Modeling the propagation, scanning and optimization of focused light beams in scattering media

DISSEPTION

zur Erlangung des akademischen Grades eines

DOKTOR-INGENIEURS

(DR.-ING.)

der Fakultät für Ingenieurwissenschaften, Informatik und Psychologie der Universität Ulm

von

Ahmed Elmaklizi

aus Kairo, Ägypten

Gutachter: Prof. Dr. rer. nat. Raimund Hibst
Prof. Dr.-Ing. Wolfgang Menzel

Amtierende Dekanin: Prof. Dr. phil. Tina Seufert

Ulm, 16.11.2015
Abstract

In our pursue for better resolution in imaging inside scattering media in all sort of scientific and industrial fields, we hit a barrier. Namely, the destruction of the focus of the illuminating beam. This limitation can be circumvented by better understanding the interaction between focused illumination systems and the scattering media.

In this work each of the incident light beams was decomposed into a summation of plane waves using the angular spectrum of plane waves (ASPW) description. This allows us to model focused beams with an arbitrary numerical aperture (NA) without the limitations found in the paraxial approximation. Said beams are simulated using a finite-difference time-domain (FDTD) tool that was developed during the work and further enhanced to simulate the scanning of focused beams in a more efficient way compared to other FDTD solvers.

Using the developed tools, it was possible to show that using small NA beams for imaging deep inside scattering media proved more advantageous than high NA beams. Also due to the usage of the ASPW formalism, it was possible to model and verify the mechanism of wave-front shaping. Such a tool that uses the exact solution of Maxwell’s equations can be used in the future to further our development of applications such as phase optimization, photo-acoustics and many more techniques that are expected to keep pushing the boundaries of deep imaging inside and through turbid media.
Acknowledgements

I would like to thank my parents who made sure that I had the chance to follow my dreams. Also my friends in the laser institute who made me feel home away from home.

Special thanks to the supervisors of the work Prof. Dr. Raimund Hibst and Prof. Dr. Alwin Kienle and my colleagues Dr. Ansgar Hohmann, Arnd Brandes, Dominik Reitzle, Julian Stark, Philipp Krauter, and Thomas Brenner for all the academic support and the fruitful scientific discussion.
Glossary

\(\lambda\) wavelength

\(\mu\) Magnetic permeability (henrys/meter)

\(\mu_0\) Free-space permeability (4 \(\pi\ 10^7\) henrys/meter)

\(\mu_r\) Relative permeability (dimensionless scalar)

\(\rho\) mean free path

\(\varepsilon\) Electrical permittivity (farads/meter)

\(\varepsilon_0\) Free-space permittivity (8.8541012 farads/meter)

\(\varepsilon_r\) Relative permittivity (dimensionless scalar)

\(C_i\) concentration ratios of the refractive indices of the medium \(i\)

\(j\) \(\sqrt{-1}\)

\(n_m\) refractive index of medium

\(n_s\) refractive index of scatterer

2-D Two dimension

3-D Three dimension

A Area

r \((x,y,z)\)

A Amplitude of a wave

ABC absorbing boundary condition

ASPW Angular spectrum of plane waves

B Magnetic flux density (webers/meter\(^2\))

**Beam-waist**\(_{1/e^2}\) The point at which the intensity of the beam drops to \(1/e^2\) of the maximum intensity of the beam.

\(c\) speed of light (meter/second)

CFRP Carbon fiber-reinforced plastics

conc. volume concentration

cyl cylinder

D Electric flux density (coulombs/meter\(^2\))

DMD Digital micromirror device

E Electric field (volts/meter)

FDTD Finite-difference time-domain

FFT fast Fourier transform

fs femtosecond

H Magnetic field (amperes/meter)

MC Monte-Carlo

med medium

n refractive index

NA Numerical aperture

NFFF Near- to far-field transformation

OPC optical phase conjugation

PET positron emission tomography

PML perfectly matched layer

PSTD Pseudo-spectral time-domain

SLM Spatial light modulator

TE transverse electric field

TF/SF Total-field/scattered-field

TM transverse magnetic field
Contents

Glossary v

List of Figures ix

1 Introduction 1

2 Theory 5

2.1 Angular spectrum of plane waves ................................................. 5
    2.1.1 Geometric intensity law .................................................... 9
    2.1.2 Focused and Gaussian beams .............................................. 12
    2.1.3 Quasi-Bessel beam ........................................................... 12
    2.1.4 Radially polarized beam (ring beam) .................................... 12

2.2 Beam scanning .............................................................................. 14

2.3 Applying ASPW in the multiple cylinders scattering analytical solution .... 15

2.4 Mode-locking using analytical solution ......................................... 18

2.5 Phase optimization ................................................................. 18

2.6 The direct extinction method ...................................................... 23
    2.6.1 The direct extinction method within the Monte Carlo algorithm .... 24
    2.6.2 Modeling the absorption ........................................................ 25
    2.6.3 Ray direction: The Poynting vector ....................................... 26
    2.6.4 Modeling the scattering ........................................................ 27

3 Numerical methods 29

3.1 Introduction to FDTD ............................................................... 29

3.2 Discretization of Maxwell’s equations ......................................... 30

3.3 Total-field/scattered-field technique ............................................ 31
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4</td>
<td>Modeling of beams in 2-D</td>
<td>34</td>
</tr>
<tr>
<td>3.5</td>
<td>Numerical dispersion</td>
<td>35</td>
</tr>
<tr>
<td>3.6</td>
<td>Absorbing boundary condition</td>
<td>36</td>
</tr>
<tr>
<td>3.7</td>
<td>Near- to far-field transformation</td>
<td>38</td>
</tr>
<tr>
<td>3.8</td>
<td>Verification</td>
<td>39</td>
</tr>
<tr>
<td>4</td>
<td>Results and applications</td>
<td>43</td>
</tr>
<tr>
<td>4.1</td>
<td>Light beam scanning</td>
<td>44</td>
</tr>
<tr>
<td>4.2</td>
<td>Depth profile study for multiple beams</td>
<td>47</td>
</tr>
<tr>
<td>4.2.1</td>
<td>Scattering media</td>
<td>48</td>
</tr>
<tr>
<td>4.2.2</td>
<td>The illumination</td>
<td>48</td>
</tr>
<tr>
<td>4.2.3</td>
<td>Results</td>
<td>49</td>
</tr>
<tr>
<td>4.3</td>
<td>Phase optimization</td>
<td>59</td>
</tr>
<tr>
<td>4.4</td>
<td>Time reversal and phase conjugation</td>
<td>65</td>
</tr>
<tr>
<td>4.4.1</td>
<td>Optical phase conjugation</td>
<td>67</td>
</tr>
<tr>
<td>4.4.2</td>
<td>Time reversal</td>
<td>72</td>
</tr>
<tr>
<td>4.5</td>
<td>Carbon fiber</td>
<td>78</td>
</tr>
<tr>
<td>4.5.1</td>
<td>Comparison of different simulation models for light propagation in CFRP</td>
<td>78</td>
</tr>
<tr>
<td>4.5.2</td>
<td>Far-field results of the different simulation models and discussion</td>
<td>80</td>
</tr>
<tr>
<td>4.5.3</td>
<td>Near-field results of the different simulation models and discussion</td>
<td>81</td>
</tr>
<tr>
<td>4.5.4</td>
<td>Measurements of remitted light from CFRP in the backward direction</td>
<td>85</td>
</tr>
<tr>
<td>4.5.5</td>
<td>Results and discussion of the measurements and comparison with simulations</td>
<td>88</td>
</tr>
<tr>
<td>4.6</td>
<td>The direct extinction method</td>
<td>92</td>
</tr>
<tr>
<td>4.6.1</td>
<td>Principle - <em>in vacuo</em></td>
<td>92</td>
</tr>
<tr>
<td>4.6.2</td>
<td>In absorbing media</td>
<td>94</td>
</tr>
<tr>
<td>4.6.3</td>
<td>In scattering media</td>
<td>96</td>
</tr>
<tr>
<td>4.6.4</td>
<td>Direction of the Poynting vectors</td>
<td>99</td>
</tr>
<tr>
<td>5</td>
<td>Discussion and outlook</td>
<td>103</td>
</tr>
<tr>
<td>References</td>
<td></td>
<td>109</td>
</tr>
</tbody>
</table>
List of Figures

