagation of plane wave in ZnO NPs is compared with the simulation of the propagation of plane wave in free space. The electric and magnetic field variations were numerically calculated in both free space and in ZnO NPs by discretizing Maxwell's equations. For electrical conductivity of $7x10^{-6}$ S/m and $1.5x10^{-5}$S/m the numerical simulation of the plane wave in ZnO NPs shows the propagation of plane wave does not attenuate, because the conductivity of ZnO NPs is very small. However, the magnitude of electric and magnetic fields in ZnO NPs is attenuated for large electrical conductivity of 0.04 S/m and ZnO NPs absorb both electric and magnetic fields.

Abbreviations Used in the thesis

1-D: One-Dimension

eV: electron Volt

FDTD: Finite-Difference Time-Domain

meV: mili electron Volt

MATLAB: Matrix Laboratory

nm: nanometer

NP: nano particle

TEM: Transition Electron Microscope

ZnO: Zinc Oxide

ZnO NPS: Zinc oxide Nanoparticles

CHAPTER ONE

INTRODUCTION

1.1 Background of the study

The development in the field of nano science and nanotechnology has opened new nano scale technological applications. Nanotechnology is the ability to observe measure, use and manufacture things at the nano scale (10^{-9} m) range. Metal oxide nano particles have attracted considerable attention in technological applications due to unique properties originating from their particle sizes in nano scale. Zinc oxide is one of the well-known semiconductor metal oxides with the formula ZnO. Generally ZnO has several favorable properties and applications like high room-temperature luminescence; wide band gap with band gap energy of 3.37 eV which provides to operate in the blue and ultra-violet optical devices. Its large exciton binding energy of 60 meV gives ZnO several advantages including better radiation resistance for devices used in space and nuclear applications. Large exciton binding energy of ZnO provides the exciton stability and enhances luminescence efficiency. Because of its nontoxic nature it is used as antibacterial drug agent and in cosmetics. The wide band gap enables it to be used as ultraviolet light protector in eyeglasses. It is routinely used in optoelectronic application, its hardness and rigidity make it useful in ceramics industry [1, 2, 3, 4]. Due to these diverse applications and properties, there has been a strong interest in the investigation of ZnO in photonic devices and we have chosen ZnO NPs for the simulation of electromagnetic waves by using one dimensional Finite-Difference Time-Domain (FDTD) method.

1.2 FDTD Method

Kane Yee introduced the Finite-Difference Time-Domain (FDTD) method in 1966. FDTD Method is based on the approximation of derivatives by using finite difference method. It is a numerical means of directly solving Maxwell's time dependent equations and those equations are discretized in the time and spacial domains by using the finite difference method. The FDTD method solves for both electric and magnetic fields in time and space using the coupled Maxwell's curl equations, rather than solving for the electric field alone or the magnetic field alone with a wave equation. It is the most popular method in electromagnetic wave propagation simulation [5, 6, 7]. Due to its popularity, conceptual simplicity, the time-domain nature and accuracy in computation, we have used the FDTD method for the visualization of the evolution of complex electromagnetic phenomena such as the propagation of electromagnetic waves in ZnO NPs.

1.3 Maxwell's equations

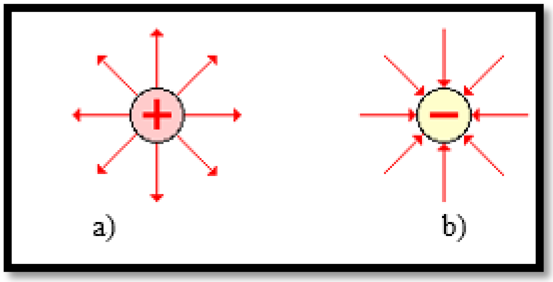


Figure 1. 1: The direction of the electric field is away from a positive test charge (a) and towards for a negative test charge (b) [8].

James clerk Maxwell was born in Edinburgh in 1831and formulated four basic Maxwell's equations in 1873. Nowadays these equations are called Maxwell's equations. In material medium these four equations are described as, the first equation (1.1) is known as Gauss' law and describes about electric charges are the sources of electric field as shown in Figure 1.1. The second equation (1.2) describes about a magnetic monopole does not exist as shown in figure 1.2 and is known as Gauss' law for magnetism. The third equation (1.3) is known as Faraday's law and explains about a time varying magnetic field induces a spacial varying electric field as shown in Figure 1.3. The fourth equation (1.4) describes about time varying electric field and current generate magnetic field, and is known as Ampere-Maxwell law as shown in Figure 1.4 [9,10].

$$\nabla \cdot E = \frac{\rho}{\varepsilon_0} \qquad 1.1$$

$$\nabla \cdot H = 0 \qquad 1.2$$

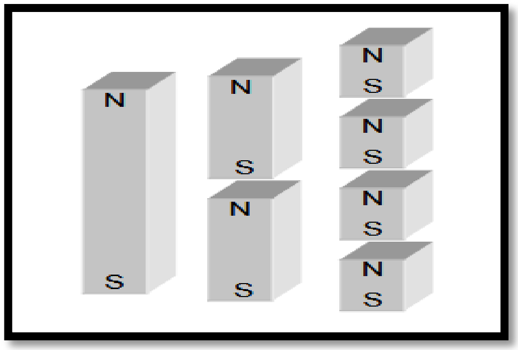


Figure 1. 2: Cutting of a large permanent magnet in to smaller ones [11].

It is impossible to separate the North Pole from the South Pole of a magnet.

$$\nabla \times \mathrm{E} = -\mu \frac{\partial \mathrm{H}}{\partial \mathrm{t}} \quad 1.3$$

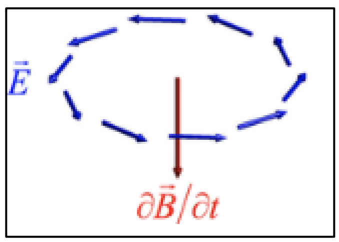


Figure 1. 3: Time varying magnetic field generates induces circulating electric field orcirculating electric fields induces time varing magnetic fields [12].

From the figure above B is magnetic field intensity.

$$\nabla \times \mathrm{H} = \mathrm{J} + \varepsilon \frac{\partial \mathrm{E}}{\partial \mathrm{t}} \quad 1.4$$

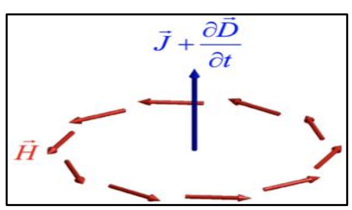


Figure 1. 4: Circulating magnetic fields induce currents and or time varying electric fields. Currents and or time varying electric fields induce circulating magnetic fields [12].

From the figure above D is electric displacement.

Where, $\nabla = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$ is the del operator expressed in Cartesian coordinates; E is electric field in volts/meter; H is magnetic field in amperes/meter; J is current density in amperes/meter^2; ε_0 is free space permittivity (8.85×10^{-12} farads/meter); ε is electrical permittivity in farads/meter; μ is magnetic permeability ($4\pi \times 10^{-7}$ henrys/meter) and ρ is the electric charge density in coulombs per cubic meter [13].

1.4 Electromagnetic Waves

From Maxwell's equation, a changing magnetic field produces an electric field and a changing electric field produces a magnetic field and these fields (waves) are perpendicular to each other and to the direction of propagation. These propagating fields are called electromagnetic waves. To examine the propagation of the electromagnetic waves, consider a plane electromagnetic wave propagating in the +z -direction, with the electric field E pointing in the +x-direction and the magnetic field H in the +y-direction, as shown in Figure 1.5 below. At any time both E and H are uniform over any plane perpendicular to the direction of propagation [14].

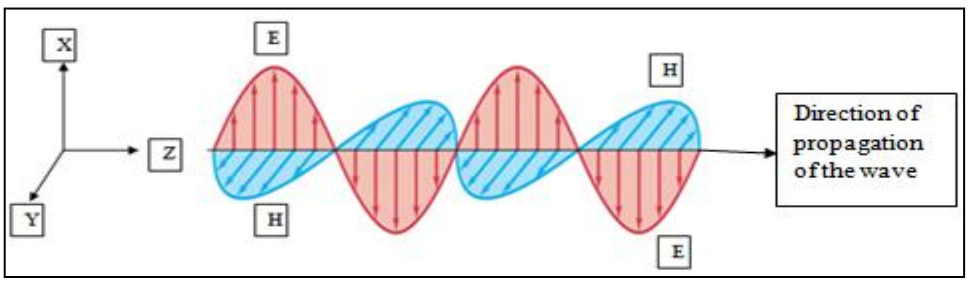


Figure 1. 5: A plane electromagnetic wave [14]

1.5 Motivation

The wide band gap (3.37 eV) and high exciton binding energy (60 meV) of ZnO NPs has variety of applications in the visible and near ultraviolet regions. Since nanometer-size zinc oxide has many new exciting properties and wide technological applications such as transparent electrodes, laser diodes, light emitting diodes (LEDs), water purification, solar energy conversion, quantum dot devices, and cosmetics. ZnO is better suited for use in photonic deceives as a local switch for light. Recent interest in low dimensional materials for the photonic application has motivated us to simulate the possibility of light propagation in ZnO NP so as to check the possibility of use in photonic devices like miniature interferometers.

1.6 Statement of the problem

In case of optical switches and EDFA (Erbium doped Fiber Amplifier) mostly glasses are being used. Most researchers work is based on the effect of bulk materials on traditional optical instruments like glasses. Since bulk properties of materials does not explain quantum-optical circumstances at the nanoscale level, the current work focuses on the analysis of light propagation in ZnO NPs.

1.7 Objective of the thesis

1.7.1 General objective

To numerically simulate and compare the Electric and Magnetic field variations in free space and in ZnO NPs using one dimensional FDTD method.

1.7.2 Specific objectives

- To know how to discretize Maxwell's equations in time domain.
- To develop MATLAB code for the application of wave propagation.
- To compare and contrast the propagation of the electric and magnetic field variations in free space and ZnO NPs for different electrical conductivity value of ZnO NPs.
- To investigating the effect of electric and magnetic propagation in ZnO NPs.

1.8 Significance of the study

ZnO NP is characterized by its direct and wide band gap at room temperature thus, enabling its use in optoelectronic applications such as light emitting diodes, laser diodes and photo detectors. Most notable, among these properties is its high excitonic binding energy of 60 meV at room temperature which makes it a promising material for optical devices that are based on excitonic effects. And also the antibacterial activity of ZnO NP is known to increase with a decrease in particle size and such an action can be stimulated by visible light. Because of this ZnO NP is the most studied oxides in its nano-particle range. Because we are planning to build a Mach-Zehnder interferometer for all optical communication devices, in this regard it is expected to understand the field variations and its effect in ZnO NPs.

CHAPTER TWO

LITERATURE REVIEW

This section presents a review of thesis works done by different researchers related to ZnO NPs and the FDTD method in one dimension used in the simulation of electromagnetic fields in free space and in material medium.

2.1 ZnO NPs

ZnO NPs have multifunctional industrial applications such as solar cells, UV light-emitting devices, photo catalysts, gas sensors, pharmaceutical, transparent conducting oxide, and cosmetic industries have attracted a significant interest in worldwide. ZnO NP is a wide band gap of 3.4 eV and direct semiconductor with a stable wurtzite structure [15 16]. The structure of ZnO NP is hexagonal wurtzite as shown in Fig 2.1.

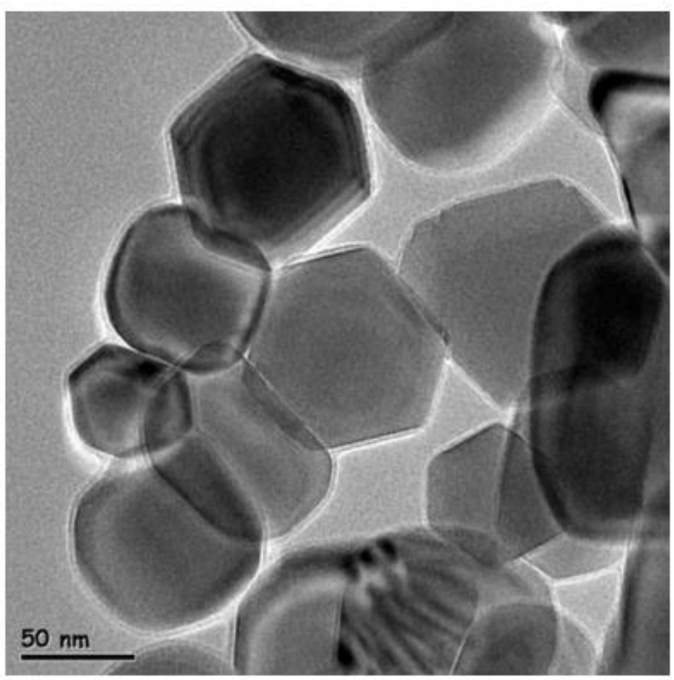
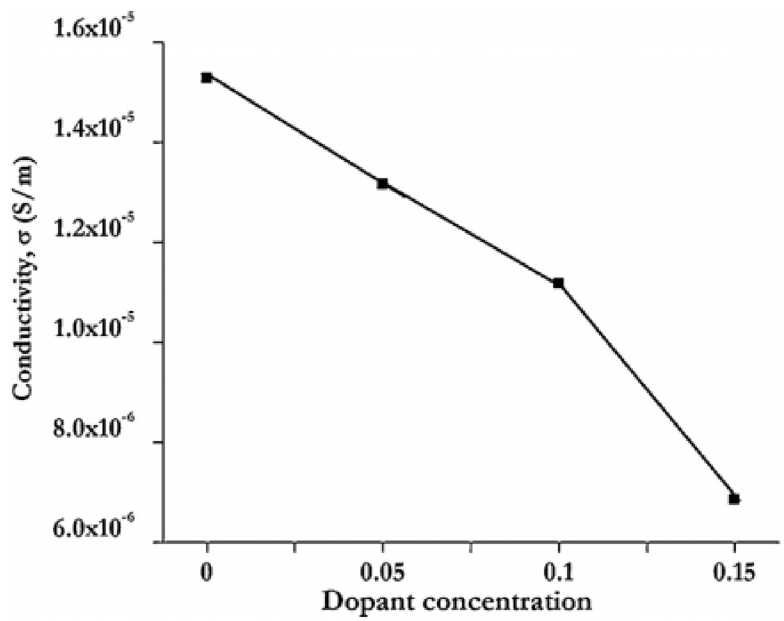
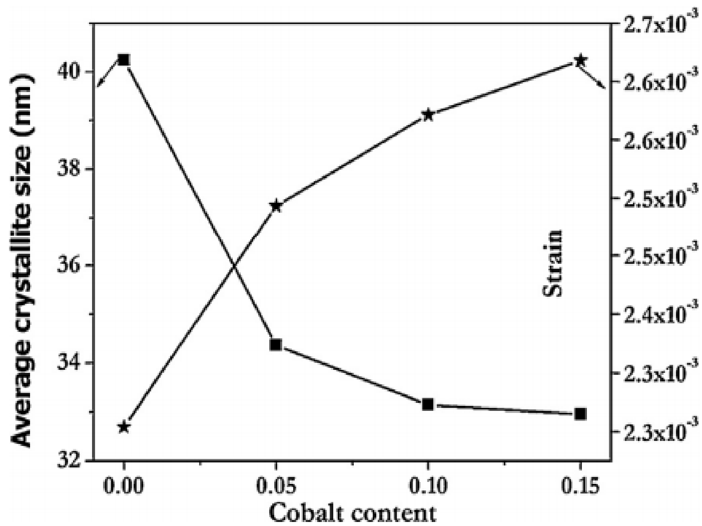


Figure 2. 1: TEM image of hexagonal wurtzite ZnO NPs [17].

