دانشگاه شیراز

دانشکده علوم

پایان‌نامه دکتری در رشته فیزیک (اپتیک و لیزر)

بهبود روش FDTD:کاربرد در نانواپتیک و نانوفوتونیک

توسط

احمد محمدی

استاد راهنما:

دکتر حمید نادگران

شهریور ماه ۱۳۸۵

Shiraz University
Faculty of Science

Ph.D. Dissertation
In Physics (Optics and Laser)

THE NOVEL IMPROVEMENTS TO FINITE DIFFERENCE TIME DOMAIN MODELING: APPLICATIONS IN NANOOPTICS AND NANOPHOTONICS

By

AHMAD MOHAMMADI

Supervised by
Dr. HAMID NADGARAN

September 2006

IN THE NAME OF GOD

THE NOVEL IMPROVEMENTS TO FININT DIFFERENCE TIME DOMAIN MODELING: APPLICATIONS IN NANOOPTICS AND NANOPHOTONICS

BY

AHMAD MOHAMMADI

THESIS

SUBMITTED TO THE SCHOOL OF GRADUATE STUDIES IN PARTIAL FULFILMENT OF THR REQUIREMENTS FOR THE DEGREE OF PH.D.

IN

ATOMIC PHYSICS
(OPTICS AND LASER)

SHIRAZ UNIVERSITY

SHIRAZ

ISLAMIC REPUBLIC OF IRAN

EVALUATED AND APROVED BY THE THESIS COMMITTEE AS : excellent

.... H. NADGARAN, PH.D. ASSOCIATE PROF. OF PHYSICS (CHAIRMAN)

................M. BARATI, PH.D. PROF. OF PHYSICS

.... M. M. GOLSHAN, PH.D. ASSISTANT PROF. OF PHYSICS

:.M. MORADI, PH.D. PROF. OF PHYSICS

...... A. ZAKERY, PH.D. ASSOCIATE PROF. OF PHYSICS

M. ZARGAR. SHOUSHTARI, PH.D. PROF. OF PHYSICS, SHAHID CHAMRAN UNIVERSITY

SEPTEMBER 2006

This dissertation is dedicated to my family

and

The memory of my parents and my brother

Acknowledgements

I am deeply indebted to my supervisor Dr. Hamid Nadgaran for giving me a large amount of creative freedom to pursue various curiosities along the way to investigate this interesting topic, for his academic, financial and moral support, and for his patience and understanding. At certain points, it was just his advice and support that enabled me to continue with my work.

I also thank my PhD committee members: Dr. Mahmood Barati, Dr. Mohammad Mehdi Golshan, Dr. Mahmood. Moradi, Dr. Abdonaser Zakeri and Dr. Morteza Zargar Shoushtari for the time and effort they put forth in reviewing my thesis.

This thesis is the continuation of works which had been started in Laser and Optics group, Shiraz University, and pursued at the NanoOptics group of the Swiss Federal Institute of Technology (ETH) where I stayed for one year as a visiting scholar. I wish to express my gratitude to Professor Vahid Sandoghdar for giving me the opportunity to work in his research group, for providing me access to all the tools necessary for completing this project, and for arranging the financial support. His vast knowledge and experience have been invaluable. I will always be thankful to Prof. Christian Hafner for being the one who managed my visit to ETH. Moreover, I am grateful to him for all the stimulating discussions enriching my knowledge about Computational Optics as well as Optimization techniques.

I owe most of the skills I acquired during this project to Dr. Mario Agio whose strong backgrounds in Optics were of great help. Many thanks to him for the excellent cooperation, and for guiding my research career. It is my pleasure to work among a group of international researchers in an excellent working atmosphere where I learned many things other than my main work. Particularly, I would like to thank Rik Harbers whose encouragement and guidance helped me to learn the implementation of computational techniques on high performance computing machinery. Furthermore, I thank Ray Ballisti, the system administrator, who assisted me in installation and maintenance of software packages.

I am also especially thankful to Margrit Joerger, Veronika Sieger, and Ruth Zaehringer who arranged all official tasks.

During my stay in Zurich, I was lucky to be surrounded by a number of terrific fellow students from nearly all parts of the world gathered in a wonderful student house called Vinzenzheim (I would call it Hotel California: where you can check out, but you can never leave!). Naming all of them would actually not allow me to complete this job. I would particularly thank them for never allowing me to feel homesick, for the pleasant moments exploring the beautiful nature of Switzerland, and for nightly discussions which opened new worlds before my eyes.