1.1 Conceptual comparison between wide-field illumination and focused illumination when both are are used in microscopy. .............................................. 2

2.1 Geometry of light focusing in 3-D. A plane wave is incident on a lens, which focuses the light. Afterwards, the light starts to diverge. An aperture in front of the lens is omitted for clarity. .......................................................... 6

2.2 Geometry of the simulations, as carried out in this work in 2-D. The setup is infinite in \(z\)-direction. The electric field is propagating in \(x\) direction while being polarized in \(z\) direction. The dark red region visualizes the focusing effect after going through the lens. ................................................................. 8

2.3 Comparison of different distributions of Huygens’ point sources depending on the integration domain. Both (a) and (b) are describing the illumination of an aperture using spatial (a) and angular (b) domain integration, while (c) is for the angular integration for a lens. In all cases the illumination consists of a plane wave. 10

2.4 Description of the two main conditions for aplanatic lenses. (a) The sine rule, where the ray emerging from an aplanatic lens meets the focal sphere at the same height as the corresponding ray entered the lens. (b) The intensity law where the energy flux along a ray must stay constant. \(f\) is the focus length of the aplanatic lens and \(h\) is the distance between the ray under consideration and the optical axis. 11

2.5 A schematic of the orientation of plane waves in order to form beams of different polarization. \(\hat{E}\) is the direction of polarization and \(\hat{k}\) is the direction of propagation. 13

2.6 A comparison between the linearly and radially polarized beams. The figures were generated using 3-D FDTD by propagating 100 plane waves in the scheme of ASPW. The beam waist and the wavelength were equal to 1 \(\mu \text{m}\). ............... 14
LIST OF FIGURES

2.7 Simulation (Monte Carlo and Maxwell method) of the differential scattering cross section of a 40 µm by 40 µm carbon fiber sample irradiated by a Gaussian beam with a beam waist of 15 µm. .................................................. 16
2.8 Two time shots for a plane wave of wavelength of 1 µm incident on a cylinder of diameter of 1 µm and \( n_s = 1.33 \). .......................................................... 19
2.9 Schematic of how the phase optimization works (both off-mode in Fig. (a) and on-mode in Fig. (b)). The SLM is assumed to work in reflection mode for better visibility only. Also, the SLM is taken here as an example. In principle any wave front modulation device can be used in this setup. ......................... 20
2.9 Schematic of how the phase optimization works (both off-mode in Fig. (a) and on-mode in Fig. (b)). The SLM is assumed to work in reflection mode for better visibility only. Also the SLM is taken here as an example. In principle any wave front modulation device can be used in this setup. ......................... 21
2.10 The effect of the realization number on the accuracy of the intensity enhancement at the focus. \( n_s \) is equal to 1.4 while the depth where the optimization occurred was 35 µm. ....................................................... 22
2.11 Comparing the enhancement factor \( \eta \) for a low scattering scenario \((n_s = 1.4)\), and a high scattering scenario \((n_s = 1.5)\). \( x \) is the detection depth inside the material. 23
3.1 The 2-D FDTD grid with the TF/SF regions. The bold black letters on the side \((L,M-L,\ldots)\) are the indices used in the implementation. ......................... 33
3.2 Introduction of the incident field. (a) Generation of a 2-D incident field by the projection of a 1-D vector for \( \phi \) less than 90°. (b) Generation of 2-D incident fields by the projection of a 1-D vector for \( \phi \) more than 90°. ......................... 34
3.3 The implementation of the ASPW method in the FDTD method. The plane wave propagates in the x-direction and passes through a lens where a focused beam is formed at position \((x_0,y_0)\). The FDTD grid is divided into a total field region that contains both the incident and the scattered fields and a scattered field region which contains only the scattered fields. The incoming wave enters the FDTD grid at the interface between total and scattered field. \( y_m \) represents the maximum distance from the focus of the beam to the lateral boundary of the total field and scattered field regions. ................................. 35
3.4 The 2-D FDTD grid with the near- to far-field transformer boundary. ....... 39
3.5 Comparison of the normalized intensity of the $E_z$-component of the electric field for scattering by a cylinder of diameter 1 $\mu$m for an incident plane wave: (a) FDTD simulation, (b) analytical solution, (c) the relative difference between the first two figures. Figures (a) and (b) are normalized to the maximum of the intensity for each case, and the cylinder is located at $x/\lambda = y/\lambda = 0$.

3.6 The differential scattering cross section of a cylinder with a diameter of 1 $\mu$m for an incident plane wave and a focused beam. The focused beam has a maximum divergence angle of 45 degrees while both the focused beam and the plane wave have the wavelength of 1 $\mu$m. The refractive index of the cylinder is 1.33 surrounded by air ($n = 1$) in both cases. The spatial resolution in the FDTD simulation is equal to $\lambda/80$.

3.7 Comparison between the grid sizes of FDTD and MC.

3.8 Three different FDTD grid sizes (from left to right: $y = 8\lambda$, $16\lambda$ and $32\lambda$) displayed in logarithmic scale over the range $8\lambda \times 8\lambda$ for the linearly polarized beam.

4.1 The normalized intensity of the $E_z$ component of the electric field at different positions of the focused beam. The desired focus positions in the figures (a) to (f) are at: $(x_0/\lambda = -4, y_0/\lambda = 0)$, $(x_0/\lambda = -4, y_0/\lambda = -4)$, $(x_0/\lambda = 0, y_0/\lambda = 0)$, $(x_0/\lambda = 0, y_0/\lambda = -4)$, $(x_0/\lambda = 3, y_0/\lambda = 3)$, and $(x_0/\lambda = 5, y_0/\lambda = 1)$. The intensity is normalized to the intensity of the non disturbed $E_z$ component at the focus of the beam. The maximum divergence angle is $45^\circ$ and the wavelength of the incident light is 1 $\mu$m. The spatial resolution in the FDTD simulation is equal to $\lambda/20$ and $n_m = 1$.

4.2 The normalized intensity of the $E_z$ component of the electric field for axial scanning ($x$ direction) at $y_0 = 0$. The normalization is relative to the maximum intensity of the incident non-scattered focused beam. Figure (a) shows the scatterers in red, while they are omitted in the latter pictures for better visibility of the beam shape. The figures from (a) to (f) show focus positions at: $y_0/\lambda = 0$ and $x_0/\lambda = (-8, -6, -2, 2, 4, 9)$. 21 plane waves are used to form the beam. The refractive indices are $n_s = 1.45$ and $n_m = 1.33$, the radius of the cylinders is 0.5 $\mu$m, the wavelength of the incident light is 1 $\mu$m, and $\theta_{max} = 45^\circ$. The spatial resolution in the FDTD simulation is equal to $\lambda/20$. 
4.3 The normalized intensity of the $E_z$ component of the electric field for lateral scanning ($y$ direction) at $x_0 = 0$. The normalization is relative to the maximum intensity of the incident non-scattered focused beam. Figure (a) shows the scatterers in red, while they are omitted in the latter pictures for better visibility of the beam shape. The figures from (a) to (f) show focus positions at: $x_0/\lambda = -10$ and $y_0/\lambda = 2$, and then $x_0/\lambda = 0$ and $y_0/\lambda = (-8, 4, 0, -4, 8)$. 21 plane waves are used to form the beam. The refractive indices are $n_s = 1.45$ and $n_m = 1.33$, $r = 0.5 \mu m$, the wavelength of the incident light is $1 \mu m$, and $\theta_{max} = 45^\circ$. The spatial resolution in the FDTD simulation is equal to $\lambda/20$. 

4.4 The intensity (W/m$^2$) of a focused beam at different focus positions for an incident beam of 1 W/m power ($|\theta| = [0^\circ : 45^\circ]$). The upper left picture shows the scatterers in blue while they are omitted in the latter pictures for better visibility of the beam shape. The origin in the longitudinal direction is placed at the starting point of the scatterers. The refractive indices are $n_m = 1.33$ and $n_s = 1.5$. $x_0$ is the focal position. 