The average crystal size and electrical conductivity of ZnO NPs is shown in figure 2.2 (a) and (b) respectively. As shown in Figure 2.2, decrease in conductivity with increase in doping concentration of cobalt in ZnO [18].



(a)



(b)

Figure 2. 2: (a).Variation of conductivity, σ(S/m) with dopant concentration, (b). Average crystallite size and strain Vs Co content of $Zn_{1-x}Co_xO$ NP [18].

The refractive index n of ZnO NP is, $n = 2.025$ from this, relative permittivity $\mathcal{E}_r$of ZnO nanoparticle is $\mathcal{E}_{r=}n^2 = (2.025)^2 = 4.1006$ at a wavelength of 600 nm as shown in Figure 2.3 [19].

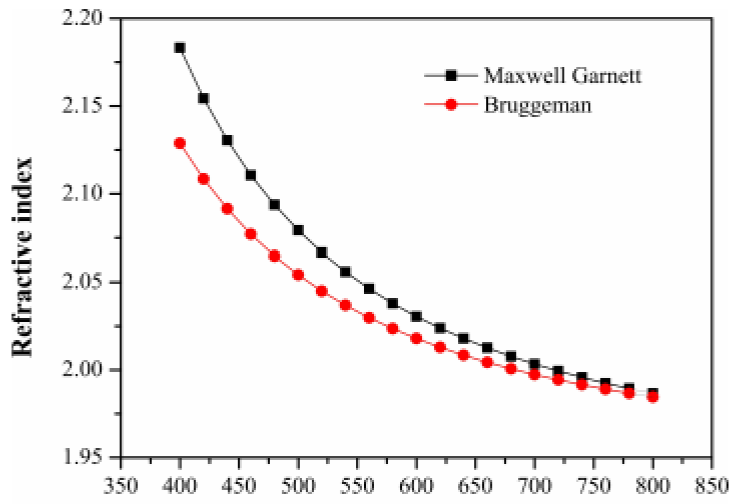


Figure 2. 3: Sellmeier approximation of the dispersion dependences of the refractive index of ZnO NP obtained by Maxwell Garnett and Bruggeman relations [19].

2.2 The Yee Algorithm

The FDTD algorithm as first proposed by Kane Yee in 1966 employs second-order central differences. The algorithm can be summarized as follows:

1. Replace all the derivatives in Ampere's and Faraday's laws with finite differences. Discretize space and time so that the electric and magnetic fields are staggered in both space and time.

2. Solve the resulting difference equations to obtain "update equations" that express the (unknown) future fields in terms of (known) past fields.

3. Evaluate the magnetic fields one time-step into the future so they are now known (effectively they become past fields).

4. Evaluate the electric fields one time-step into the future so they are now known (effectively they become past fields).

5. Repeat the previous two steps until the fields have been obtained over the desired duration [20].

2.3 Source Setup in an FDTD Simulation

FDTD algorithms require initial conditions, which mean that values of the fields must be specified throughout the lattice at the start of the simulation. Typically, all fields are initialized to zero. To perform a simulation, energy has to be introduced into the problem space; i.e., an electromagnetic wave source has to be created. The EM wave sources used in the FDTD method includes Gaussian pulse and sinusoidal source in one dimensional grid [21].

2.4 One-dimensional plane wave propagation in free space

Pranay Valson has studied a one-dimensional FDTD simulation in free space. He has simulated the result using Gaussian pulse [22] as shown in figure 2.4

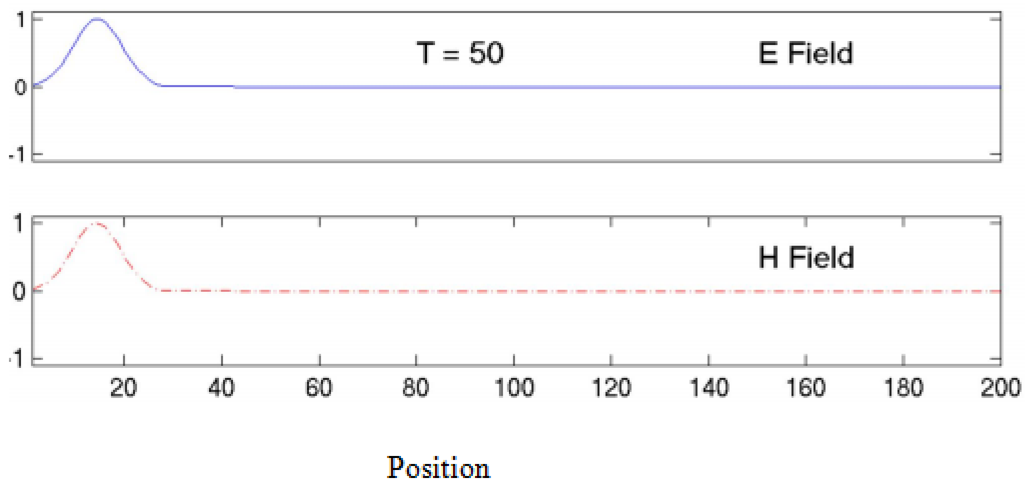


Figure 2. 4: A one-dimensional FDTD simulation in free space, at time step T = 50 the Gaussian pulse is propagating to the x+ direction [22].

A. Z. Elsherbeni and V. Demir reported that a one-dimensional FDTD implementation of electric and magnetic field components generated by a z-directed current sheet, J_z, placed at the center of a problem space filled with air between two parallel, perfect electric conductor (PEC) plates extending to infinity in the y and z dimensions. They have used Gaussian pulse source in both directions from the centre of the FDTD grid. Figure 2.5 shows simulation of E_z and H_y within the FDTD computational domain demonstrating the propagation of the fields [23].

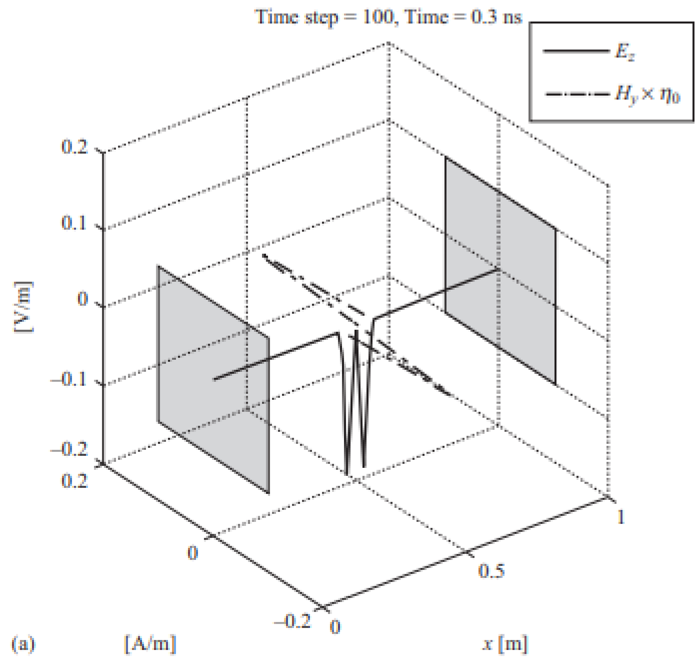
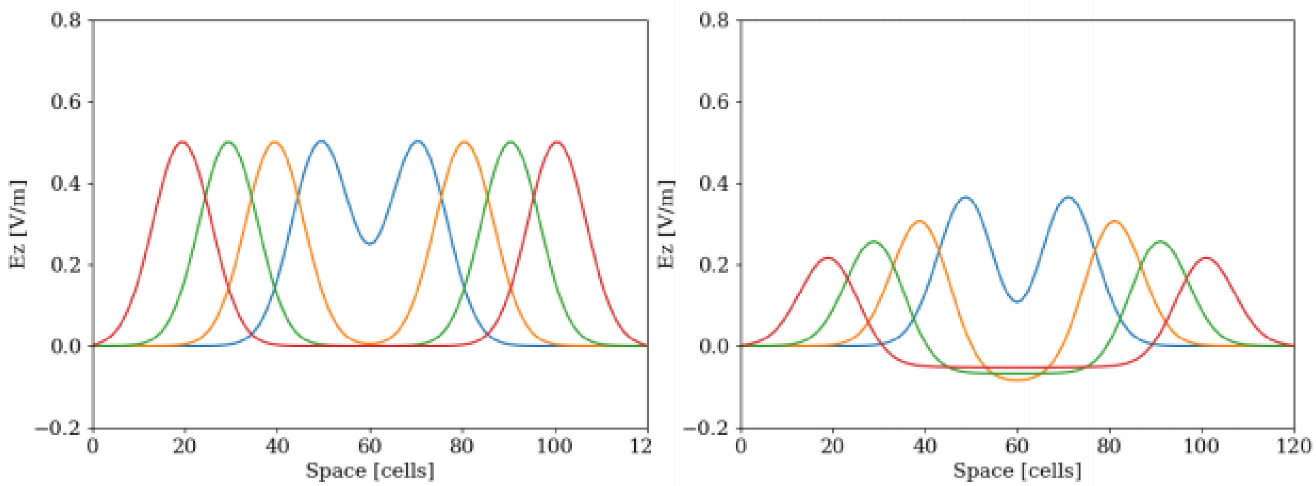


Figure 2. 5: Snapshots of a one-dimensional FDTD simulation: (a) fields observed after 100 time steps; (b) fields observed after 300 time steps [23].

2.5 One-dimensional plane wave propagation in a dielectric medium with conductivity

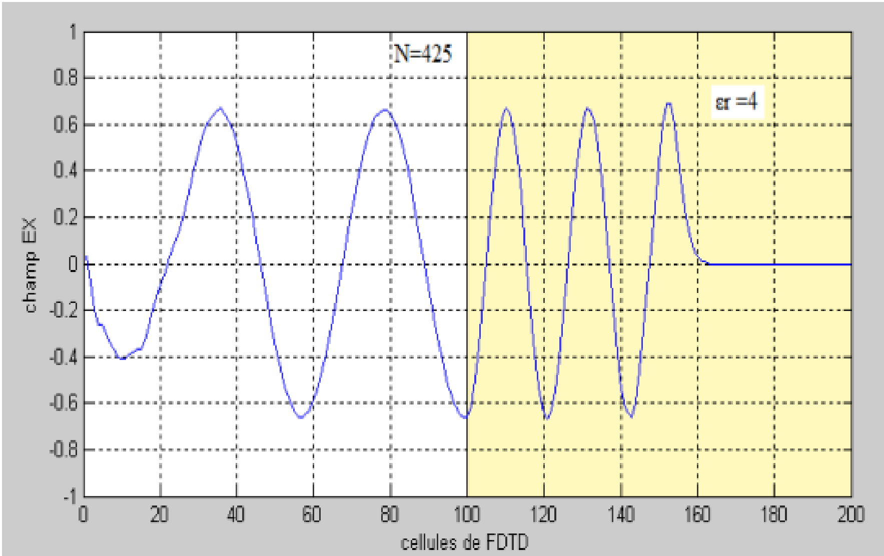
Gregory A et al have studied optical scatter in from isolated metal NP and array of gold and silver NPs. They have simulated the result using FDTD and experimentally verified it using Nedar-field scanning optical microscopy (NSOM) [24]. Maxim Sukharev and Tamar Seideman have theoretically studied coherent control of light propagation via NP arrays [25]. Gernot Ohner found that one dimensional simulation without and with electrical losses as shown in Fig 2.6 [26]. For Fig 2.6: (a) since the electrical conductivity is zero the magnitude of the electric field is not attenuate and the medium will not absorb the magnetic field. However for Fig 2.6: (b) since the medium has an electrical conductivity of 0.05 S/m the magnitude of the electric field is attenuate and absorbeded by the medium.