No gratitude is sufficient to repay the unceasing love and unconditional support of my big family who has provided me delightful and secure environment in which I could grow up. Along this line a special word of thanks go to Reza who has directly contributed to this work and Tahmineh for taking care of me and everything else so that I could concentrate on my work. Most of all, I owe my education to my father who did his best to constantly support my educational endeavours till the moment I could stand on my feet.

Last but not least, I gratefully acknowledge financial support from the Iranian Ministry of Science and ETH Zurich. This work was performed within the Innovation Initiative project Composite Doped Metamaterials (CDM) of ETH Zurich.

Abstract

The Novel Improvements to Finite Difference Time Domain Modeling: Applications in NanoOptics and NanoPhotonics

The Finite Difference Time Domain (FDTD) method is a robust computational technique that can be applied to a wide range of applications in optics. However, due to the staircasing problem, very fine meshes, and consequently high computing resources are required to model curved interfaces, especially for metals. This thesis deals with the development of a systematic framework for modeling dielectric and dispersive materials' boundaries so that one can obtain accurate results from FDTD simulation using personal computers. Effective permittivities for the two-dimensional FDTD method are derived using a contour path approach that accounts for the boundary conditions of the electromagnetic fields at dielectric interfaces. Our schemes are validated using Mie theory for the light scattering from a dielectric cylinder. Significant improvements in terms of accuracy and error fluctuations are observed, especially in the calculation of resonances. To deal with dispersive materials, we combine a contour-path approach with Z transform to handle both the electromagnetic boundary conditions at the interface and the negative dispersive dielectric function of the material. We compare the accuracy of the standard two-dimensional FDTD method in modelling Surface Plasmon Polaritons (SPPs). The results show a considerable reduction of relative error by an order of magnitude. Finally, we investigate the accuracy of these approaches by applying them to some common problems in Nano-Optics and Nano-Photonics. This set of systematic tests demonstrates the accuracy and efficiency of our methods.

Table of Contents

List of Figures and Illustrations

List of Symbols, Abbreviations and Nomenclature

ABC	Absorbing Boundary Condition
ADE	Auxiliary Differential Equation
CDA	Coupled Dipole Approximation
CFL	Courant-Freidrichs-Lewy
CFS	Complex Frequency Shift
CP	Contour Path
CPEP	Contour Path Effective Permittivities
CPML	Convolutional Perfectly Matched Layer
DDA	Dipole Dipole Approximation
DFT	Discrete Fourier Transform
EP	Effective Permittivities
FD	Finite Difference or Frequency Domain
FDTD	Finite Difference Time Domain
FE	Finite-Element
FEM	Finite-Element Method
FITD	Finite Integral Time Domain
FWHM	Full Width Half Maximum
GA	Genetic Algorithm
GMT	Generalized Multipole Technique
LR-SPP	Long Range Surface Plasmon Polariton
LSP	Localized Surface Plasmon
MAS	Method of Auxiliary Sources
MMP	Multiple Multipole Program
MoM	Method of Moment
PBG	Photonic Band Gap
PC	Photonic Crystal
PEC	Perfect Electric Conductor
PLRC	Piecewise Linear Recursive Convolution
PML	Perfectly Matched Layer
PWE	Plane Wave Expansion
RC	Recursive Convolution

SCS	Scattering Cross Section
SERS	Surface Enhanced Raman Scattering
SNOM	Scanning Near-Field Optical Microscopy
SPP	Surface Plasmon Polariton
TD	Time Domain
TE	Transverse Electric
TF/SF	Total Filed/Scattered Field
TLM	Transmission Line Matrix
TM	Transverse Magnetic
V-EP	Volume Average Effective Permittivity
VP-EP	Volume Average Polarized Effective Permittivity