4.5 The intensity (W/m$^2$) of a quasi-Bessel beam at different focus positions for an incident beam of 1 W/m power ($|\theta| = [25^\circ : 45^\circ]$). The upper left picture shows the scatterers in blue while they are omitted in the latter pictures for better visibility of the beam shape. The origin in the longitudinal direction is placed at the starting point of the scatterers. The refractive indices are $n_m = 1.33$ and $n_s = 1.5$. $x_0$ is the focal position. 

4.6 The intensity (W/m$^2$) for the focused beam in Fig. 4.4 averaged over a lateral range of $\pm 20 \mu m$. $x_0$ is the focal position. 

4.7 The intensity (W/m$^2$) for the quasi-Bessel beam in Fig. 4.5 averaged over a lateral range of $\pm 20 \mu m$. $x_0$ is the focal position. 

4.8 The on-axis intensity for the focused, Gaussian (Beam-waist$_{1/e^2} = 1.5 \mu m$), and Bessel beams for the same incident differential power. The refractive indices are $n_m = 1.33$ and $n_s = 1.5$. 

4.9 The lateral profile of the beams at different depths for $n_m = 1.33$ and $n_s = 1.5$. The differential power of each beam is equal to 1 Watt/m. The first three focused beams have $\theta_{max} = 45^\circ$(blue), $25^\circ$(green), $15^\circ$(red). The quasi-Bessel beam has $|\theta| = [25^\circ : 45^\circ]$, while the Gaussian beam has a FWHM = 0.86 $\mu m$. 

xii
4.10 The on-axis intensity for the beams while using two sizes of cylindrical scatterers (solid lines for Dia. = 1 µm and dashed lines for 2 µm) while $n_s$ is kept equal to 1.45 and $n_m = 1.33$. ................................. 54

4.11 Beam profiles at three different depths using the analytical solution for the non-scattered light ($\rho = 3.4 \, \mu m$). ................................................................. 55

4.12 Ratio of the intensities for different beams using the analytical solution for the non-scattered light for the case when $\rho$ is equal to 3.4 µm. ................................. 56

4.13 The intensity of the focused beam ($\theta_{max} = 45^\circ$) from the FDTD (dashed lines) while being scanned through scattering media for different concentrations of scatterers. The intensity is compared with the Beer-Lambert law using the direct extinction method (solid lines with squares). ................................. 57

4.14 Comparing the validity of the Beer-Lambert law using the direct extinction method compared to FDTD for different scattering parameters and for the same incident focused beam and volume concentration ($\theta_{max} = 45^\circ$, conc. = 5%). The tilde sign in the legend of the last curve is to show the range excluded from the interpolation. This is done to avoid taking the main peak, thus, taking only the multiple scattering contribution. ................................. 59

4.15 The effect of using lateral scanning to average over several incoherent intensities. The refractive indices are $n_s = 1.5$ and $n_m = 1.33$. In both cases, the intensity of the focus is shown after being scanned in depth direction. The wavelength is $\lambda = 1 \, \mu m$. ................................. 60

4.16 The procedure to analyze the effect of phase optimization on the enhancement of intensity. In the first column, the incident light is scattered. By shifting the beam laterally, the beam interacts with different configurations of the scatterers. In the second column, the phase of the beam is optimized. All the results from the second column are averaged by adding them incoherently to reach the desired focal plane in the third column. This procedure is repeated after going to the following depth point by shifting the focus of the beam in the longitudinal direction. The main advantage of this method is the usage of one set of simulation data to get the optimization of several realizations. ................................. 62
4.17 FDTD simulations to show the effect of phase optimization. Two samples with two different concentrations are investigated while keeping the mean free path as close as possible while assuming single scattering. The dashed lines are the FDTD simulations without optimization. The circle symbols show the optimized case with a range of $2\pi$ for the phase, while the square symbols show the optimized case with a range of $\pi$. The solid lines show the combination of FDTD simulations for a homogenous medium (to have the information about the non-disturbed focus) and the FDTD simulations with scatterers, but without phase optimization. The agreement between the dashed lines and the circle curves shows that the optimization process merely corrects the phase of the focus which was disturbed due to the scattering process.

4.18 A combined image of the intensity $[\text{W/m}^2]$ in focal planes after depth scanning through a scattering medium of $n_m = 1.33$ and $n_s = 1.5$. In each subfigure the normal propagation of the beam is shown, followed by the phase optimized propagation. The combination was done according to the scheme shown in Fig. 4.16 and $\lambda = 1 \mu\text{m}$.

4.19 Comparing the near field intensity $[\text{W/m}^2]$ for the optimized and non-optimized cases for two different depths and for a focused beam with $\theta_{max} = 45^\circ$. The refractive indices were $n_m = 1.33$ and $n_s = 1.5$. The wavelength was $1 \mu\text{m}$. Fig. (c) is identical to Fig. (b) with the sole difference of keeping the same scale to better see and compare the low intensities away from the focus.

4.20 Schematic of time reversal of a point source. (a) An outgoing wave that gets scattered by an arbitrarily shaped scatterer which is drawn in gray. (b) The outgoing wave has been reversed and is directed back towards its original source.

4.21 The normalized intensity [a.u.] of a converging radial wave. Assuming no scatterers, a dipole would have been formed in the middle of the grid with an intensity of 1. The refractive indices are $n_m = 1$, $n_s = 1.33$, and $\lambda = 1 \mu\text{m}$.

4.22 The normalized intensity [a.u.] of a converging radial wave after correcting the phases by detecting an outgoing dipole. The refractive indices are $n_m = 1$, $n_s = 1.33$, and $\lambda = 1 \mu\text{m}$.

4.23 The intensity $[\text{W/m}^2]$ of a dipole propagating out of the point of interest to be detected using the NFFF. The parameters used are $n_m = 1$, $n_s = 1.33$, $r = 0.5 \mu\text{m}$ and $\lambda = 1 \mu\text{m}$.
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.24</td>
<td>The intensity ([\text{W/m}^2]) of a reversed dipole using the phase information from Fig. 4.23, trying to achieve focusing at the point (y = 0 \mu m, x = -4.75 \mu m). In the case of (t = 75 \text{ fs}) we get the moment of best focus.</td>
<td>77</td>
</tr>
<tr>
<td>4.25</td>
<td>The setup of the carbon fiber simulations.</td>
<td>79</td>
</tr>
<tr>
<td>4.26</td>
<td>(\log_{10}) of the intensity of the scattered light [a.u.] in the 40 by 40 (\mu m) carbon fiber sample calculated by the Maxwell solution (polarization parallel to the carbon fibers) using 50 different realizations to average the results. The results are normalized by the intensity of the incident Gaussian beam.</td>
<td>82</td>
</tr>
<tr>
<td>4.27</td>
<td>Absorbed power density in the 40 by 40 (\mu m) carbon fiber sample according to four different simulation models (polarization parallel to the carbon fibers).</td>
<td>83</td>
</tr>
<tr>
<td>4.28</td>
<td>A Gaussian beam with beam-waist of 15 (\mu m) illuminating a sample of parallel cylinders of diameter equal to 7 (\mu m). The wavelength is 515 nm and the matrix containing the cylinders is vacuum ((n_m = 1)). The beam is incident from the left hand side of the sample. The color bar represents the logarithm to base 10 of the intensity of the light ((</td>
<td>E_z</td>
</tr>
<tr>
<td>4.29</td>
<td>The same intensity and Poynting vectors as in Fig. 4.28c and 4.28d but with an extended scale to show more details deep in the sample.</td>
<td>87</td>
</tr>
<tr>
<td>4.30</td>
<td>Measurement and simulation of the differential scattering cross section of a carbon fiber sample irradiated by a Gaussian beam with a beam waist of 15 (\mu m) ((\lambda = 515 \text{ nm})).</td>
<td>88</td>
</tr>
<tr>
<td>4.31</td>
<td>Absorbed light for a Gaussian beam rotated by (\theta_{\text{tilt}}).</td>
<td>91</td>
</tr>
<tr>
<td>4.32</td>
<td>Differential scattering cross section results ([\log_{10}(\text{value})]) for a Gaussian beam incident on a carbon fiber sample with different tilting directions. The radially polarized beam has a tilting angle of 0°.</td>
<td>92</td>
</tr>
</tbody>
</table>
4.33 Comparison of the probability distributions yielded by the MC simulations (the number of sampled “target positions” are $10^6$ and $10^9$ on the left and on the right, respectively) and the FDTD simulations for the linearly polarized beam focused in vacuo in the $x$-direction. These distributions are displayed here in logarithmic scale over the range $8\lambda \times 8\lambda$. The MC simulations are shown for $y/\lambda > 0$ and FDTD simulations for $y/\lambda \leq 0$ for both figures. The blue curves are cross-sections of the probability profiles at the focal plane $x = x_{ph} = 4\lambda$, while the green curves are cross-sections of the FDTD results.