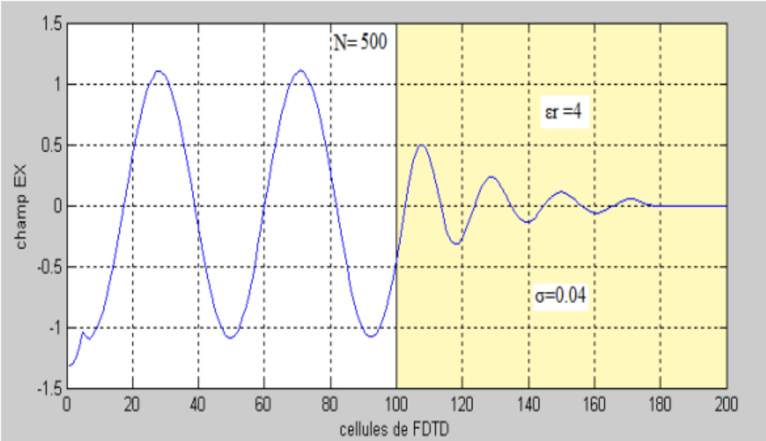
(a) (b)

Figure 2. 6: A one dimensional simulation a) without (σ=0 S/m) and b) with electrical losses (σ=0.005 S/m) Each colored line represents the value of the electric field at a different time step, after 10 (blue), 20 (orange), 30 (green) and 40 (red) time steps [26].

Ahmed Faize et al studied that numerical simulation of electromagnetic problems using FDTD method. Figure 2.7: (a) show the numerical results of the electric field Ex of the source in Sinusoidal form and the simulation of the propagation for this wave in a lossless dielectric medium εr. Figure 2.7: (b) show a dielectric medium with losses characterized with a conductivity σ and relative dielectric constant εr. The magnitude of the electric field is attenuate and absorbed by the medium due to electrical conductivity σ [27].



(a)



(b)

Figure 2. 7:.(a) Simulation of propagation of a sinusoidal wave incident on a medium of relative dielectric constant ε_r=4. (b)Simulation of propagating a sinusoidal wave hitting a lossy dielectric material and a dielectric constant ε_r=4, with a conductivity σ = 0.04 (S / m) [27].

CHAPTER THREE

METHODOLOGY

This section presents the formulation of the finite difference methods as well as formulations of the FDTD method that is used in this thesis.

3.1 Forward difference method

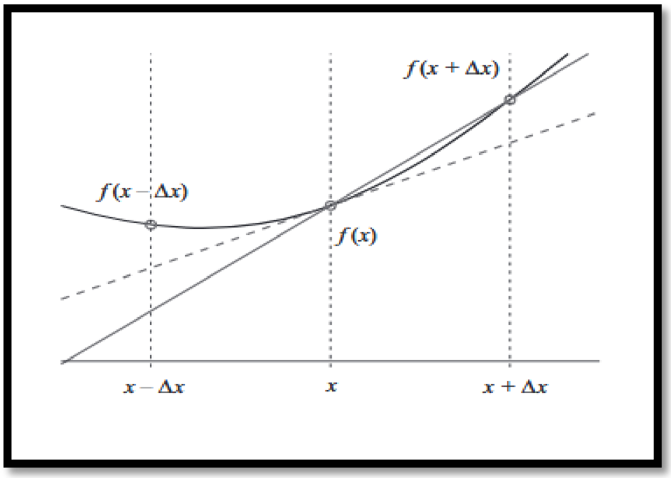


Figure 3. 1: Forward difference method approximation of the $\mathbf{f'(x)}$ of f(x) [23]

Forward difference method is obtained from the definition of the first derivative of a continuous function f(x) differentiable at x as shown in Figure 3.1 [12]

By using the forward point $f(x+\Delta x)$ the expression of the first derivative is written as

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Since Δx is very small the expression for first derivative is approximated by usingTaylor's series expansion of the forward point $f(x+\Delta x)$.

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{1}{2}f''(x)\Delta x^2 + \frac{1}{6}f'''(x)\Delta x^3 + \cdots \qquad 3.1$$

Since we want to express the expression of the first derivative, from equation (3.1) the terms written after first derivative are approximated. Therefore, equation (3.1) can be written as

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + O(\Delta x)^2$$

Divide both sides by Δx and rearrange it, we get that

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} + O(\Delta x) \qquad 3.2$$

Equation (3.2) is called forward difference formula and the expression $O(\Delta x)$ indicates that the error of approximation is in the order of Δx.

3.2 Backward difference method

In a similar manner by using a backward point, as shown in figure 3.2$f(x - \Delta x)$, we can approximate$f'(x)$ using Taylor series expansion.

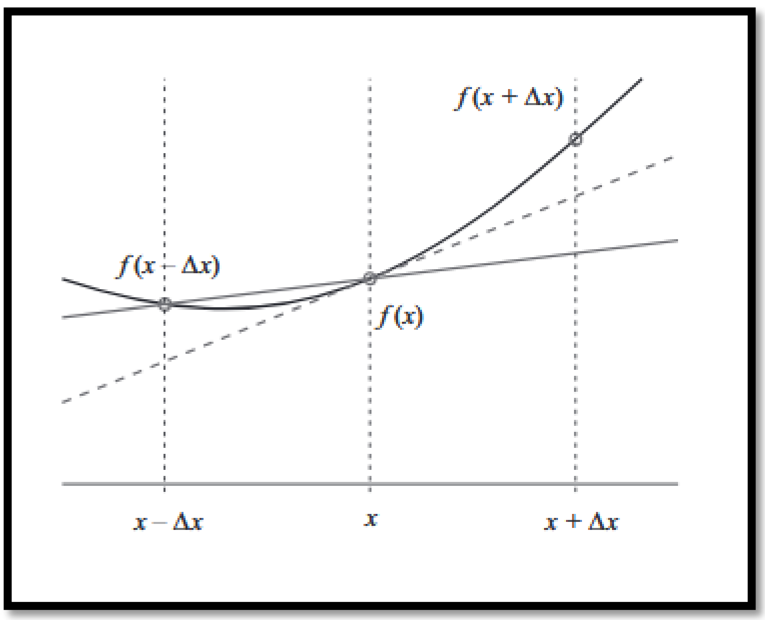


Figure 3. 2: Backward difference method approximation of the **f′(x)** of f(x) [23]

$$f(x - \Delta x) = f(x) - f'(x)\Delta x + \frac{1}{2}f''(x)\Delta x^2 - \frac{1}{6}f'''(x)\Delta x^3 + \cdots \qquad 3.3$$

The terms after $f'(x)$are called errors

$$f(x-\Delta x)-f(x)=-f'(x)\Delta x+O(\Delta x)^2$$

After divide both sides by Δx and rearrange it we get

$$f'(x)=\frac{f(x-\Delta x)-f(x)}{\Delta x}+O(\Delta x) \qquad 3.4$$

3.3 Central difference method

The formula for central difference method is obtained by using the forward point $f(x+\Delta x)$and back ward point$f(x-\Delta x)$ as shown in figure 3.3.

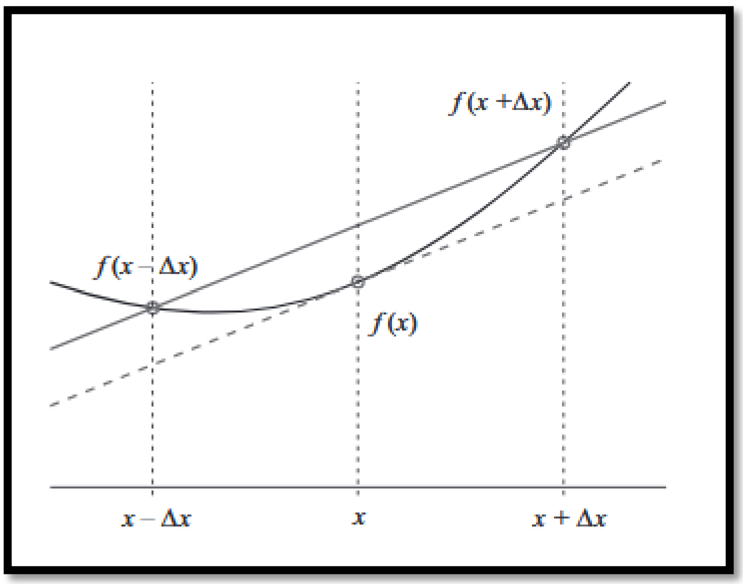


Figure 3. 3: Central difference method approximation of the $\mathbf{f'(x)}$ of f(x) [23]

Subtract equation (3.3) from (3.1)

$$f(x+\Delta x)-f(x-\Delta x)=f(x)+f'(x)\Delta x+\tfrac{1}{2}f''(x)\Delta x^2+\tfrac{1}{6}f'''(x)\Delta x^3+\cdots\text{-}(f(x)-f'(x)\Delta x+\tfrac{1}{2}f''(x)\Delta x^2-\tfrac{1}{6}f'''(x)\Delta x^3+\cdots)$$

$$f(x+\Delta x)-f(x-\Delta x)$$
$$=f(x)-f(x)+f'(x)\Delta x+f'(x)\Delta x+\frac{1}{2}f''(x)\Delta x^2-\frac{1}{2}f''(x)\Delta x^2+\frac{1}{6}f'''(x)\Delta x^3+\frac{1}{6}f'''(x)\Delta x^3+\cdots$$

$$f(x+\Delta x) - f(x-\Delta x) = 2f'(x)\Delta x + 2\frac{1}{6}f'''(x)\Delta x^3 + \cdots$$

The term after $f'(x)$ is approximated term because Δx is very small and $\Delta x^3$is very very small.

$$f(x+\Delta x) - f(x-\Delta x) = 2f'(x)\Delta x + O(\Delta x)^3$$

$$\frac{f(x+\Delta x) - f(x-\Delta x)}{2\ \Delta x} = f'(x) + O(\Delta x)^2$$

$$f'(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + O(\Delta x)^2 \qquad 3.5$$

Equation (3.5) indicates that the central difference approximation is second order accurate, meaning the error is less. While forward and backward approximations are first order accurate and the error is greater than central difference approximation. As a result, central difference approximation is the best approximation method.

3.4 The FDTD Method and discretization of Maxwell’s curl equations

The FDTD method is one of the most popular numerical methods of modeling electromagnetic wave propagations. Since it is a numerical method of directly solving Maxwell's time dependent equations using the finite difference method those equations are discretized in the time and spacial domains by using the finite difference method.

The FDTD method is formulated by converting Maxwell’s curl equations into a discrete form. Maxwell’s equations represent the propagation of an electromagnetic wave and the relationship between the electric and magnetic fields. The medium is linear, uniform, isotropic, and homogeneous with conduction current. Maxwell’s curl equations (1.3 and 1.4) become:

$$\nabla \times \mathrm{H} = \varepsilon \frac{\partial \mathrm{E}}{\partial \mathrm{t}} + J \qquad 3.6$$

$$\nabla \times \mathrm{E} = -\mu \frac{\partial \mathrm{H}}{\partial \mathrm{t}} - M \qquad 3.7$$

$M = M_c + M_i$is the magnetic current density and $M_c = \sigma_m H$ is the conduction magnetic density and M_i is the imposed magnetic density. And $J = J_c + J_i$is the electric current density;$J_c = \sigma_e E$ is the conduction current density and J_i is the imposed current density. Therefore equation 3.6 and 3.7 can be rewritten as

$$\nabla \times \mathrm{H} = \varepsilon \frac{\partial \mathrm{E}}{\partial \mathrm{t}} + \sigma_e E + J_i \qquad 3.8$$

$$\nabla \times \mathrm{E} = -\mu \frac{\partial \mathrm{H}}{\partial \mathrm{t}} - \sigma_m H - M_i \qquad 3.9$$

For one dimensional case equations (3.8) and (3.9) in a Cartesian coordinate system can be expressed as

$$\nabla \times \mathrm{H} = \varepsilon \frac{\partial \mathrm{E}}{\partial \mathrm{t}} + \sigma_e E + J_i$$

$$\begin{pmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ \frac{\partial}{\partial x} & 0 & 0 \\ 0 & H_y & 0 \end{pmatrix} = \varepsilon \frac{\partial}{\partial t} \begin{pmatrix} 0 \\ 0 \\ \mathrm{E}_z \end{pmatrix} + \sigma_e \begin{pmatrix} 0 \\ 0 \\ \mathrm{E}_z \end{pmatrix} + J_i$$

$$\left(\frac{\partial H_y}{\partial x} \right) \hat{k} = \varepsilon \frac{\partial \mathrm{E}_z}{\partial t} + \sigma_e \mathrm{E}_z + J_i$$

$$\frac{\partial \mathrm{E}_z}{\partial t} = \frac{1}{\varepsilon} \left(\frac{\partial H_y}{\partial x} - \sigma_e \mathrm{E}_z - J_i \right) \qquad 3.10$$

$$\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t} - \sigma_m H - M_i$$

$$\begin{pmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ \frac{\partial}{\partial x} & 0 & 0 \\ 0 & 0 & \mathrm{E}_z \end{pmatrix} = -\mu \frac{\partial}{\partial t} \begin{pmatrix} 0 \\ \mathrm{H}_y \\ 0 \end{pmatrix} - \sigma_m \begin{pmatrix} 0 \\ \mathrm{H}_y \\ 0 \end{pmatrix} - M_i$$

$$-\hat{j}\left(\frac{\partial \mathrm{E_z}}{\partial x}\right) = -\mu\frac{\partial \mathrm{H_y}}{\partial t} - \sigma_m \mathrm{H_y} - M_i$$

$$\frac{\partial \mathrm{H_y}}{\partial t} = \frac{1}{\mu}\left(\frac{\partial \mathrm{E_z}}{\partial x} - \sigma_m \mathrm{H_y} - M_i\right) \qquad 3.11$$