Chapter One
Introduction and Overview of Thesis

1.1 Towards Nanoscale Optics

In recent years, there have been increasing efforts to replace traditional electron-based devices by the photon-based counterparts. The existing electronic devices are very slow devices compared to photonic ones. Moreover, there is a fundamental limit on the miniaturization of electronic devices, leading to a bound on the maximum data transportation and data processing speed. Several photonic devices have already been realized and employed in real-world technology to overcome limitations of the traditional devices. In particular, one can name photonic devices exploiting optical fibers with applications in signal transmission, amplification, routing, filtering, etc. Extraordinary optical properties of materials such as nonlinearity, electro-optics properties, and types of anisotropies allow us to try alternatives for nearly all active and passive electronic devices. Although these photonic devices will solve the problem of slow operation, they are too large to allow the fabrication of all-optical chips analogous to their electronic counterparts, i.e. electronic integrated circuits. Scaling down photonic devices to nanometric dimensions is a major goal of current researches in Photonics, leading to a new emerging field called *NanoPhotonics*. Controlling light at the nanoscale is the major subject in NanoPhotonics. Recent advances in nanotechnology, in particular, fabricating nanoscale structures allow the realization of novel photonic devices which can confine and guide electromagnetic energy in sub-wavelength scales. In this context, perhaps, Photonic Crystals (PCs) are paid most widely attentions. Yablonovitch [1] and John [2] independently introduced the concept of PCs as means which offer the possibility of inhibition of spontaneous light emission and strong photon localization by modifying the mode structure and the density of states. They exhibit a photonic band-gap, i.e., a region with vanishing density of states and prohibited propagation. Therefore, an emitter with a transition frequency within the band-gap is not able to emit photons. Very soon, it was revealed that controlling the spontaneous emission is just one of many exciting possibilities which PCs can offer. The subsequent ideas were mainly based on the purely classical propagation properties of photonic crystals. By controlled inclusion of point or line defects into an otherwise perfect PC, various novel photonic devices have been realized. A point-like defect results in a very high quality factor cavity with very small mode volumes [3] and line defects provide a possibility to manipulate the propagation of light. The PC waveguides have several advantageous compared to the conventional optical waveguides based on the principle of total internal reflection. The guiding in PC waveguides can happen in low index materials or even in air providing very low absorption losses and material dispersion. Moreover, very high intensities can be guided without unwanted nonlinear interaction. They can guide light through very sharp bend (even of 90 degree) with extremely low transmission losses for a wide range of frequencies [4, 5]. Therefore PCs can provide efficient interconnection between elements of photonic circuits such as filters, waveguides, nanocavities, etc. In addition, the possible integration of active devices, such as defect mode lasers into photonic crystals [6] has triggered intensified research activities for the development of highly integrated optical circuits. It is beyond the scope of this introduction to cite all possible applications and devices proposed in recent years.

The diffraction limit for the guiding of electromagnetic energy imposes a lower limit of a few hundred nanometers for the size on these optical devices. However, to realize the optical analogy of highly integrated electronic devices with lateral dimensions of a few tens of nanometers, we must reduce the size of photonic devices beyond the diffraction limit. One approach to overcome the diffraction limit is based on the so-called Surface Plasmon Polariton (SPP) optics which offers the possibility of achieving a strong spatial confinement of electromagnetic fields. SPPs are collective electron oscillations coupled to a light field which are propagating along a dielectric-metal interface and decay exponentially perpendicular to the interface into both neighboring media [7]. The guided electromagnetic energy is trapped on the surface of the metal and confined to dimensions below the diffraction limit. Furthermore, SPPs offer a way of reducing optics to two dimensions. Due to their particular near-field characters and huge field enhancement effects, SPPs are being explored for their potential applications in sub-wavelength Optics, data storage, light generation, quantum information, microscopy and bio-photonics, etc [8, 9]. Two-dimensional surface plasmon (SP) photonic crystals exhibiting a plasmonic band-gap have also been reported [10-12]. Moreover, SP waveguiding in SP crystals, enhanced optical transmission through nanosize holes, as well as light-controlled optical switching have been demonstrated [11-14]. It is now widely expected that SPs will play an important role in future integrated NanoPhotonics.

Another approach to light guiding beyond diffraction limit is to exploit metal nanoparticles which sustain the so-called Localized Surface Plasmons (LSPs). LSPs are collective oscillations of charge density in bounded metallic nanostructures which are resonantly excited by an electromagnetic field with appropriate frequency and polarization [15-17]. The extremely large and localized electromagnetic fields associated with the plasmon resonances together with the large scattering cross sections (SCSs) at specific wavelengths have stimulated research in recent years. For instance, Plasmon coupling along a chain of particles can lead to the coherent propagation of electromagnetic energy below the diffraction limit [18-21].

Parallel to the development in the confinement and guiding light in nanostructures, the studies of optical phenomena at the nanometer scale has triggered remarkable progress in other fields like Spectroscopy, Biology, Medicine, etc. In this context, one can name Scanning Near Field Optical

Microscopy, NanoAntenna, Bilogical labeling and tracking, Tumor therapy, Laser spectroscopy of a single molecule, studying the influence of a single gold nanoparticle on a single molecule, controlled coupling of a nano-emitter to a single mode of a microcavity, study of single organic molecules as quantum optical systems, and many other emerging and exciting fields. All these subtopics are treated within the scope of NanoOptics [8, 22-26], which, in general, studies the interaction of light and matter at the nanometer scale.