4.34 Comparison of the probability distributions displayed here in logarithmic scale over the range $8\lambda \times 8\lambda$ and yielded by the MC simulations (with $10^9$ “target positions” sampled) and the FDTD simulations (grid size $8\lambda \times 32\lambda$) for the linearly polarized beam focused in the $x$-direction in increasingly absorbing media. From left to right and top to bottom: $\mu_a = (16\lambda)^{-1}$, $(8\lambda)^{-1}$, $(4\lambda)^{-1}$ and $(2\lambda)^{-1}$ (the corresponding values for the imaginary component $\kappa$ of the material’s refractive index are $(64\pi)^{-1}$, $(32\pi)^{-1}$, $(16\pi)^{-1}$, and $(8\pi)^{-1}$, respectively). The curves are cross-sections of the probability profiles at the focal plane $x = x_{ph}$ (MC in blue and FDTD in green).

4.35 Quantitative representation of the results shown in Fig. 4.34. The probability profiles corresponding to the different absorbing materials are cross-sections close to the illumination face (left), at $x = 0.01\lambda$ and in the focal plane at $x = x_{ph} = 4\lambda$ (right).

4.36 The normalized intensity of the $E_x$-component for a Gaussian (a), a focused (b), and a Bessel (c) beam and the intensity of the lateral component of the electric field ($I_r = |E_x|^2 + |E_y|^2$) for a radially polarized beam (d). All beams are formed using equation (2.27) while propagating in a non-scattering medium ($n_m = 1$). For the Gaussian and the radially polarized beams, the beam waist is set to $1 \mu m$. In each case the desired focus depth is $40 \mu m$. All the beams are normalized to the maximum intensity for each individual case and the scale is logarithmic.
LIST OF FIGURES

4.37 The normalized intensity of the $E_x$-component for a Gaussian (a), a focused (b), and a Bessel beam (c) and the normalized intensity of the lateral component of the electric field ($I_r = |E_x|^2 + |E_y|^2$) for a radially polarized beam (d). All beams are formed using equation (2.27) while propagating in a scattering medium of $\rho = 10 \, \mu m$. For the Gaussian and the radially polarized beams the beam waist is set to $1 \, \mu m$. In each case the desired focus depth is $40 \, \mu m$. All the beams are normalized to the maximum intensity for each individual case and the scale is logarithmic.

4.38 Direction of the normalized Poynting vectors $\mathbf{S}(\mathbf{r})$ plotted over probability distributions displayed here in logarithmic scale over the range $3\lambda \times 3\lambda$, and calculated with both MC simulations ($10^9$ “target positions” sampled) and FDTD simulations (grid size of $8\lambda \times 32\lambda$). Left: The linearly polarized beam is focused in vacuo. Right: The same beam is focused in an absorbing medium, where $\mu_a = (2\lambda)^{-1}$. In MC simulations, the binning size is kept at $\Delta x = \Delta y = \lambda/25$.

4.39 A radially polarized beam is focused in vacuo. On the left: Distribution of the non-normalized Poynting vectors $\mathbf{S}(\mathbf{r})$ plotted over the probability distribution displayed here in logarithmic scale over the range $4\lambda \times 4\lambda$ and calculated with FDTD simulations (grid size of $8\lambda \times 32\lambda$). On the right: same distribution of the normalized Poynting vectors obtained with both MC simulations ($10^8$ “target positions” sampled) and the FDTD simulations plotted over the probability distribution displayed here in logarithmic scale over the range $8\lambda \times 8\lambda$. The Poynting vectors are normalized in the figure on the right to better show the results in regions with extremely small intensity (the points of destructive interference).
Chapter 1

Introduction

In the recent few years, a great deal of progress has been made in the fields of microscopy (e.g. confocal microscopy [1], two photon microscopy [2, 3]), optical coherence tomography [4], photo-acoustic imaging [5, 6, 7, 8], and photo-thermal therapy [9, 10, 11, 12, 13, 14, 15]. This is mainly due to the fact that using light is non-invasive, accurate (more than e.g. sonar due to the higher frequency of the light), and much more safe compared to other means of three-dimensional imaging which usually has a high dose of radiation (e.g. X-rays and PET). The main obstacle to wider usage of light in the mentioned fields is scattering [16]. Refractive index inhomogeneities cause light to be strongly scattered. What makes the problem even more convoluted is the continuous pursuit of better resolution. This can be achieved mostly by focusing light into tight beams, to limit the interaction between the incident light and the sample being examined to the smallest possible area. [17] (see Fig. 1.1).

This work has two main targets. First is the modeling of the incident light as focused beams of different profiles. This is done by following in the footsteps of the work by Çapoğlu, Taflove, and Backman [18, 19]. The angular spectrum of plane waves (ASPW) is used to decompose the complex structure of the beams into a summation of - simpler to describe - plane waves. This model is then applied in a finite-difference time-domain (FDTD) code written specifically for this purpose. The results are verified using different analytical solutions for the scattering of light (both plane waves and beams) by a single dielectric cylinder [20, 21]. A simulation technique is then used to model the scanning of light beams through the scattering media by manipulating the phases of the plane waves that constitute the beam being used [22].

Secondly the developed code is used to simulate several techniques to enhance the intensity of the light focus inside the scattering media. One method is the optimization of the wave front
1. INTRODUCTION

Figure 1.1: Conceptual comparison between wide-field illumination and focused illumination when both are are used in microscopy.

of the incident light [23, 24, 25], where light is modulated in such a way that the individual components of the beam would add up constructively at the point of interest. The second method is the usage of a guiding star inside the scattering medium which is then phase conjugated to get the best wave-front shaping to reach deep inside the scattering medium [26, 27, 28]. The term “guiding star” is taken from the field of astronomy where the light from a star is taken as a reference to calibrate the adaptive optics used in telescopes. Obviously it is complicated to study such techniques inside a material in an experimental setup, and until now most of the simulations have only used the T-matrix method or other approximation approaches like the paraxial approximation [27, 28]. This shows another advantage of this work since the simulations solve Maxwell’s equations for a certain situation, providing us with an exact solution and giving us a tool that can facilitate the investigation of the intrinsic characteristics of light scattering. There are other similar works using tools based on the numerical solution of Maxwell’s equations [29, 30], but in the case of the current study there is more emphasis on how to visualize the connection between the simulation tool and the experimental devices that are used to implement such setups. Furthermore, the tool developed in this work is intended to help in understanding
if such methods would work for a certain set of parameters (e.g., refractive index of the particles, size and concentration of said particles, etc.).

Several other examples for how the code was used are also given to further our understanding of some physical problems that we are facing (e.g., the characterization of carbon fibers using light), and to verify other types of numerical solutions (e.g., the Monte Carlo method).