3.5 FDTD updating equations for one dimension

Those time-dependent Maxwell's curl equations (3.10 and 3.11) can be represented in discrete form, both in space and time, using the second-order accurate central difference formula. The electric and magnetic field components are sampled at discrete positions both in time and space. The FDTD algorithm calculates the fields at discrete time instants; however, the electric and magnetic field components are not sampled at the same time instants. For a time-sampling period Δt, the electric field components are sampled at time instants $0, \Delta t, 2\Delta t \ldots, n\Delta t, \ldots$; however, the magnetic field components are sampled at time instants $\frac{1}{2}\Delta t$, $(1+\frac{1}{2})\Delta t$, …,$(n+\frac{1}{2})$….Therefore, the electric field components are calculated at integer time steps, and magnetic field components are calculated at half-integer time steps, and they are offset from each other by $\frac{\Delta t}{2}$. The field components need to be referred not only by their spatial indices which indicate their positions in space, but also by their temporal indices, which indicate their time instants. Therefore, a superscript notation is adopted to indicate the time instant. For instance, the *z* component of an electric field vector positioned at$((i-1)\Delta x, (j-1)\Delta y, (k-1)\Delta z)$ and sampled at time instant $n\Delta t$ is referred to as$E_z^n(\mathrm{i,j,k})$. Similarly, the y component of a magnetic field vector positioned at $(\left(i-\frac{1}{2}\right)\Delta x, (j-1)\Delta y, \left(k-\frac{1}{2}\right)\Delta z)$ and sampled at time instant $(n+\frac{1}{2})\Delta t$ is referred to as $H_y^{n+\frac{1}{2}}(i,j,k)$. Maxwell's curl equations can be expressed in terms of finite differences. For equation (3.10)

$$\frac{\partial \mathrm{E}_z}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \sigma_e \mathrm{E}_z - J_i\right)$$

The derivatives in this equation can be approximated by using the central difference formula with the position of $\mathrm{E}_z(\mathrm{i})$ being the center point for the central difference formula in space and time instant $(n+\frac{1}{2})\Delta t$ as being the center point in time.

$$\frac{E_z^{n+1}(i) - E_z^{n}(i)}{\Delta t} = \frac{1}{\mathcal{E}} \frac{H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)}{\Delta x} - \frac{\sigma_e}{\mathcal{E}} E_z^{n+\frac{1}{2}}(i) - \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}} \qquad 3.12$$

Since (3.12) contain $E_z^{n+\frac{1}{2}}(i)$, this term can be written as the average of the terms at time instants $(n+1)\Delta t$ and $n\Delta t$ as

$$E_z^{n+\frac{1}{2}}(i) = \frac{E_z^{n+1}(i) - E_z^{n}(i)}{2} \qquad 3.13$$

Using equation (3.13) into (3.12) and by arranging the terms we can write

$$\frac{E_z^{n+1}(i,j,k)}{\Delta t} - \frac{E_z^{n}(i,j,k}{\Delta t} = \frac{1}{\mathcal{E}} \frac{H_y^{n+\frac{1}{2}}(i,j,k) - H_y^{n+\frac{1}{2}}(i-1,j,k)}{\Delta x} - \frac{\sigma_e}{\mathcal{E}} \left(\frac{E_z^{n+1}(i,j,k) + E_z^{n}(i,j,k)}{2}\right) - \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}}$$

$$\frac{E_z^{n+1}(i)}{\Delta t} - \frac{E_z^{n}(i)}{\Delta t} = \frac{1}{\mathcal{E}} \frac{H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)}{\Delta x} - \frac{\sigma_e}{2\mathcal{E}} E_z^{n+1}(i) - \frac{\sigma_e}{2\mathcal{E}} E_z^{n}(i) - \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}} \left(\frac{1}{\Delta t} + \frac{\sigma_e}{2\mathcal{E}}\right) E_z^{n+1}(i)$$

$$= \frac{1}{\mathcal{E}\Delta x} \left(H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)\right) + \left(\frac{1}{\Delta t} - \frac{\sigma_e}{2\mathcal{E}}\right) E_z^{n}(i) - \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}}$$

$$\left(\frac{2\mathcal{E} + \Delta t \sigma_e}{2\mathcal{E}\Delta t}\right) E_z^{n+1}(i) = \frac{1}{\mathcal{E}\Delta x} \left(H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)\right) + \left(\frac{2\mathcal{E} - \Delta t \sigma_e}{2\mathcal{E}\Delta t}\right) E_z^{n}(i) - \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}}$$

$$E_z^{n+1}(i) = \left(\frac{2\mathcal{E}\Delta t}{2\mathcal{E} + \Delta t \sigma_e}\right) \frac{1}{\mathcal{E}\Delta x} \left(H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)\right) + \left(\frac{2\mathcal{E}\Delta t}{2\mathcal{E} + \Delta t \sigma_e}\right) \left(\frac{2\mathcal{E} - \Delta t \sigma_e}{2\mathcal{E}\Delta t}\right) E_z^{n}(i) - \left(\frac{2\mathcal{E}\Delta t}{2\mathcal{E} + \Delta t \sigma_e}\right) \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}}$$

$$E_z^{n+1}(i) = \left(\frac{2\mathcal{E}\Delta t}{2\mathcal{E} + \Delta t \sigma_e}\right) \left(\frac{2\mathcal{E} - \Delta t \sigma_e}{2\mathcal{E}\Delta t}\right) E_z^{n}(i) + \left(\frac{2\mathcal{E}\Delta t}{2\mathcal{E} + \Delta t \sigma_e}\right) \frac{1}{\mathcal{E}\Delta x} \left(H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)\right) - \left(\frac{2\mathcal{E}\Delta t}{2\mathcal{E} + \Delta t \sigma_e}\right) \frac{1}{\mathcal{E}} J_i^{n+\frac{1}{2}}$$

$$E_z^{n+1}(i) = \frac{2\mathcal{E} - \Delta t\sigma_e}{2\mathcal{E} + \Delta t\sigma_e} E_z^n(i) + \frac{2\Delta t}{(2\mathcal{E} + \Delta t\sigma_e)\Delta x} (H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1))$$

$$- \frac{2\Delta t}{2\mathcal{E} + \Delta t\sigma_e} J_i^{n+\frac{1}{2}} \qquad 3.14$$

$$\text{Let } \frac{2\mathcal{E} - \Delta t\sigma_e}{2\mathcal{E} + \Delta t\sigma_e} = \text{Ceze}, \frac{2\Delta t}{(2\mathcal{E} + \Delta t\sigma_e)\Delta x} = \text{Cezhy and } -\frac{2\Delta t}{2\mathcal{E} + \Delta t\sigma_e} = \text{Cezj}$$

Therefore (3.14) can be written as

$$E_z^{n+1}(i) = \text{Ceze} \times E_z^n(i) + \text{Cezhy} \times (H_y^{n+\frac{1}{2}}(i) - H_y^{n+\frac{1}{2}}(i-1)) + \text{Cezj} \times J_i^{n+\frac{1}{2}} \qquad 3.15$$

Similarly, updating equations can be obtained for magnetic field components following the same methodology. However, while applying the central difference formula to the time derivative of the magnetic field components, the central point in time shall be taken as $n\Delta t$. Equation (3.11)

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_z}{\partial x} - \sigma_m H_y - M_i\right)$$

Must be approximated using finite differences

$$\frac{H_y^{n+\frac{1}{2}}(i) - H_y^{n-\frac{1}{2}}(i)}{\Delta t} = \frac{1}{\mu}\frac{E_z^{n+1}(i+1) - E_z^n(i)}{\Delta x} - \frac{\sigma_m}{\mu} H_y^n(i) - \frac{1}{\mu} M_i^n \qquad 3.16$$

$$\text{But,} \qquad H_y^n(i) = \frac{H_y^{n+\frac{1}{2}} + H_y^{n-\frac{1}{2}}}{2}$$

$$\frac{H_y^{n+\frac{1}{2}}(i)}{\Delta t} - \frac{H_y^{n-\frac{1}{2}}(i)}{\Delta t} = \frac{1}{\mu\Delta x} E_z^{n+1}(i+1) - \frac{1}{\mu\Delta x} E_z^n(i) - \frac{\sigma_m}{\mu}\left(\frac{H_y^{n+\frac{1}{2}} + H_y^{n-\frac{1}{2}}}{2}\right) - \frac{1}{\mu} M_i^n$$

$$\frac{H_y^{n+\frac{1}{2}}(i)}{\Delta t} - \frac{H_y^{n-\frac{1}{2}}(i)}{\Delta t} = -\frac{\sigma_m}{2\mu} H_y^{n+\frac{1}{2}} - \frac{\sigma_m}{2\mu} H_y^{n-\frac{1}{2}} + \frac{1}{\mu\Delta x} E_z^{n+1}(i+1) - \frac{1}{\mu\Delta x} E_z^n(i) - \frac{1}{\mu} M_i^n$$

$$\frac{1}{\Delta t}H_y^{n+\frac{1}{2}}(i)+\frac{\sigma_m}{2\mu}H_y^{n+\frac{1}{2}}=\frac{1}{\Delta t}H_y^{n-\frac{1}{2}}(i)-\frac{\sigma_m}{2\mu}H_y^{n-\frac{1}{2}}+\frac{1}{\mu\Delta x}E_z^{n+1}(i+1)-\frac{1}{\mu\Delta x}E_z^{n}(i)-\frac{1}{\mu}M_i^n$$

$$\left(\frac{1}{\Delta t}+\frac{\sigma_m}{2\mu}\right)H_y^{n+\frac{1}{2}}(i)=\left(\frac{1}{\Delta t}-\frac{\sigma_m}{2\mu}\right)H_y^{n-\frac{1}{2}}+\frac{1}{\mu\Delta x}\left(E_z^{n+1}(i+1)-E_z^{n}(i)\right)-\frac{1}{\mu}M_i^n$$

$$\left(\frac{2\mu+\Delta t\sigma_m}{2\mu\Delta t}\right)H_y^{n+\frac{1}{2}}(i)=\frac{2\mu-\Delta t\sigma_m}{2\mu\Delta t}H_y^{n-\frac{1}{2}}(i)+\frac{1}{\mu\Delta x}\left(E_z^{n+1}(i+1)-E_z^{n}(i)\right)-\frac{1}{\mu}M_i^n$$

$$H_y^{n+\frac{1}{2}}(i)=\left(\frac{2\mu\Delta t}{2\mu+\Delta t\sigma_m}\right)\frac{2\mu-\Delta t\sigma_m}{2\mu\Delta t}H_y^{n-\frac{1}{2}}(i)+\left(\frac{2\mu\Delta t}{2\mu+\Delta t\sigma_m}\right)\frac{1}{\mu\Delta x}\left(E_z^{n+1}(i+1)-E_z^{n}(i)\right)-\left(\frac{2\mu\Delta t}{2\mu+\Delta t\sigma_m}\right)\frac{1}{\mu}M_i^n$$

$$H_y^{n+\frac{1}{2}}(i)=\left(\frac{2\mu-\Delta t\sigma_m}{2\mu+\Delta t\sigma_m}\right)H_y^{n-\frac{1}{2}}(i)+\frac{2\Delta t}{(2\mu+\Delta t\sigma_m)\Delta x}\left(E_z^{n+1}(i+1)-E_z^{n}(i)\right)-\left(\frac{2\Delta t}{2\mu+\Delta t\sigma_m}\right)M_i^n \qquad 3.17$$

Let $\frac{2\mu-\Delta t\sigma_m}{2\mu+\Delta t\sigma_m}=Chyh$, $\frac{2\Delta t}{(2\mu+\Delta t\sigma_m)\Delta x}=Chyez$ and $\frac{2\Delta t}{2\mu+\Delta t\sigma_m}=Chym$

Therefore (3.17) can be written as

$$H_y^{n+\frac{1}{2}}(i)=Chyh\times H_y^{n-\frac{1}{2}}(i)+Chyez\times\left(E_z^{n+1}(i+1)-E_z^{n}(i)\right)-Chym\times M_i^n \qquad 3.18$$

3.6 Flow chart of 1-D FDTD method

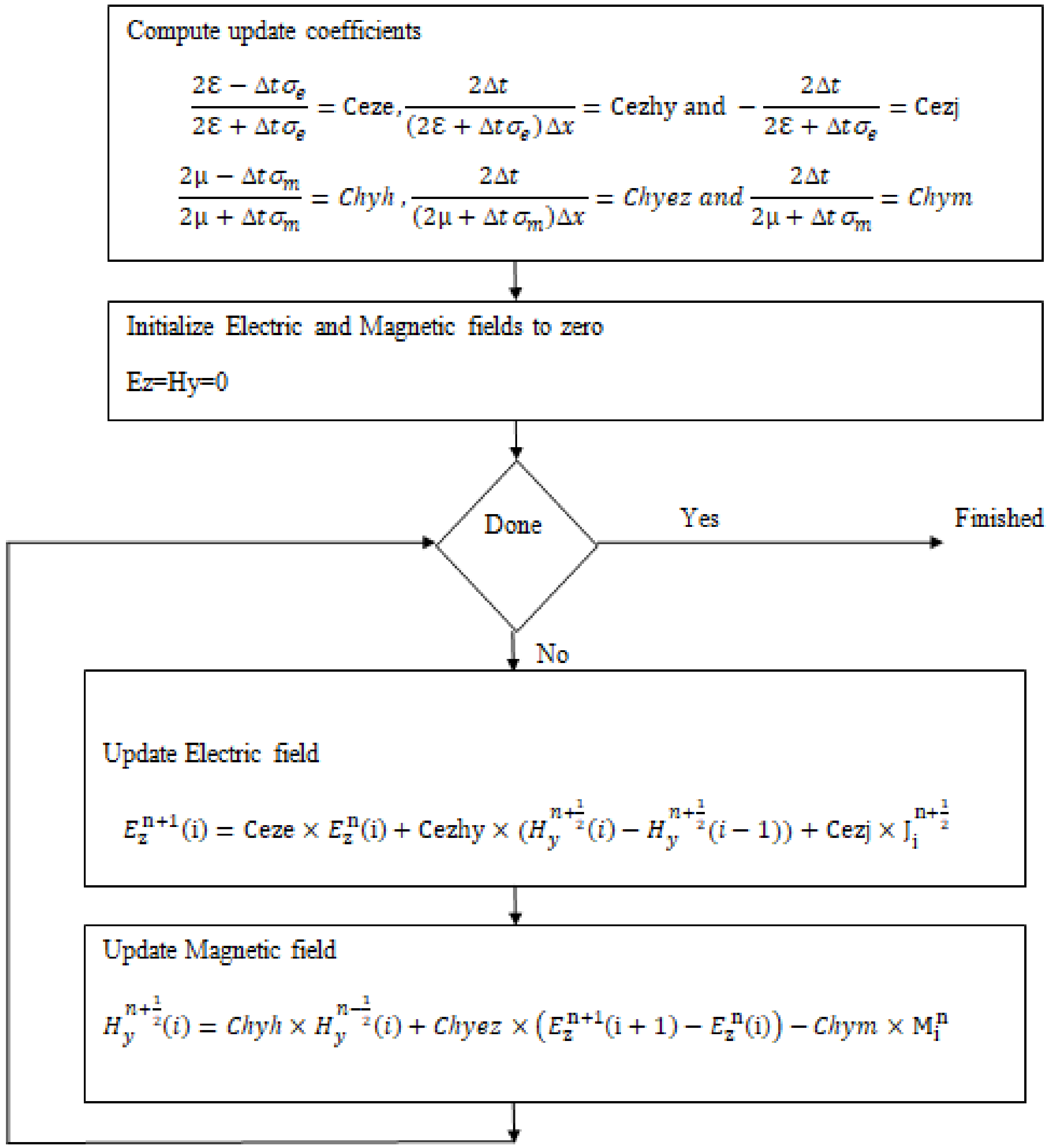


Figure 3. 4: Flow chart of FDTD method.