1.2 NanoOptics: Theoretical Considerations

Since optical phenomena are straightforward to observe, from ancient times people have investigated the nature of light and developed theories to explain the light behavior. The invention of novel optical instruments initiated breakthrough in optical theories. In 1621, Willebrord Snell (1591-1626) found the law of refraction from which the theory of geometrical optics was developed. Robert Hooke (1635-1703) formulated the wave theory of light. Christiaan Huygens (1629-1695) developed the well-known Huygens principle. The wave theory was improved further by Augustin Jean Fresnel (1788-1827), Joseph Fraunhofer (1787-1826), and Gustav Robert Kirchhoff (1824-1887) who completed the theory of diffraction. Based on the experiments by Heinrich Rudolf Hertz (1857-1894) in 1888, the nature of light was understood to be a transverse electromagnetic wave and Optics was introduced as a branch of Electrodynamics. James Clerk Maxwell (1831-1879) derived the fundamental equations of Electrodynamics. Very soon after the wave theory of light was completely formulated, Max Planck (1858-1947) introduced the concept of quantum theory and showed that Maxwell's equations are not accurate in describing the nature and the properties of light.

Although we are aware that Quantum Theory is nowadays the most complete theory, we still use and study the old and incomplete theories: We use geometrical optics to calculate the refraction, Huygens principle to explain the interference, Kirchhoff's diffraction theory to compute the diffraction of light by macroscopic objects and finally Maxwell's equation to describe the light-matter interaction. The reason is that the more developed theories are more complicated and we prefer to work with the simpler one as long as it is valid to describe the optical phenomena under investigation.

Now, the question is: "Which theory can be properly adopted for NanoOptics?" To answer this question, we should investigate the validity scope of each theory regarding the light wavelength and the size of interacting object. When wavelength is much smaller than the object size, Geometrical Optics is a first approximation which ignores the wave behavior of light. A better but more complicated option would be Kirchhoff's diffraction theory which allows for the wave nature of light. Kirchhoff's theory attributes ideal properties to the object such as perfect conductivity or real refractive index and assumes a scalar approximation. When the wavelength and the object size are comparable, or the vector properties of the fields are important, we should switch to Classical Electrodynamics. At atomic level, however, the only possibility is Quantum Theory. As the term "NanoOptics" implies, we are dealing with objects smaller than one micron which are comparable to the wavelength of light in optical region of electromagnetic spectrum. Therefore, we are not allowed to take advantage of simplifications offered by Geometrical Theory or Diffraction Theory and we have to live with Classical Electrodynamics or Quantum Theory of light. Fortunately, most optical phenomena at the nanoscale can be well described by Classical Electrodynamics. However, when the precise formulation of the emission or absorption of photons is important or when photon-particle interactions are essential, the classical solutions become inaccurate and we have to replace the Maxwell description of light by a pure quantum description or by semiclassical theories.

1.3 Computational Electrodynamics

Having adopted the Classical Electrodynamics, one has to find the solutions to the Maxwell's equations. Although, these equations look simple, there are only a few rare electromagnetic cases where they can be solved exactly. Therefore, approximate mathematical methods have been developed. When computers became available, a new class of methods began to evolve; *Computational Electrodynamics.* Computer techniques have revolutionized the way in which electromagnetic problems are analyzed. Besides, they are widely utilized in technology as powerful design tools which offer a relatively inexpensive way of designing safe and reliable modern devices by testing a large number of different constructions without actually building them. A pure heuristic try and error approach without supporting simulation would be waste of time and resources.

Development and analysis of computational methods for solving the Maxwell's equations are today very active fields of research and varieties of numerical techniques have been proposed. Each technique has its advantages and disadvantages, no unique method covers all applications. One may choose a suitable method regarding the required accuracy, the total simulation time, the type of results required, the frequency region, and so on. There are different classifications for computational techniques, and each technique may be categorized in more than one group. Instead of discussing the individual methods, we present a brief description of these classifications, together with the advantages and drawbacks of each category which apply as well to its members. Then, we briefly review most commonly computational techniques currently applied to NanoOptics problems.

a) Analytical Techniques versus Numerical Techniques. As emphasized earlier, there are a few cases where Maxwell's equations can be solved in a closed-form. Therefore, for almost all real world problems we need to exploit numerical techniques which solve fundamental field equations directly, subject to the boundary constraints posed by the geometry.