The thesis is organized in four main chapters. After the introduction chapter 2 describes the ASPW method which is the main theoretical tool that is used to model the light beams used. Also other related utilities are introduced in subsequent sections such as the ability to scan beams that are modeled using the ASPW and the optimization of the phase of such beams to achieve enhanced intensity inside scattering media. In chapter 3, the FDTD method is described and its verification is presented. Several different applications are shown in chapter 4, where the ASPW is used to model some specific problems. For example in section 4.2, the depth scanning of beams with different profiles is simulated to show what kind of beams perform better for illuminating deep inside a scattering medium. Each section has its own conclusions depending on its results, and in the end of the work there is a chapter for a more general discussion.
1. INTRODUCTION
Chapter 2

Theory

Abstract

The main challenges in modeling light propagation can be summarized in two points. The first one is the complex interaction between the incident light and the scatterers. In this work this problem is dealt with either by using a specific geometry for the scatterers (e.g., cylinders) in order to use the analytical solution of such a problem, or by implementing a numerical method like FDTD to solve the discretized Maxwell’s equations. The second challenge is the modeling of the incident light. It is possible to use the paraxial description of a Gaussian beam while adding extra terms to take into account the higher numerical appreture [31]. However, even with these correction terms, the beam still suffers from some errors. Moreover, it becomes more tricky to simulate other kind of beams with different spatial profiles like ring beams or Bessel beams. For this purpose the angular spectrum of plane waves (ASPW) method [32] is utilized in this work. The ASPW of an optical field is the representation of that field as a superposition of plane waves.

2.1 Angular spectrum of plane waves

In this work, the field distribution that is studied in the near-field - and in particular in the focal plane - is formed from light illuminating a lens in the far-field (Fig. 2.1). This means that a beam with a complex structure is transformed into a summation of converging plane waves. The formalism used here is based on the work of Novotny and Hecht [33]. The first step is to
write the spatial dependence of the fields on the spatial frequencies of the electric field in the focal plane

\[ E(x, y, z) = \int \int \hat{E}(k_x, k_y; z = 0) e^{j(k_x x + k_y y \pm k_z z)} dk_x dk_y, \quad (2.1) \]

where \( E \) is the electric field at the point \((x, y, z)\) and \( \hat{E} \) is the electric field for the spatial frequencies \((k_x, k_y; z = 0)\) in the focal plane. The spatial frequency \( k_z \) depends on the other components according to the relation \( k_z = \sqrt{k_0^2 - k_x^2 - k_y^2} \), following the Helmholtz equation.

By defining \( r = |r_\infty| = \sqrt{x^2 + y^2 + z^2} \) which is the distance from the point of evaluation in the far-field to the origin at the focus of the beam, we get

\[ E_\infty(s_x, s_y, s_z) = \lim_{kr \to \infty} \int \int \hat{E}(k_x, k_y; z = 0) e^{jkr(\frac{k_x}{r} s_x + \frac{k_y}{r} s_y + \frac{k_z}{r} s_z)} dk_x dk_y, \quad (2.2) \]

where \( s = (s_x, s_y, s_z) = (\frac{x}{r}, \frac{y}{r}, \frac{z}{r}) \) is a dimensionless unit vector in direction of \( r_\infty \) and \( E_\infty \) is the field distribution \( E \) at \( r_\infty \). By going to the far-field we lose the information about the evanescent waves - which are described by the high spatial frequencies - due to their exponential decay. Therefore, in equation (2.2), the limits of the integration have been limited to \( k_x^2 + k_y^2 \leq \)
2.1 Angular spectrum of plane waves

\( k^2 \). \( k = (k_x, k_y, k_z) \) is the wave vector and \( k = |k| \) is the wave number. The integration in equation (2.2) can be evaluated using the method of stationary phase to give:

\[
E_\infty(s_x, s_y, s_z) = -2\pi jks_z \hat{E}(ks_x, ks_y; z = 0)e^{jkr/r}.
\] (2.3)

Equation (2.3) shows that the far-field is completely defined by the spatial frequency description of the field in the focal plane by replacing \( k_x \rightarrow ks_x \) and \( k_y \rightarrow ks_y \). This simply means that the unit vector \( s \) fulfills:

\[
s = (s_x, s_y, s_z) = \left( \frac{k_x}{k}, \frac{k_y}{k}, \frac{k_z}{k} \right).
\] (2.4)

This gives us the near-field spatial frequencies in the focal plane as a function of the far-field distribution:

\[
\hat{E}(k_x, k_y; z = 0) = \frac{jre^{-jkr}}{2\pi k_z} \hat{E}_\infty(k_x, k_y).
\] (2.5)

By substituting equation (2.5) into equation (2.1) (and keeping in mind that now equation (2.1) is completely defined in the far-field after the usage of the limit operator in equation (2.2)), we get

\[
E(x, y, z) = \frac{jre^{-jkr}}{2\pi} \int \int_{k_x^2 + k_y^2 \leq k^2} \hat{E}_\infty(k_x, k_y) e^{j(k_x x + k_y y + k_z z)} \frac{1}{k_z} dk_x dk_y,
\] (2.6)

which is the spatial distribution in the near-field as a function of the far-field distribution. However, the far-field is still described as a function of the spatial frequencies. A more convenient way is to transform it into the angular domain. This is done by replacing the differentials as

\[
dk_x dk_y = \cos \theta (k^2 \sin \theta d\theta d\phi),
\] (2.7)

where \( \phi \) is the angle measured from \( x \)-axis in the \( x-y \) plane and \( \theta \) is the angle from \( z \)-axis to the \( x-y \) plane. This transforms the integration from a plane to a spherical surface. By substituting equation (2.7) into equation (2.6), where the \( k \cos \theta \) term in equation (2.7) cancels out with the term \( 1/k_z = 1/(k \cos \theta) \) in equation (2.6), and by using \( \hat{E}_\infty = \hat{E}_{inc}/\sqrt{\cos \theta} \) to ensure
2. THEORY

the conservation of energy while going through the lens \[33, 34\] (explained in detail in section 2.1.1), we reach

\[
E(x, y, z) = \frac{jre^{-jkr}}{2\pi} \int_0^{\theta_{\text{max}}} \int_{-\pi}^{\pi} \hat{E}_{\text{inc}}(\theta, \phi) e^{jk(x\sin\theta\cos\phi + y\sin\theta\sin\phi \pm z\cos\theta)} \sqrt{\cos\theta} \sin\theta d\phi d\theta. \tag{2.8}
\]

The previous formulation is for a three-dimensional setup. In this work a two dimensional description is mostly used (Fig. 2.2) to decrease the computational load. By following the same procedure that is used for equation \(2.8\), we arrive at

\[
E_z(x, y) = \frac{-re^{-jkr}}{\sqrt{\lambda^2}} \int_{-\theta_{\text{max}}}^{\theta_{\text{max}}} \hat{E}_{z,\text{inc}}(\theta) e^{jk(y\sin\theta \pm x\cos\theta)} \sqrt{\cos\theta} d\theta, \tag{2.9}
\]

**Figure 2.2:** Geometry of the simulations, as carried out in this work in 2-D. The setup is infinite in \(z\)-direction. The electric field is propagating in \(x\) direction while being polarized in \(z\) direction. The dark red region visualizes the focusing effect after going through the lens.

where the fields in the \(z\)-direction are constant and the angle \(\theta\) is now the angle measured from the \(x\)-axis in the \(x-y\) plane (see Fig. 2.2). The investigated two-dimensional case decouples Maxwell’s equations into two independent polarizations, the transverse electric (TE) and the transverse magnetic (TM) polarizations. In this study only the TM-polarization will be discussed since the numerical treatment of both polarizations is identical. Therefore, only the component of the electric field parallel to the \(z\)-axis is regarded. For this reason, we find the subscript
2.1 Angular spectrum of plane waves

This subscript is suppressed from now on since we only deal with that component. Equation (2.9) illustrates that the field distribution of the required beam in the focal plane can be manipulated by controlling the $\hat{E}_{\text{inc}}$ term in the far-field. The propagation direction in the 2-D case is the $x$-direction while $y$ denotes the lateral direction. Equation (2.9) is further discretized to be usable in the computational parts of this work and normalized to have a maximum of $E_0$ for the incident beam:

$$E_z(x, y) = \sum_{m=1}^{M} \hat{E}_{z, \text{inc}}(\theta_m) e^{j(y \sin \theta_m \pm x \cos \theta_m) \sqrt{\cos \theta_m}},$$

where $M$ is the number of plane waves used to construct the beam under test. The normalization factor is inside the angular description of the beam as will be shown in section 2.1.2.