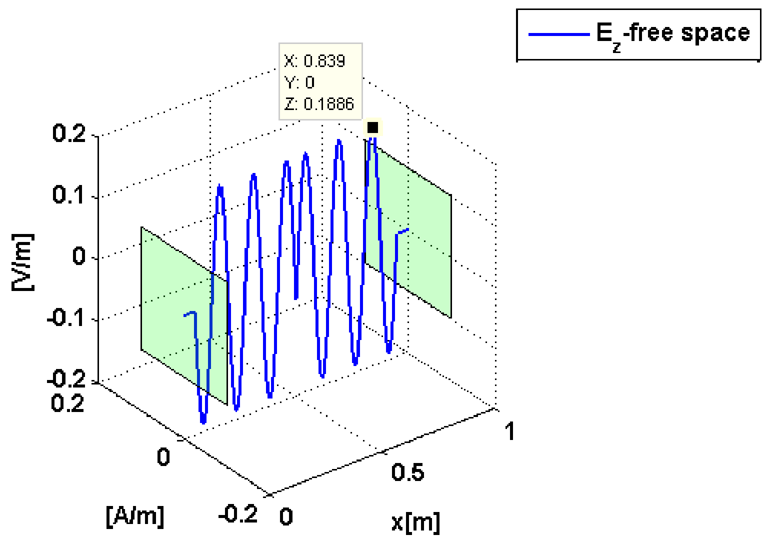
CHAPTER FOUR

RESULTS AND DISCUSSION

In this thesis we have simulated the propagation of electric and magnetic field. Mainly we have simulated electric and magnetic field propagation in free space and in ZnO NP by using the FDTD algorithm as explained in [20]. Pranay Valson [22] and A. Z. Elsherbeni and V. Demir [23] uses Gaussian pulse sources, but since sinusoidal wave form sources express the correct propagation of electric and magnetic field than Gaussian pulse sources. Therefore we have used sinusoidal wave form sources. The basic findings of our investigations are presented as follows.

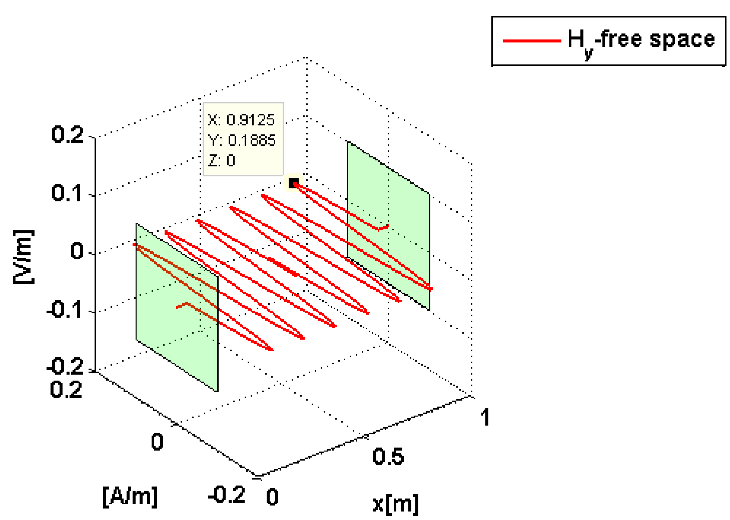
4.1 Simulation of electric and magnetic field in free space

Using the permittivity and permeability of free space, which is obtained from [13], in the updating equations (3.15) and (3.18) MATLAB code is generated using MATLAB software. Using the generated code electric and magnetic fields are simulated by a z-directed sinusoidal current source, Jz, placed at the center of a problem space filled with air between two parallel, perfect electric conductor (PEC) plates extending to infinity in the y and z directions. The simulation of electric and magnetic field within the FDTD computational domain demonstrating the propagation of the fields and is shown in Figure 4.1. From the figure both the magnitude of the electric and magnetic field does not attenuate, because of the conductivity of free space is zero this result is the same as shown in figure 2.7: (a) [27]. A MATLAB code is given in Appendix for a one-dimensional FDTD simulation for free space.



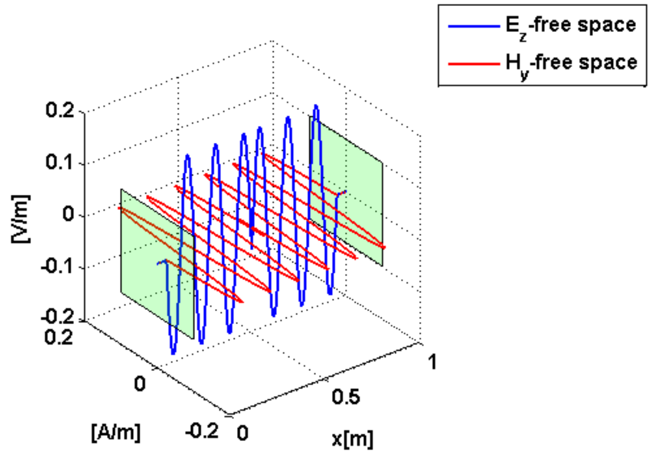
Ez-free space
X: 0.839
Y: 0
Z: 0.1886
0.2
0.1
0
-0.1
-0.2
[V/m]
0.2
0
-0.2
[A/m]
0
0.5
1
x[m]

(a)



Hy-free space
X: 0.9125
Y: 0.1885
Z: 0
0.2
0.1
0
-0.1
-0.2
[V/m]
0.2
0
-0.2
[A/m]
0
0.5
1
x[m]

(b)



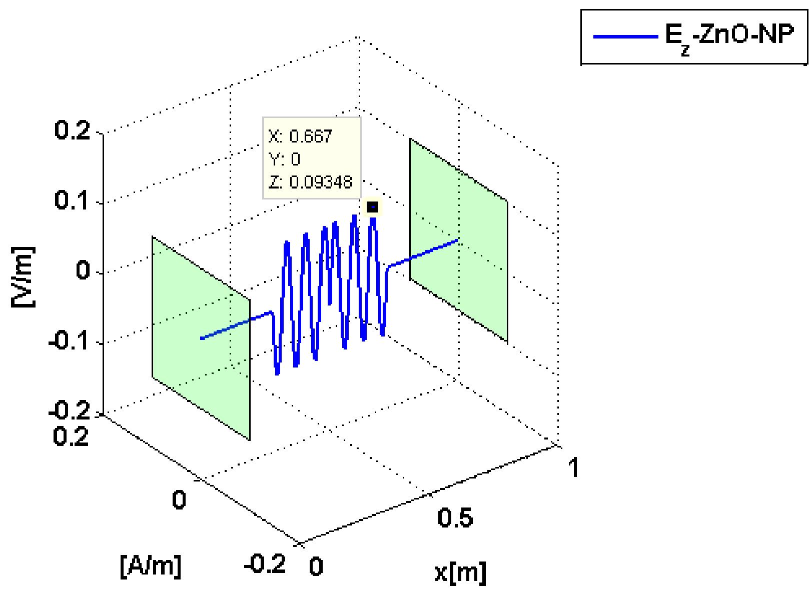
(c)

Figure 4. 1: One-dimensional FDTD simulation in free space: (a) electric field observed after 500 time steps; (b) magnetic field observed after 500 time steps; (c) both electric and magnetic field.

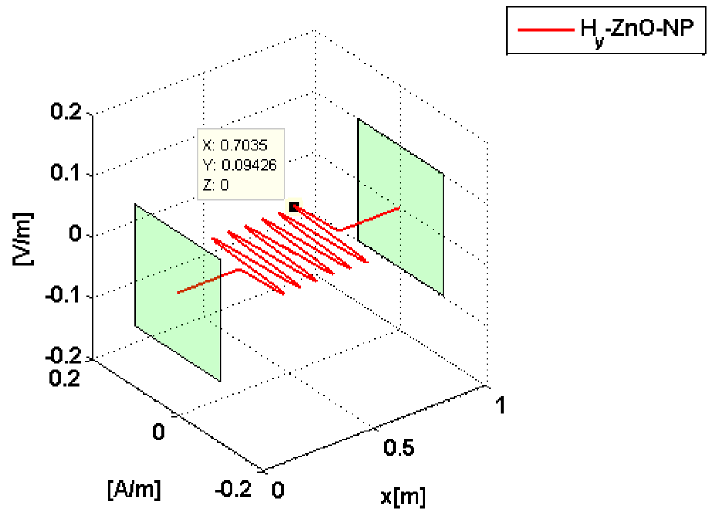
4.2 Simulation of electric and magnetic field in ZnO NPs of different electrical conductivity

The dielectric constant of ZnO NPs is 4.001 and is obtained from [19]. Using the permittivity and permeability of free space, which is obtained from [13], in the updating equations (3.15) and (3.18) MATLAB code was generated using MATLAB software. Using the generated code electric and magnetic fields are simulated by a z-directed sinusoidal current source, J_z, placed at the center of a problem space filled with ZnO NP between two parallel, perfect electric conductor (PEC) plates extending to infinity in the y and z directions. The simulation of E_z and H_y within the FDTD computational domain demonstrating the propagation of the fields and is shown in Fig 4.2.

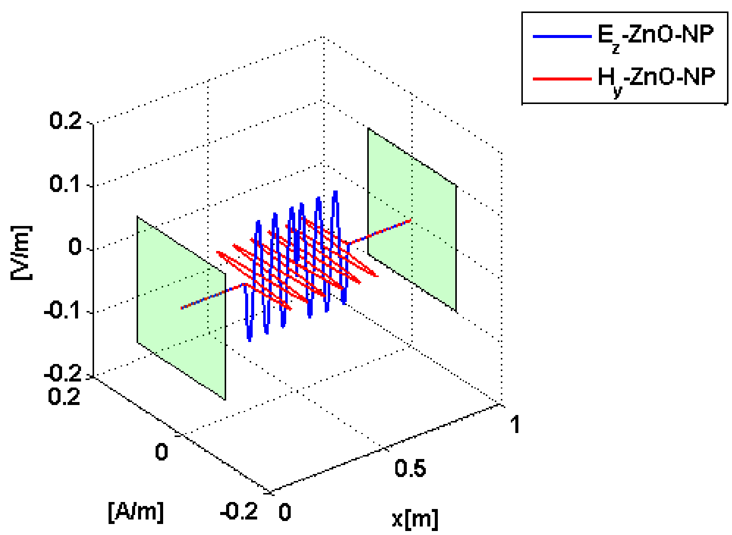
For ZnO NPs doped with cobalt ($Zn_{1-x}Co_xO$) when x=0.15, the electrical conductivity is $7x10^{-6}$ S/m [18]. We have used this electrical conductivity value and we get the simulation result as shown in Fig 4.2. For Fig 4.2: (a) the magnitude of the electric field is 0.09348 V/m. As compared to the magnitude of the electric field in free space (0.1886 V/m), the magnitude of electric field in ZnO NPs is slightly decreased but not attenuated. Materials having small value of electrical conductivity absorb small amount of energy. Since we have used small value of electrical conductivity for ZnO NPs, we get a minimum absorption and attenuation level of the magnitude of the electric field. Therefore the difference between 0.1886 V/m and 0.09348 V/m is 0.09512 V/m and this is the amount of electric field absorbed by ZnO NPs. For Fig 4.2: (b) the magnitude of the magnetic field is 0.09426 A/m. As compared to the magnitude of the magnetic field in free space (0.1885 A/m), the magnitude of magnetic field in ZnO NPs is slightly decreased but not attenuated. Since we have used small value of electrical conductivity for ZnO NPs, we get a minimum absorption and attenuation level of the magnitude of the magnetic field. Therefore the difference between 0.1885 A/m and 0.09426 A/m is 0.09424 A/m and this is the amount of magnetic field absorbed by ZnO NPs



(a)



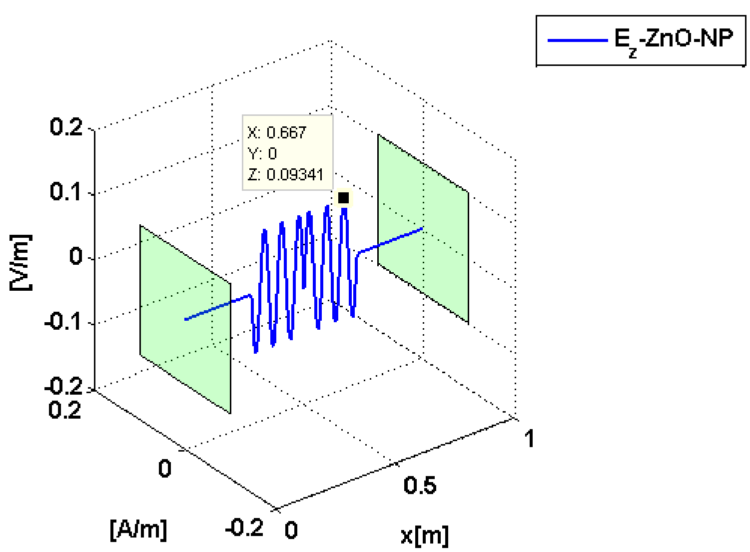
(b)



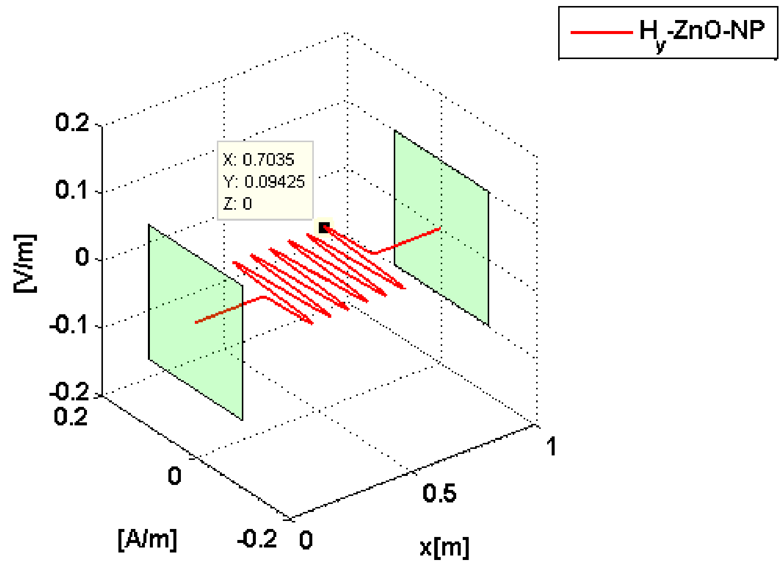
(c)

Figure 4. 2: One-dimensional FDTD simulation in ZnO NPs: (a) electric field observed after 500 time steps ; (b) magnetic fields observed after 500 time steps ; (c) both electric and magnetic field.

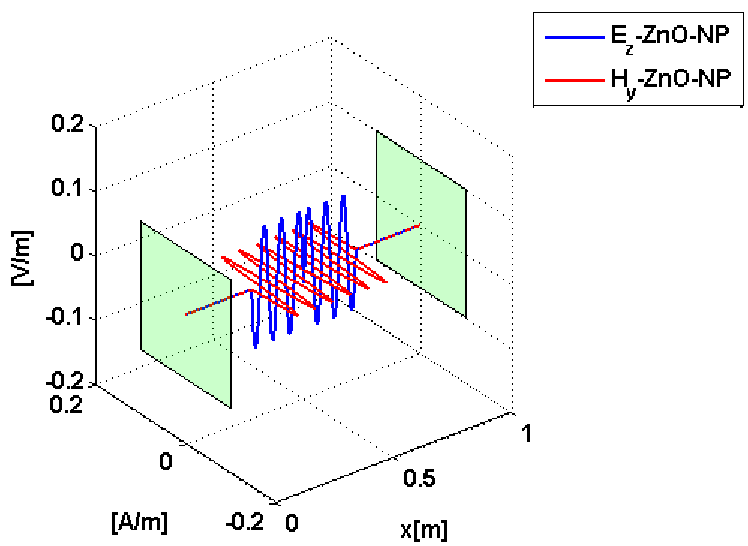
When x=0, in ZnO NPs doped with cobalt ($Zn_{1-x}Co_xO$), it becomes pure ZnO NPs and the electrical conductivity of pure ZnO NPs is 1.5×10^{-5} S/m [18]. The simulation result is shown in Fig 4.3. For Fig 4.3: (a) the magnitude of the electric field is 0.09341 V/m. As compared to the magnitude of the electric field in free space (0.1886 V/m), the magnitude of electric field in pure ZnO NPs is decreased but not attenuated. Since we have used small value of electrical conductivity for ZnO NPs, we get a minimum absorption and attenuation level of the magnitude of the electric field. Therefore the difference between 0.1886 V/m and 0.09341 V/m is 0.09519 V/m and this is the amount of electric field absorbed by pure ZnO NPs. For Fig 4.3: (b) the magnitude of the magnetic field is 0.09425 A/m. As compared to the magnitude of the magnetic field in free space (0.1885 A/m), the magnitude of magnetic field in ZnO NPs is decreased. Since we have used small value of electrical conductivity for pure ZnO NPs, we get a minimum absorption and attenuation level of the magnitude of the magnetic field. Therefore the difference between 0.1885 A/m and 0.09425 A/m is 0.09425 A/m and this is the amount of magnetic field absorbed by pure ZnO NPs. The absorption level of the electric and magnetic field in Fig 4.3 is greater than in Fig 4.2, because the electrical conductivity for Fig 4.3 is greater than for Fig 4.2.



(a)



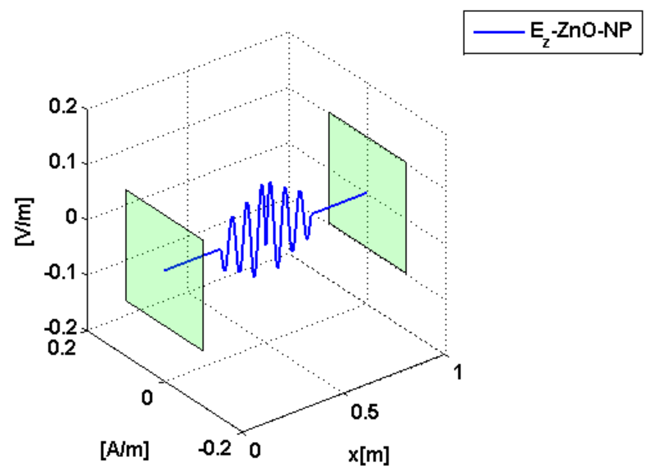
(b)



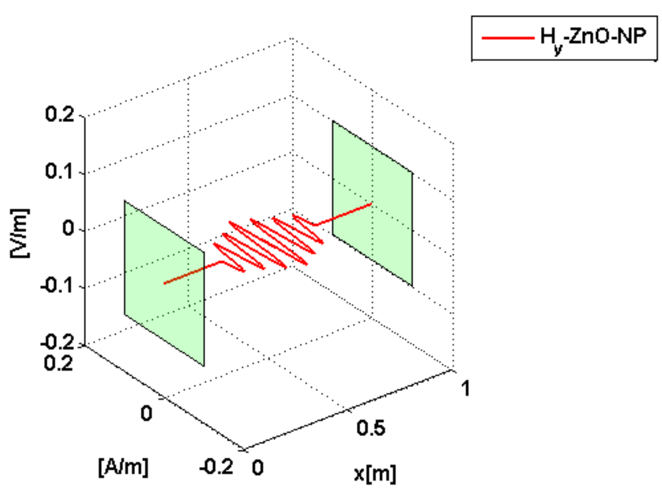
(c)

Figure 4. 3: One-dimensional FDTD simulation in ZnO NPs: (a) electric field observed after 500 time steps; (b) magnetic fields observed after 500 time steps; (c) both electric and magnetic field.

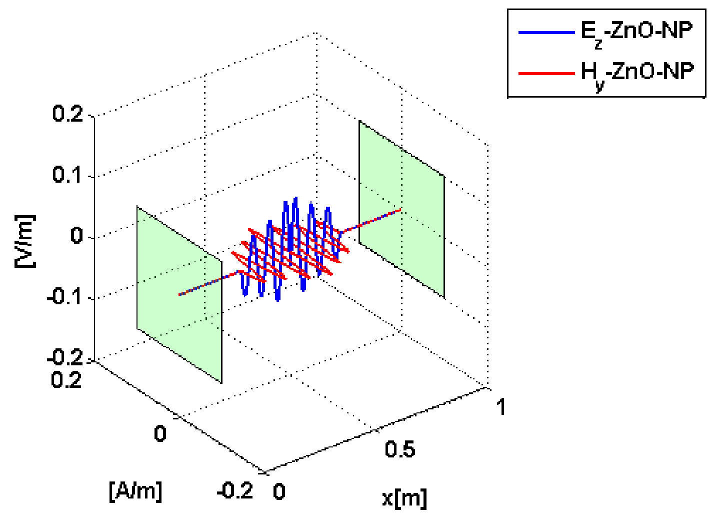
When we have used the electrical conductivity (0.04 S/m) of A. Faize et al., [27] into the code generated for ZnO NPs the simulation result is shown in Fig 4.4. Fig 4.4: (a) is the simulation result of the magnitude of the electric field. Since the electrical conductivity (0.04 S/m) is greater than both the conductivity of $7x10^{-5}$ S/m and $1.5x10^{-5}$ S/m, we get a maximum absorption and attenuation level of the magnitude of the electric field. As a result the magnitude of the electric field is damping and the simulation result of the electric field is analogous to that of A. Faize et al., as shown in Fig 2.7: (b) [27].



(a)



(b)



(c)

Figure 4. 4: One-dimensional FDTD simulation in ZnO NPs: (a) electric field observed after 500 time steps; (b) magnetic fields observed after 500 time steps; (c) both electric and magnetic field.

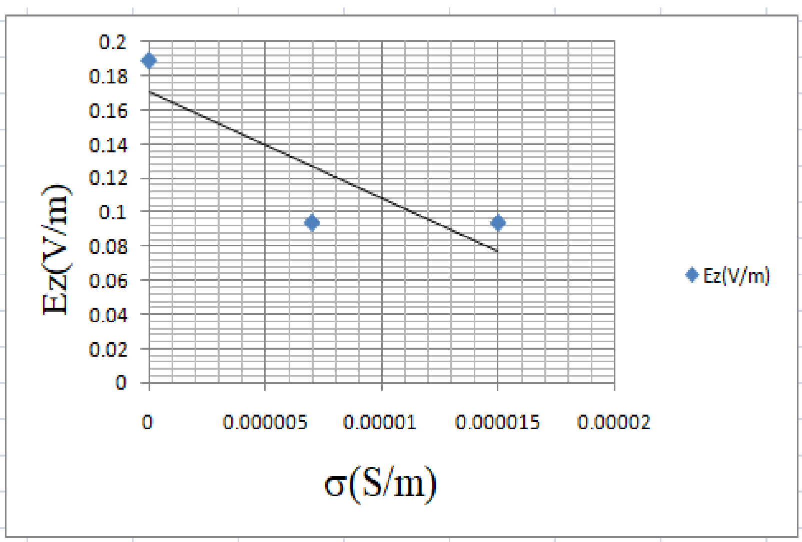
4.3 Comparison of the electric and magnetic field variations in free space and in ZnO NPs

The simulated result of the magnitude of electric and magnetic field in free space is 0.1886 and 0.1885 as shown in Figure 4.1: (a) and (b) respectively for a conductivity of 0 S/m. The magnitude of electric and magnetic field in ZnO NP is 0.09341 and 0.09425 respectively as shown in Figure 4.2: (a) and (b) for a conductivity value of $1.5x10^{-5}$. And as shown in figure 4.4: (a) and (b) the magnitude of the electric and magnetic field is 0.09348 and 0.09426 respectively for a conductivity value of $7x10^{-6}$. The numerical result of the magnitude of electric and magnetic field with corresponding electrical conductivity is tabulated in Table 4.1.

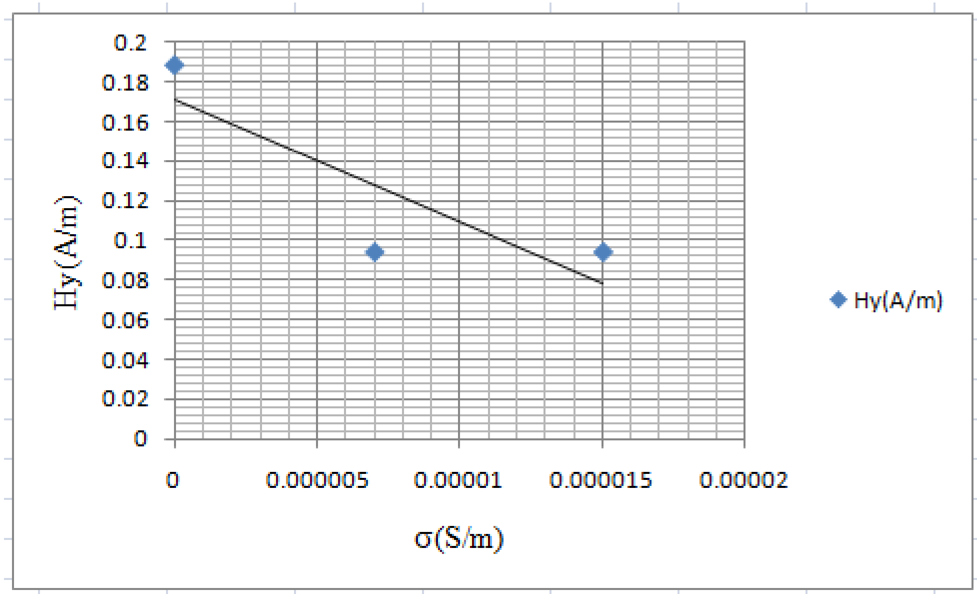
Table 4. 1: Electrical conductivity Vs Electric field

σ(S/m)	0	7.00E-06	1.5E-05
Ez(V/m)	0.1886	0.09348	0.09341
Hy(A/m)	0.1885	0.09426	0.09425

The relationship between the magnitude of electric and magnetic field versus electrical conductivity is plotted in Fig 4.5. From the Figure we get, as electrical conductivity increases electric field decreases. Both the magnitude of the electric and magnetic field in free space is greater than in ZnO NPs, this is because of the electrical conductivity of free space is zero and ZnO NP is $1.5x10^{-5}$ as a result as electrical conductivity increases the magnitude of electric and magnetic field decreases.