In summary, the ASPW describes the optical fields of the focused beams as a superposition of propagating plane waves [32]. First, the spatial distribution of the electric field $E(x = 0, y)$ in the focal plane is given. Then, by using a Fourier transform, the electric field versus spatial frequency $\hat{E}(k_y)$ is calculated. By substituting the integrands in the Fourier transform, the angular description $\hat{E}(\theta)$ in the far-field is obtained [33]. Following the work of Richards and Wolf, we model the focusing effect by using an aplanatic lens. Thus, we need to take the geometric intensity law into account [34]. After these mathematical manipulations, we write the spatial electric field as a function of the angular far-field in a discretized form to facilitate the simulations later on using plane waves incident at discrete angles.

2.1.1 Geometric intensity law

As mentioned in section 2.1, it is necessary to consider the energy conservation when light passes through a lens. A simple aperture (or a pin hole) is assumed which is illuminated by a plane wave. The wave-front that passes to the other side of the aperture can be imagined as the coherent summation of an infinite number of Huygens’ point sources placed equidistantly from each other as illustrated in Fig. 2.3(a). This is done by integrating over the point sources. However, to perform this integration in the angular domain, we need the proper differential term. This can be seen as having a constant $\delta \theta$ in Fig. 2.3(b). This correction term can be easily derived from equation (2.7) to be simply a $\cos(\theta)$ term which is multiplied by the differential $d\theta$.

The previous argument can be applied to the case of a lens as well as can be seen in Fig. 2.3(c) (this figure is only for illustration since it is assumed that the light refracts directly at the plane of the lens which is not true in the case of this study due to the transformation to the far-field.
2. THEORY

\[ \delta \theta_1 \neq \delta \theta_2 \]
\[ \delta y_1 \neq \delta y_2 \]
\[ \delta y_1 \neq \delta y_2 \]

\( (a) \) \( (b) \) \( (c) \)

\[ \delta \theta_1 \neq \delta \theta_2 \]
\[ \delta y_1 \neq \delta y_2 \]
\[ \delta y_1 \neq \delta y_2 \]

Figure 2.3: Comparison of different distributions of Huygens’ point sources depending on the integration domain. Both (a) and (b) are describing the illumination of an aperture using spatial (a) and angular (b) domain integration, while (c) is for the angular integration for a lens. In all cases the illumination consists of a plane wave.

that was discussed in the previous section). However, there is one difference that needs to be taken into account when dealing with lenses. The wave-front of the light coming out of the lens is curved in such a way that we get the same phase for all the infinitely small sources at the focus of the lens. This is in contrast to the aperture case where we simply had the same wave-front on both sides of the aperture. In Fig. 2.4 this can be seen more clearly by looking at the refraction of light on the surface of a Gaussian reference sphere [33, 34] (Fig. 2.4(a)). We can use such a sphere due to the application of the sine rule since we deal with an aplanatic lens in the far-field. Since energy needs to be conserved, the energy flux infront of and behind the
Figure 2.4: Description of the two main conditions for aplanatic lenses. (a) The sine rule, where the ray emerging from an aplanatic lens meets the focal sphere at the same height as the corresponding ray entered the lens. (b) The intensity law where the energy flux along a ray must stay constant. $f$ is the focus length of the aplanatic lens and $h$ is the distance between the ray under consideration and the optical axis.

A planar wave needs to be constant (Fig. 2.4(b)). This means:

\[ \delta P_i = \delta P_o, \]
\[ I_i \delta A_i = I_o \delta A_o, \]
\[ I_o = I_i \frac{\delta A_i}{\delta A_o}, \]
\[ I_o = I_i \cos(\theta), \]

(2.11)

where $i$ and $o$ stand for the input and the output sides of the reference sphere respectively, $A$ denotes the differential area on the sphere and $P$ is the power of the light illuminating the area $A$. This leads to

\[ a_o = a_i \sqrt{\cos(\theta)} \]

(2.12)

where $a$ is the amplitude of the wave. This is the so-called intensity law of geometrical optics [33, 34]. This means that the beam distribution after the lens in the focal plane will not be identical to the desired distribution ($\hat{E}_{inc}(\theta)$). To solve this problem, the $\hat{E}_{inc}(\theta)$ term can be divided by $\sqrt{\cos \theta}$. Usually such a distortion can be neglected for beams with small divergence angles. This correction would in turn affect the spatial distribution of the illumination light on the surface of the lens.
2. THEORY

2.1.2 Focused and Gaussian beams

To model a specific beam, the angular distribution of the fields in the far-field needs to be defined. We start with the electric field distribution of a Gaussian profile in the spatial domain [35]:

\[ E_z(x = 0, y) = E_0 e^{-\beta^2 y^2}, \quad (2.13) \]

where \( \beta^2 \) corresponds to the inverse of the square of the beam waist, and \( E_0 \) is the amplitude of the Gaussian beam (which will be dropped from any further equations since it is only a scaling factor). Knowing the distribution of the fields in space, we reach the angular distribution by performing a Fourier transform. In the angular domain, we get

\[ \hat{E}_{z,\text{inc}}(\theta) = \frac{E_0}{2\sqrt{\pi} \beta} e^{-\left(\frac{k \sin \theta}{2\beta}\right)^2}. \quad (2.14) \]

The previous equation is capable of modeling the focal plane of a Gaussian beam. However, once the beam waist of the beam approaches the wavelength \( (1/\beta \approx \lambda) \), the whole expression tends towards 1. Said limit is a good description for a plane wave passing through an aperture (top-hat profile in the angular spectrum), where the aperture is described by the maximum divergence angle allowed \( (\theta_{\text{max}}) \).

2.1.3 Quasi-Bessel beam

In 3-D a Bessel beam can be generated by illuminating an annular aperture [36]. Due to the loss of cylindrical symmetry (since the simulations are performed in 2-D) a quasi-Bessel beam [37] can be formed by the light incident from two angular ranges. To model this mathematically, we use the formula

\[ \hat{E}_{z,\text{inc}}(\theta) = E_0 \left( \text{rect} \left( \frac{2(\theta - \theta_{\text{max}}) + \Delta \theta}{2\Delta \theta} \right) + \text{rect} \left( \frac{2(\theta + \theta_{\text{max}}) - \Delta \theta}{2\Delta \theta} \right) \right), \quad (2.15) \]

where \( \theta_{\text{max}} \) is the maximum divergence angle and \( \Delta \theta \) is the angular width of the beam.

2.1.4 Radially polarized beam (ring beam)

Beams with radial polarization (or cylindrical vector beams) have recently been of particular interest in several fields including microscopy, metrology [38], optical trapping and manipulation [39], and lithography [40]. This is due to the high numerical aperture (NA) of these beams.
which leads to its focusing property and the small size of the focus spot of the longitudinal component compared to the transverse component \cite{41,42}. These characteristics make such beams highly important for current research, as can be seen from the many previous investigations, both theoretically and experimentally \cite{39,40,41,42,43,44,45,46}.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure2_5.png}
\caption{A schematic of the orientation of plane waves in order to form beams of different polarization. \(\hat{E}\) is the direction of polarization and \(\hat{k}\) is the direction of propagation.}
\end{figure}

To implement a radially polarized beam, we need to fully understand the case of the linearly polarized beam. In the latter case, each plane wave that constitutes part of the beam is rotated around its propagation axis to keep the polarization of each plane wave directed along the same direction (see Fig. 2.5a). For the radially polarized beam, each plane wave is polarized radially \cite{42} in such a way that the direction of the electric field of each plane waves points towards the direction of propagation (see Fig. 2.5b). This will result in a hole at the center of the beam, since all the plane waves that are being added have opposite phase and add up to zero. A simulation using a 3-D FDTD with no scatterers is shown in Fig. 2.6 as an example of how the two beams (Gaussian beam in Fig. \ref{2.6a} and ring beam in Fig. \ref{2.6b}) differ in their structure.

For the 2-D case being studied here, we get a radially polarized beam by modifying equa-
2. THEORY

(a) A 3-D linearly polarized Gaussian beam. (b) A 3-D radially polarized ring beam.