(a)



(b)

Figure 4. 5: (a) Plot of electric and (b) magnetic field vs electrical conductivity.

CHAPTER FIVE

CONCLUSION AND FUTURE WORK

FDTD method is used for the simulation of electromagnetic wave propagation. In this study, a solution of Maxwell's equations by using FDTD method is simulated. Codes were generated and subsequently implemented in the MATLAB software. The code is applied to investigate propagation of electric and magnetic fields in ZnO NPs and in free space. Through simulation in free space, it was found that the magnitude of the electric and magnetic fields of the propagated plane waves never decrease. Since the conductivity of free space is zero both electric and magnetic field will not be absorbed by free space. For small values of electrical conductivity ($7x10^{-6}$ S/m and $1.5x10^{-5}$S/m) the magnitude of electric and magnetic fields in ZnO NPs will not be attenuated, but were found to be less than that of free space. However, the magnitude of electric and magnetic fields in ZnO NPs is attenuated for higher values of electrical conductivity, such as 0.04 S/m and ZnO NPs absorb both electric and magnetic fields. For ZnO NPs the problem is addressed by us for the first time and therefore the result is open for validation and comment.

Future work

We want to generate 2-D FDTD MATLAB code for the simulation of MZ interferometer made by ZnO NP array. Also, the exact value of the electrical conductivity for ZnO NPs should be investigated.