Figure 2.6: A comparison between the linearly and radially polarized beams. The figures were generated using 3-D FDTD by propagating 100 plane waves in the scheme of ASPW. The beam waist and the wavelength were equal to 1 µm.

Equation (2.14) with a sign function:

\[ \hat{E}_{\text{inc},\text{rad}} = \hat{E}_{\text{inc}} \text{sgn}(\theta). \] (2.16)

2.2 Beam scanning

Scanning a beam through a scattering medium is one of the main points of interest when studying techniques like laser scanning microscopy, as we have seen in Fig. 1.1. Simulating a focused beam is achieved by using equation (2.10). Carrying out a simulation for every focus point is very time consuming. Instead, we can use another advantage of the ASPW description of the beams. By performing the steady state simulation of each individual plane wave \( E_m \) separately, we can scan the beam through the medium by multiplying the data from a single simulation set by the appropriate phase shift as explained in detail in our previous work [22]. As such, the complete solution of the scanned beam is calculated according to,
2.3 Applying ASPW in the multiple cylinders scattering analytical solution

\[ E_{\text{shift}}(x, y) = \sum_{m=1}^{M} \bar{E}_m(\theta) \exp(jk(x\cos\theta_m + y\sin\theta_m)) \cdot \exp(jk(x_{\text{sh}}\cos\theta_m + y_{\text{sh}}\sin\theta_m)) \sqrt{\cos\theta_m}, \]  

(2.17)

where \( E_{\text{shift}} \) is the steady state electric field for a longitudinal shift \( x_{\text{sh}} \) and a lateral shift \( y_{\text{sh}} \) of the focus position.

The discretization of the number of plane waves in the ASPW approach places a lower limit for the number of plane waves that has to be taken into account to achieve proper wave front shaping. This sampling problem has been addressed before in general terms [19]. An expression for the minimum number of plane waves (\( M_{\text{min}} \)) needed to get a focus with no numerical artifacts due to sampling for a maximum incident angle \( \theta_{\text{max}} \) was derived in this study:

\[ M_{\text{min}} = \frac{2y_m \sin(\theta_{\text{max}})}{\lambda} + 1, \]  

(2.18)

where \( y_m \) is the maximum distance between the focal point and the simulation grid boundary in y-direction. The first term in the equation is due to sampling theory, while the second term takes into account the odd number of plane waves (the wave incident at angle zero). If the number of plane waves used is less than this number, then a distorted repeated image of the beam will appear beside the beam [47]. The usage of equation (2.18) does not totally negate the problem, rather it pushes the secondary aliases (that would appear due to the low sampling rate) out of the simulation grid in order to suppress the distortion of the fields.

2.3 Applying ASPW in the multiple cylinders scattering analytical solution

In some situations, certain numerical methods are not the best tools to be used to investigate light propagation. One example is the propagation of light through carbon fibers. This is an important investigation since lasers are often used to treat carbon fibers during manufacturing processes [48]. The problem in this case is that due to the high concentration (up to 60 percent volume concentration) it is not possible to use solutions based on transport theory. This is shown in Fig. 2.7 where the transport theory (simulated by MC\(^1\)) and the Maxwell solution [49]

\(^1\)The Monte Carlo code is written and maintained by Dr. Ansgar Hohmann
2. THEORY

![Graphs showing differential scattering cross section](image)

(a) TM case (polarization parallel to the carbon fibers).

(b) TE case (polarization perpendicular to the carbon fibers).

**Figure 2.7:** Simulation (Monte Carlo and Maxwell method) of the differential scattering cross section of a 40 µm by 40 µm carbon fiber sample irradiated by a Gaussian beam with a beam waist of 15 µm.

are compared. It can be seen that the two solutions deviate from each other despite the fact that the MC solution uses the phase function that takes into account the Gaussian profile of the beam. A possible explanation for this deviation is the fact that the analytical solution uses several different distributions of cylinders. The MC on the other hand uses a homogenous medium. This means that the MC loses some of the characteristics of the cylinders that appear especially for the high absorption case. One such phenomenon is the increase of transmission at high absorption due to the transmission channels found in scattering media [50]. This can only be observed for inhomogeneous media. On the other hand, due to the high absorption of the fibers, the FDTD fails to simulate unless a very high resolution is used. This is mainly due to the much shorter plasmon wavelength which requires higher temporal resolution to be able to resolve this higher frequency component of the scattered wave [51]. This will be discussed more in section 4.5.

The analytical solution of light scattering by multiple cylinders has already been developed [52, 53, 54] and implemented [55]. This solution avoids all the problems that we have mentioned. However, the solution is limited to an incident plane wave, which is not a suitable model for the laser beams used in industry. In this work, the Gaussian beam is implemented
2.3 Applying ASPW in the multiple cylinders scattering analytical solution

in the analytical solution for the scattering from multiple cylinders using the ASPW method. The core code for the analytical solution has already been implemented in [55]. After that, equation (2.10) is used to initialize the code for plane waves with different incident angles. The solutions of the scattering of all plane waves are summed up coherently to get the desired solution.

An important aspect here is the normalization of the beam. There are two conventions that can be used depending on the problem being studied. The first is to normalize the maximum of the incident beam to 1. This is used when the phenomena under consideration needs to be compared with the case of an incident plane wave (since the main defining characteristic of a plane wave is its intensity, while the power in the plane wave is infinite by definition). This can be done by the following steps:

- Start the simulation for each plane wave that constitutes the beam while scaling the amplitude of each plane wave according to the ASPW method.
- Compute the Fourier transform of the amplitudes of the beam by *e.g.* using a fast Fourier transform (FFT).
- Calculate the normalization factor which is the maximum of the output of the FFT. Note that for focused or Gaussian beams, this value is in the middle of the beam. However, by stating that we always take the maximum value, the algorithm becomes more general. Thus, other types of beams can be simulated too, *e.g.* radially polarized beams which have their maxima away from the center of the beam.
- Divide the electric field of the beam by the calculated normalization factor.

This first method (the normalization to a maximum intensity of 1) is used later on in section 4.5. The second normalization method, is to normalize to a power of 1. This is very useful when trying to study real life applications where the source power is usually limited to a certain value as done in section 4.2. This normalization process is done as follows:

- Start the simulation for each plane wave that constitutes the beam, while scaling the amplitude of each plane wave according to the ASPW method.

---

1. The multiple cylinder analytical code used in this section was programmed by Dr. Jan Schäfer for the purpose of single incident plane wave [55] and further developed and maintained for beams and scanning beams by the author.
2. THEORY

- Calculate the normalization factor by summing up over the absolute square of the amplitudes used for the plane waves.
- Divide the absolute square of the electric field by the normalization factor.

2.4 Mode-locking using analytical solution

As was mentioned already in section 2.3 using the analytical solution of light scattering from multiple cylinders offers a lot of advantages especially, when combined with the ASPW method. However, so far the solutions were obtained in the steady state. In this section we show how to combine this solution with the mode-locking technique to get the analytical solution in time domain. The mode-locking method is essentially based on an inverse Fourier transform. It combines several steady state solutions for different frequencies, and gives the result in time domain. This is similar to a simple laser where each of the laser modes oscillates independently, with no fixed relationship between those modes. This can be visualized as a set of independent lasers all emitting light at slightly different frequencies [56]. The equation that governs the mode-locking is

$$E(r, t) = \sum_{\lambda=\lambda_{\text{min}}}^{\lambda_{\text{max}}} E(r, \lambda) \exp(j2\pi ct/\lambda). \quad (2.19)$$

The variable $t$ spans a vector from $t_{\text{init}} = D/(2cn_s)$ - where $D$ is the total depth of the sample under the assumption that the phase origin is in the middle of the grid - to $T$ with a time step $\Delta t = (\Delta x)/(\sqrt{2}c)$. The $\Delta t$ condition originates from the stability of the FDTD method and is used here for consistency, but it is in no way a limiting condition. A more insistent condition comes from sampling theorem which requires the use of a number of wavelengths above a certain limit [57] to avoid numerical artifacts. Fig. 2.8 shows two time shots for a plane wave incident on a dielectric cylinder to show the behavior of this technique. The simulation has been calculated with 300 wavelengths ranging from 0.85 $\mu$m to 1.15 $\mu$m.