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APPENDIX

```
% Electric field in free space One-Dimensional FDTD Code
```

```
 % Define initial constants
eps_0=8.85e-12;                    % permittivity of free space
 mu_0 = 4*pi*1e-7;                        % permeability of free space
% Define problem geometry and parameters
domain_size = 1;                        % 1D problem space length in micrometers
dx = 1e-3;
dt = 3e-12;                         % duration of time step in seconds
number_of_time_steps = 500;               % number of iterations
 nx =round(domain_size / dx ) ;             % number of cells in 1D problem space
source_position = 0.5;                  % position of the current source Jz
% Initialize field and material arrays
Ceze=zeros(nx+1,1);
Cezhy=zeros(nx+1,1);
Cezj=zeros(nx+1,1);
Ez=zeros(nx+1,1);
Jz =zeros(nx+1,1);
eps_r_z = ones ( nx +1 ,1);                 % free space
sigma_e_z =zeros ( nx +1 ,1);                 % free space
Chyh =zeros(nx,1);
Chyez =zeros(nx,1);
Chym =zeros(nx,1);
Hy =zeros(nx,1);
My =zeros(nx,1);
mu_r_y=ones(nx,1); % free space
sigma_m_y=zeros(nx,1); % free space399
%calculate FDTD updating c o e f f i c i e n t s
Ceze = (2.*eps_r_z.*eps_0-dt.*sigma_e_z)./(2*eps_r_z.*eps_0 +dt.*sigma_e_z );
```

```
Cezhy= (2*dt/dx)./(2*eps_r_z*eps_0 + dt * sigma_e_z ) ;
Cezj=(-2*dt)./(2*eps_r_z*eps_0 +dt* sigma_e_z);
Chyh = (2*mu_r_y*mu_0-dt*sigma_m_y)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chyez=(2*dt/dx)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chym=(-2*dt)./(2*mu_r_y*mu_0+dt* sigma_m_y);
% Define the sinusoidal source waveform
 time = dt *(0: number_of_time_steps-1);
Jz_waveform =sin(((2/pi*time)/5e-11));
 source_position_index = round(nx*source_position/domain_size )+1;
% FDTD loop
for time_step = 1: number_of_time_steps
% Update Jz for the current time step
 Jz(source_position_index)=Jz_waveform(time_step ) ;
% Update magnetic field
 Hy(1:nx)=Chyh(1:nx).*Hy(1:nx)+Chyez(1:nx).*(Ez(2:nx+1)-Ez(1:nx))+Chym(1:nx).*My(1:nx);
%  Update electric field
Ez(2:nx)=Ceze(2:nx).* Ez(2:nx)+Cezhy(2:nx).*(Hy(2:nx)-Hy(1:nx-1))+Cezj(2:nx).*Jz(2:nx);
Ez(1) = 0; % Apply PEC boundary condition at x = 0 micrometer
Ez(nx+1) = 0; % Apply PEC boundary condition at x = 1 micrometer
 end
 % initialize 1D plotting parameters
Ez_positions=[0:nx]*dx;
Hy_positions=([0:nx-1]+0.5)*dx ;
v=[0 -0.1 -0.1;
    0 -0.1 0.1;
    0 0.1 0.1;
    0 0.1 -0.1;
    1 -0.1 -0.1;
    1 -0.1 0.1;
    1 0.1 0.1;
    1 0.1 -0.1];
```

```
f = [1 2 3 4; 5 6 7 8];
axis([0 1 -0.2 0.2 -0.2 0.2]);
lez =line( Ez_positions , Ez*0 ,Ez,'Colo','b','LineWidth',1.5);
%   lhy =line( Hy_positions,377*Hy ,Hy*0,'Color','r','LineWidth',1.5,'linestyle','-');
set(gca,'fontsize',12 ,'FontWeight','bold');
axis square ;
legend('E_{z}-free space', 'Location ','NorthEast') ;
xlabel( ' x[m]');
 ylabel ('[A/m]');
zlabel('[V/m]') ;
grid on ;
p =patch('vertices',v ,'faces',f,'facecolor','g','facealpha',0.2 ) ;
text(0,1,1.1,'PEC','horizontalalignment','center',' fontweight','bold') ;
text(1,1,1.1,'PEC', ' horizontalalignment',' center','fontweight','bold');
% getframe
 drawnow;
% ##############################################################################
% Magnetic field in free space One -Dimensional FDTD Code
 % Define initial constants
eps_0=8.85e-12;                    % permittivity of free space
 mu_0 = 4*pi*1e-7;                    % permeability of free space
% Define problem geometry and parameters
domain_size = 1;                        % 1D problem space length in micrometers
dx = 1e-3;
dt = 3e-12;                           % duration of time step in seconds
number_of_time_steps = 500;               % number of iterations
 nx =round(domain_size / dx ) ;             % number of cells in 1D problem space
source_position = 0.5;                     % position of the current source Jz
% Initialize field and material arrays
Ceze=zeros(nx+1,1);
Cezhy=zeros(nx+1,1);
```

```
Cezj=zeros(nx+1,1);
Ez=zeros(nx+1,1);
Jz =zeros(nx+1,1);
eps_r_z = ones ( nx +1 ,1);                    % free space
sigma_e_z =zeros ( nx +1 ,1);                  % free space
Chyh =zeros(nx,1);
Chyez =zeros(nx,1);
Chym =zeros(nx,1);
Hy =zeros(nx,1);
My =zeros(nx,1);
mu_r_y=ones(nx,1); % free space
sigma_m_y=zeros(nx,1); % free space399
%calculate FDTD updating coefficients
Ceze = (2.*eps_r_z.*eps_0-dt.*sigma_e_z)./(2*eps_r_z.*eps_0 +dt.*sigma_e_z );
Cezhy= (2*dt/dx)./(2*eps_r_z*eps_0 + dt * sigma_e_z ) ;
Cezj=(-2*dt)./(2*eps_r_z*eps_0 +dt* sigma_e_z);
Chyh = (2*mu_r_y*mu_0-dt*sigma_m_y)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chyez=(2*dt/dx)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chym=(-2*dt)./(2*mu_r_y*mu_0+dt* sigma_m_y);
% Define the sinusoidal source waveform
 time = dt *(0: number_of_time_steps-1);
Jz_waveform =sin(((2/pi*time)/5e-11));
 source_position_index = round(nx*source_position/domain_size )+1;
% FDTD loop
for time_step = 1: number_of_time_steps
% Update Jz for the current time step
 Jz(source_position_index)=Jz_waveform(time_step ) ;
% Update magnetic field
 Hy(1:nx)=Chyh(1:nx).*Hy(1:nx)+Chyez(1:nx).*(Ez(2:nx+1)-Ez(1:nx))+Chym(1:nx).*My(1:nx);
 %  Update electric field
Ez(2:nx)=Ceze(2:nx).* Ez(2:nx)+Cezhy(2:nx).*(Hy(2:nx)-Hy(1:nx-1))+Cezj(2:nx).*Jz(2:nx);
```

```
Ez(1) = 0; % Apply PEC boundary condition at x = 0 micrometer
Ez(nx+1) = 0; % Apply PEC boundary condition at x = 1 micrometer
 end
% initialize 1D plotting parameters
Ez_positions=[0:nx]*dx;
Hy_positions=([0:nx-1]+0.5)*dx ;
v=[0 -0.1 -0.1;
   0 -0.1 0.1;
   0 0.1 0.1;
   0 0.1 -0.1;
   1 -0.1 -0.1;
   1 -0.1 0.1;
   1 0.1 0.1;
   1 0.1 -0.1];
f = [1 2 3 4; 5 6 7 8];
axis([0 1 -0.2 0.2 -0.2 0.2]);
% ez =line( Ez_positions , Ez*0 ,Ez,'Colo','b','LineWidth',1.5);
  hy =line( Hy_positions,377*Hy ,Hy*0,'Color','r','LineWidth',1.5,'linestyle','-');
set(gca,'fontsize',12 ,'FontWeight','bold');
axis square ;
legend('H_{y}-free space ' , 'Location ','NorthEast') ;
xlabel( ' x[m]');
 ylabel ('[A/m]');
zlabel('[V/m]') ;
grid on ;
p =patch('vertices',v ,'faces',f,'facecolor','g','facealpha',0.2 ) ;
text(0,1,1.1,'PEC','horizontalalignment','center',' fontweight','bold') ;
text(1,1,1.1,'PEC', ' horizontalalignment',' center','fontweight','bold');
% getframe
 drawnow;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Both Electric and Magnetic field in free space One -Dimensional FDTD Code
 % Define initial constants
eps_0=8.85e-12;                    % permittivity of free space
 mu_0 = 4*pi*1e-7;                         % permeability of free space
% Define problem geometry and parameters
domain_size = 1;                          % 1D problem space length in micrometers
dx = 1e-3;
dt = 3e-12;                              % duration of time step in seconds
number_of_time_steps = 500;                 % number of iterations
 nx =round(domain_size / dx ) ;               % number of cells in 1D problem space
source_position = 0.5;                        % position of the current source Jz
% Initialize field and material arrays
Ceze=zeros(nx+1,1);
Cezhy=zeros(nx+1,1);
Cezj=zeros(nx+1,1);
Ez=zeros(nx+1,1);
Jz =zeros(nx+1,1);
eps_r_z = ones ( nx +1 ,1);                     % free space
sigma_e_z =zeros ( nx +1 ,1);                     % free space
Chyh =zeros(nx,1);
Chyez =zeros(nx,1);
Chym =zeros(nx,1);
Hy =zeros(nx,1);
My =zeros(nx,1);
mu_r_y=ones(nx,1); % free space
sigma_m_y=zeros(nx,1); % free space
%calculate FDTD updating coefficiets
Ceze = (2.*eps_r_z.*eps_0-dt.*sigma_e_z)./(2*eps_r_z.*eps_0 +dt.*sigma_e_z );
Cezhy= (2*dt/dx)./(2*eps_r_z*eps_0 + dt * sigma_e_z ) ;
```

```
Cezj=(-2*dt)./(2*eps_r_z*eps_0 +dt* sigma_e_z);
Chyh = (2*mu_r_y*mu_0-dt*sigma_m_y)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chyez=(2*dt/dx)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chym=(-2*dt)./(2*mu_r_y*mu_0+dt* sigma_m_y);
% Define the sinusoidal source waveform
 time = dt *(0: number_of_time_steps-1);
Jz_waveform =sin(((2/pi*time)/5e-11));
 source_position_index = round(nx*source_position/domain_size )+1;
% FDTD loop
for time_step = 1: number_of_time_steps
% Update Jz for the current time step
 Jz(source_position_index)=Jz_waveform(time_step ) ;
% Update magnetic field
 Hy(1:nx)=Chyh(1:nx).*Hy(1:nx)+Chyez(1:nx).*(Ez(2:nx+1)-Ez(1:nx))+Chym(1:nx).*My(1:nx);
 %  Update electric field
Ez(2:nx)=Ceze(2:nx).* Ez(2:nx)+Cezhy(2:nx).*(Hy(2:nx)-Hy(1:nx-1))+Cezj(2:nx).*Jz(2:nx);
Ez(1) = 0; % Apply PEC boundary condition at x = 0 micrometer
Ez(nx+1) = 0; % Apply PEC boundary condition at x = 1 micrometer
 end
 % initialize 1D plotting parameters
Ez_positions=[0:nx]*dx;
Hy_positions=([0:nx-1]+0.5)*dx ;
v=[0 -0.1 -0.1;
    0 -0.1 0.1;
    0 0.1 0.1;
    0 0.1 -0.1;
    1 -0.1 -0.1;
    1 -0.1 0.1;
    1 0.1 0.1;
    1 0.1 -0.1];
f = [1 2 3 4; 5 6 7 8];
```

```
axis([0 1 -0.2 0.2 -0.2 0.2]);
ez =line( Ez_positions , Ez*0 ,Ez,'Colo','b','LineWidth',1.5);
 hy =line( Hy_positions,377*Hy ,Hy*0,'Color','r','LineWidth',1.5,'linestyle','-');
set(gca,'fontsize',12 ,'FontWeight','bold');
axis square ;
legend('E_{z}-free space','H_{y}-free space ' , 'Location ','NorthEast') ;
xlabel( ' x[m]');
 ylabel ('[A/m]');
zlabel('[V/m]') ;
grid on ;
p =patch('vertices',v ,'faces',f,'facecolor','g','facealpha',0.2 ) ;
text(0,1,1.1,'PEC','horizontalalignment','center',' fontweight','bold') ;
text(1,1,1.1,'PEC', ' horizontalalignment',' center','fontweight','bold');
 % getframe
 drawnow;
%##############################################################################
% Electric field in ZnO NP using
% the electrical conductivity of 1.5x10^-5 One-Dimensional FDTD Code
 % Define initial constants
eps_0=8.857e-12;                    % permittivity of free space
 mu_0 = 4*pi*1e-7;                       % permeability of free space
% Define problem geometry and parameters
domain_size = 1;                        % 1D problem space length in micrometers
dx = 1e-3;
dt = 3e-12;                             % duration of time step in seconds
number_of_time_steps = 500;                % number of iterations
 nx =round(domain_size / dx ) ;            % number of cells in 1D problem space
source_position = 0.5;                       % position of the current source Jz
% Initialize field and material arrays
Ceze=zeros(nx+1,1);
Cezhy=zeros(nx+1,1);
```

```
Cezj=zeros(nx+1,1);
Ez=zeros(nx+1,1);
Jz =zeros(nx+1,1);
eps_r_z = 4.1006*ones ( nx +1 ,1);
sigma_e_z =1.5*10^-5*ones( nx +1 ,1);
Chyh =zeros(nx,1);
Chyez =zeros(nx,1);
Chym =zeros(nx,1);
Hy =zeros(nx,1);
My =zeros(nx,1);
mu_r_y=ones(nx,1);
sigma_m_y=zeros(nx,1);
%calculate FDTD updating coefficients
Ceze = (2.*eps_r_z.*eps_0-dt.*sigma_e_z)./(2*eps_r_z.*eps_0 +dt.*sigma_e_z );
Cezhy= (2*dt/dx)./(2*eps_r_z*eps_0 + dt * sigma_e_z ) ;
Cezj=(-2*dt)./(2*eps_r_z*eps_0 +dt* sigma_e_z);
Chyh = (2*mu_r_y*mu_0-dt*sigma_m_y)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chyez=(2*dt/dx)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chym=(-2*dt)./(2*mu_r_y*mu_0+dt* sigma_m_y);
% Define the sinusoidal source waveform
 time = dt *(0: number_of_time_steps-1);
 Jz_waveform =sin(((2/pi*time)/5e-11));
 source_position_index = round(nx*source_position/domain_size )+1;
% FDTD loop
for time_step = 1: number_of_time_steps
% Update Jz for the current time step
 Jz(source_position_index)=Jz_waveform(time_step ) ;
% Update magnetic field
 Hy(1:nx)=Chyh(1:nx).*Hy(1:nx)+Chyez(1:nx).*(Ez(2:nx+1)-Ez(1:nx))+Chym(1:nx).*My(1:nx);
 %  Update electric field
Ez(2:nx)=Ceze(2:nx).* Ez(2:nx)+Cezhy(2:nx).*(Hy(2:nx)-Hy(1:nx-1))+Cezj(2:nx).*Jz(2:nx);
```

```
Ez(1) = 0; % Apply PEC boundary condition at x = 0 micrometer
Ez(nx+1) = 0; % Apply PEC boundary condition at x = 1 micrometer
 end
%initialize 1D plotting parameters
Ez_positions=(0:nx)*dx;
Hy_positions=((0:nx-1)+0.5)*dx ;
v=[0 -0.1 -0.1;
   0 -0.1 0.1;
   0 0.1 0.1;
   0 0.1 -0.1;
   1 -0.1 -0.1;
   1 -0.1 0.1;
   1 0.1 0.1;
   1 0.1 -0.1];
f = [1 2 3 4; 5 6 7 8];
axis([0 1 -0.2 0.2 -0.2 0.2]);
ez =line( Ez_positions , Ez*0 ,Ez,'Colo','b','LineWidth',1.5);
% hy =line( Hy_positions,186.1728*Hy ,Hy*0,'Color','r','LineWidth',1.5,'linestyle','-');
set(gca,'fontsize',12 ,'FontWeight','bold');
axis square ;
legend('E_{z}-ZnO-NP', 'Location ','NorthEast') ;
xlabel( ' x[m]');
 ylabel ('[A/m]');
zlabel('[V/m]') ;
grid on ;
p =patch('vertices',v ,'faces',f,'facecolor','g','facealpha',0.2 ) ;
text(0,1,1.1,'ABC','horizontalalignment','center',' fontweight','bold') ;
text(1,1,1.1,'ABCC', ' horizontalalignment',' center','fontweight','bold');
% getframe
 drawnow;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%  Magnetic field in ZnO NP using
% the electrical conductivity of 1.5x10^-5 One-Dimensional FDTD Code
 % Define initial constants
eps_0=8.85e-12;                    % permittivity of free space
 mu_0 = 4*pi*1e-7;                        % permeability of free space
% Define problem geometry and parameters
domain_size = 1;                          % 1D problem space length in micrometers
dx = 1e-3;
dt = 3e-12;                               % duration of time step in seconds
number_of_time_steps = 500;               % number of iterations
 nx =round(domain_size / dx ) ;           % number of cells in 1D problem space
source_position = 0.5;                    % position of the current source Jz
% Initialize field and material arrays
Ceze=zeros(nx+1,1);
Cezhy=zeros(nx+1,1);
Cezj=zeros(nx+1,1);
Ez=zeros(nx+1,1);
Jz =zeros(nx+1,1);
eps_r_z = 4.1006*ones ( nx +1 ,1);
sigma_e_z =1.5*10^-5*ones( nx +1 ,1);
Chyh =zeros(nx,1);
Chyez =zeros(nx,1);
Chym =zeros(nx,1);
Hy =zeros(nx,1);
My =zeros(nx,1);
mu_r_y=ones(nx,1);
sigma_m_y=zeros(nx,1);
%calculate FDTD updating coefficients
Ceze = (2.*eps_r_z.*eps_0-dt.*sigma_e_z)./(2*eps_r_z.*eps_0 +dt.*sigma_e_z );
```

```
Cezhy= (2*dt/dx)./(2*eps_r_z*eps_0 + dt * sigma_e_z ) ;
Cezj=(-2*dt)./(2*eps_r_z*eps_0 +dt* sigma_e_z);
Chyh = (2*mu_r_y*mu_0-dt*sigma_m_y)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chyez=(2*dt/dx)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chym=(-2*dt)./(2*mu_r_y*mu_0+dt* sigma_m_y);
% Define the sinusoidal source waveform
 time = dt *(0: number_of_time_steps-1);
 Jz_waveform =sin(((2/pi*time)/5e-11));
 source_position_index = round(nx*source_position/domain_size )+1;
% FDTD loop
for time_step = 1: number_of_time_steps
% Update Jz for the current time step
 Jz(source_position_index)=Jz_waveform(time_step ) ;
% Update magnetic field
 Hy(1:nx)=Chyh(1:nx).*Hy(1:nx)+Chyez(1:nx).*(Ez(2:nx+1)-Ez(1:nx))+Chym(1:nx).*My(1:nx);
 %  Update electric field
Ez(2:nx)=Ceze(2:nx).* Ez(2:nx)+Cezhy(2:nx).*(Hy(2:nx)-Hy(1:nx-1))+Cezj(2:nx).*Jz(2:nx);
Ez(1) = 0; % Apply PEC boundary condition at x = 0 micrometer
Ez(nx+1) = 0; % Apply PEC boundary condition at x = 1 micrometer
 end
%initialize 1D plotting parameters
Ez_positions=(0:nx)*dx;
Hy_positions=((0:nx-1)+0.5)*dx ;
v=[0 -0.1 -0.1;
    0 -0.1 0.1;
    0 0.1 0.1;
    0 0.1 -0.1;
    1 -0.1 -0.1;
    1 -0.1 0.1;
    1 0.1 0.1;
    1 0.1 -0.1];
```

```
f = [1 2 3 4; 5 6 7 8];
axis([0 1 -0.2 0.2 -0.2 0.2]);
% ez =line( Ez_positions , Ez*0 ,Ez,'Colo','b','LineWidth',1.5);
hy =line( Hy_positions, 186.1728*Hy ,Hy*0,'Color','r','LineWidth',1.5,'linestyle','-');
set(gca,'fontsize',12 ,'FontWeight','bold');
axis square ;
legend('H_{y}-ZnO-NP' , 'Location ','NorthEast') ;
xlabel( ' x[m]');
 ylabel ('[A/m]');
zlabel('[V/m]') ;
grid on ;
p =patch('vertices',v ,'faces',f,'facecolor','g','facealpha',0.2 ) ;
text(0,1,1.1,'PEC','horizontalalignment','center',' fontweight','bold') ;
text(1,1,1.1,'PEC', ' horizontalalignment',' center','fontweight','bold');
  % getframe
 drawnow;
%##############################################################################
% Both Electric and Magnetic field in ZnO NP using
% the electrical conductivity of 1.5x10^-5 One-Dimensional FDTD Code
 % Define initial constants
eps_0=8.85e-12;                    % permittivity of free space
 mu_0 = 4*pi*1e-7;                     % permeability of free space
% Define problem geometry and parameters
domain_size = 1;                          % 1D problem space length in micrometers
dx = 1e-3;
dt = 3e-12;                             % duration of time step in seconds
number_of_time_steps = 500;              % number of iterations
 nx =round(domain_size / dx ) ;             % number of cells in 1D problem space
source_position = 0.5;                     % position of the current source Jz
% Initialize field and material arrays
Ceze=zeros(nx+1,1);
```

```
Cezhy=zeros(nx+1,1);
Cezj=zeros(nx+1,1);
Ez=zeros(nx+1,1);
Jz =zeros(nx+1,1);
eps_r_z = 4.1006*ones ( nx +1 ,1);
sigma_e_z =1.5*10^-5*ones( nx +1 ,1);
Chyh =zeros(nx,1);
Chyez =zeros(nx,1);
Chym =zeros(nx,1);
Hy =zeros(nx,1);
My =zeros(nx,1);
mu_r_y=ones(nx,1);
sigma_m_y=zeros(nx,1);
%calculate FDTD updating coefficients
Ceze = (2.*eps_r_z.*eps_0-dt.*sigma_e_z)./(2*eps_r_z.*eps_0 +dt.*sigma_e_z );
Cezhy= (2*dt/dx)./(2*eps_r_z*eps_0 + dt * sigma_e_z ) ;
Cezj=(-2*dt)./(2*eps_r_z*eps_0 +dt* sigma_e_z);
Chyh = (2*mu_r_y*mu_0-dt*sigma_m_y)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chyez=(2*dt/dx)./(2*mu_r_y*mu_0+dt*sigma_m_y);
Chym=(-2*dt)./(2*mu_r_y*mu_0+dt* sigma_m_y);
% Define the sinusoidal source waveform
 time = dt *(0: number_of_time_steps-1);
 Jz_waveform =sin(((2/pi*time)/5e-11));
 source_position_index = round(nx*source_position/domain_size )+1;
% FDTD loop
for time_step = 1: number_of_time_steps
% Update Jz for the current time step
 Jz(source_position_index)=Jz_waveform(time_step ) ;
% Update magnetic field
 Hy(1:nx)=Chyh(1:nx).*Hy(1:nx)+Chyez(1:nx).*(Ez(2:nx+1)-Ez(1:nx))+Chym(1:nx).*My(1:nx);
%  Update electric field
```

```
Ez(2:nx)=Ceze(2:nx).* Ez(2:nx)+Cezhy(2:nx).*(Hy(2:nx)-Hy(1:nx-1))+Cezj(2:nx).*Jz(2:nx);
Ez(1) = 0; % Apply PEC boundary condition at x = 0 micrometer
Ez(nx+1) = 0; % Apply PEC boundary condition at x = 1 micrometer
 end
    %initialize 1D plotting parameters
Ez_positions=(0:nx)*dx;
Hy_positions=((0:nx-1)+0.5)*dx ;
v=[0 -0.1 -0.1;
   0 -0.1 0.1;
   0 0.1 0.1;
   0 0.1 -0.1;
   1 -0.1 -0.1;
   1 -0.1 0.1;
   1 0.1 0.1;
   1 0.1 -0.1];
f = [1 2 3 4; 5 6 7 8];
axis([0 1 -0.2 0.2 -0.2 0.2]);
lez =line( Ez_positions , Ez*0 ,Ez,'Colo','b','LineWidth',1.5);
lhy =line( Hy_positions, 186.1728*Hy ,Hy*0,'Color','r','LineWidth',1.5,'linestyle','-');
set(gca,'fontsize',12 ,'FontWeight','bold');
axis square ;
legend('E_{z}-ZnO-NP','H_{y}-ZnO-NP' , 'Location ','NorthEast') ;
xlabel( ' x[m]');
 ylabel ('[A/m]');
zlabel('[V/m]') ;
grid on ;
p =patch('vertices',v ,'faces',f,'facecolor','g','facealpha',0.2 ) ;
text(0,1,1.1,'ABC','horizontalalignment','center',' fontweight','bold') ;
text(1,1,1.1,'ABCC', ' horizontalalignment',' center','fontweight','bold');
% getframe
 drawnow;
```

DECLARATION

I hereby declare and confirm that the thesis entitled "Numerical simulation and comparison of the Electric and Magnetic field variations in free space and in ZnO NP using one dimensional FDTD method" is my original work and has not been presented for a degree in any other university, and that all sources of materials have been dully acknowledged. This thesis is conducted under the supervision of my advisor Dr. Gajanan Honnavar. I have followed all the ethical principles of scholars in the constructive, stimulating advice and the completion of this thesis.

___________________	___________	___________
Candidate's name	Signature	Date

As the candidate's advisor, this thesis has been submitted for examination with my approval.

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Advisor's name	Signature	Date