2.5 Phase optimization

One of the main challenges in the field of 3-D microscopy is random scattering. The opaqueness of a material is a result of the loss of spatial coherence in the incident wave-front. Looking at the intensity of the incident light after going through a scattering medium, one gets the impression
of complete random noise since only a speckle field that has no correlation is seen. It has been shown in several studies (most of which are experimental) that it is possible to unscramble these scattered fields to regain a well-structured and coherent focus with high intensity by manipulating the incident wave-fronts \cite{23, 24, 25}. Such wave-front optimization can be done by several active devices. Two of the most widely used are spatial light modulators (SLMs) which can give an enhancement of intensity at the focal spot of $\sim \pi N/4$ \cite{58, 59} for broadband sources \cite{60}, and digital micro mirror devices (DMDs) \cite{61} which offer higher modulation speed at the expense of less enhancement at the focal spot of $\sim N(2\pi)^{-1}$ \cite{59, 62, 63}. There are different ways to control the refractive index, e.g. temperature tuning, free carrier excitation, optical Kerr switching \cite{64, 65, 66, 67, 68}, or the alignment modulation of the molecules of a metallic monolayer \cite{69}. In this work, the SLM is the device that will be modeled. Also, efforts are being made to enhance the performance of SLM devices for terahertz applications \cite{70}. A recent work has been published which summarises the tailoring of light with such devices \cite{71}.

There are a lot of groups doing research now that can greatly benefit from this work, such as: (1) in OCT microscopy \cite{24}, where multi-scattered light that is being treated as noise can be used constructively to enhance the OCT signal, (2) improving the communication channels \cite{25}, (3) high resolution imaging at high depths in biomedical applications \cite{72, 73, 74, 75}, and in many other fields of science and industry. Also, an effort is currently made to deal with the main problems of these techniques, namely the need for a feedback from a detector/camera and

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2_8}
\caption{Two time shots for a plane wave of wavelength of 1 $\mu$m incident on a cylinder of diameter of 1 $\mu$m and $n_s = 1.33$.}
\end{figure}
2. THEORY

(a) Without phase optimization.

Figure 2.9: Schematic of how the phase optimization works (both off-mode in Fig. (a) and on-mode in Fig. (b)). The SLM is assumed to work in reflection mode for better visibility only. Also, the SLM is taken here as an example. In principle any wave front modulation device can be used in this setup.

the limitation to slowly varying samples [76]. Very promising results are shown in a recent study where optical diffraction-limited focusing in scattering media is achieved [77] by using nonlinear photoacoustically-guided wave-front shaping. This study attempts to solve one of the most fundamental obstacles by using a photoacoustic system as the feedback signal while optimizing the focus. Said problem is the limitation of the optimization by the diffraction of the acoustic wave. For a more recent summary of the advances in wave-front shaping techniques, reference is made to the recent work by Yu et al. [59].

In previous works, the effects of the experimental parameters on the enhancement of the intensity have been reported [78, 79]. The purpose of modeling the phase optimization technique here is to build the basis of a simulator that uses an exact solution of Maxwell’s equations that can model such focus enhancement methods. This will enable us to study situations where it is not possible to reach conclusive answers to our questions by the current experimental setups. A recent work uses a different approach. Said approach is to calculate the transmission matrix of the scattering material by modulating the incident wave-front [80]. While that method is elegant in its execution it can only be applied to non-dynamic materials. Nonetheless, it is so adaptable - after reaching the transmission matrix [81] - that it is possible to form multiple optimal foci simultaneously.

In a normal setup where a scattering sample is illuminated by a light source, we find a
2.5 Phase optimization

Figure 2.9: Schematic of how the phase optimization works (both off-mode in Fig. (a) and on-mode in Fig. (b)). The SLM is assumed to work in reflection mode for better visibility only. Also the SLM is taken here as an example. In principle any wave front modulation device can be used in this setup.

random speckle pattern on a screen behind the sample (see Fig. 2.9a). By taking the intensity of the light at a certain point as a feedback signal, we can shape the wave-front using a SLM to optimize the phase difference between the individual components of the wave front. This in effect enhances the intensity at the point of interest (see Fig. 2.9b). The scattering process itself is linear. This allows us to devise an algorithm that constructs the transmitted field in the point of interest as a linear combination of the fields coming from the individual segments of the SLM [23] so that one can optimize the phase of each of those segments. It is also worth noting that such segments can be seen as plane waves in the angular description of the incident fields [22, 82, 83]. This is important to facilitate the usage of the ASPW method to model the enhancement process numerically in the FDTD solver.

The maximum intensity enhancement $\eta$ that can be reached is defined as the ratio between the optimized intensity $I_N$ and the ensemble averaged transmitted intensity before optimization $\langle I_0 \rangle$. The factor $\eta$ depends on the number of plane waves that can be used. This can be translated as was mentioned before to the number of segments in the SLM. Assuming high enough randomness in the fields (which can be achieved by high scattering and a statistically independent distribution of scatterers), the intensity enhancement is found to be [23]

$$\eta = \frac{\pi}{4}(N - 1) + 1,$$  \hspace{1cm} (2.20)
where $N$ is the number of segments. A simulation is made in 2-D to verify this equation using the FDTD method (see Fig. 2.10 and 2.11). To calculate $\eta$, it is necessary to optimize the electric field at the point of interest and to get the ensemble average of the incident intensity. There are two ways to get such an average. One is to simulate the grid multiple times to average over several different realizations. This method is obviously too time-consuming. The second method which proves to be much more efficient is to simulate the grid only once and to randomize the phase of the electric field at the point of interest. Averaging over the intensity after this randomization of the phase of the different plane waves gives the same effect as using several realizations of the scatterers.

![Figure 2.10: The effect of the realization number on the accuracy of the intensity enhancement at the focus. $n_s$ is equal to 1.4 while the depth where the optimization occurred was 35 $\mu$m.](image)

Several observations can be made at this point. Firstly, despite the fact that in equation (2.20) a 3-D setup was assumed, the formulation still holds for the 2-D setup that is used in this work for the simulations. Secondly, the enhancement is independent of the depth of the probe that is used (as long as the probe is placed deep enough to scatter the incident light). This makes sense because of the definition of the $\eta$ which is the ratio between the optimized intensity and the intensity of the scattered light before optimization. As such, the latter already has the information about the depth. This observation is difficult to make in an experimental setup since one would need a probe inside the sample which is not practical. A third point is the presence of a deviation in Figs. 2.10 and 2.11 between the analytical formula (2.20) and the simulated data for low scattering. Once the scattering is high enough, all the assumptions made during the derivation of equation (2.20) in reference [23] hold. The main assumption in
2.6 The direct extinction method

Optical systems with high numerical aperture (NA ≥ 0.7 [17, 88]) have become important tools in the field of biophotonics, with applications ranging from optical tweezers to microscopy and spectroscopy [2, 89, 90, 91, 92]. As such, the construction of reliable simulation tools is becoming essential not only for the design of the optics, but also for a better understanding

---

Footnote:

1 The results from this section have been published [87] except subsection 2.6.4.
2. THEORY

of light-matter interactions (e.g. absorption and scattering) within the focal volume. The tight focusing of beams induces diffraction patterns in the focal volume whereby the polarization of the illumination beam plays an important role \[93, 94\]. Consequently, if the tight focusing of beams is to be modeled, the consideration of the wave nature of the light becomes paramount. This can be successfully achieved by solving Maxwell’s equations numerically, e.g. by carrying out FDTD simulations \[51\] for small volumes.

The direct extinction method constitutes an extension to the well-established scalar (i.e. non-polarized) Monte Carlo (MC) algorithm \[95\]. It enables handling the diffraction within turbid media introduced by a coherent light source. Moreover, the high sampling number required for destructive interference of a coherent source in a vectorial (i.e. polarized) MC \[96\] is rendered obsolete by this approach. In this work, we investigate the feasibility of including diffraction of the incident light into MC simulations, in order to be able to model tightly focused beams and Fraunhofer diffraction patterns in arbitrarily large simulation volumes in a relatively simple manner.

2.6.1 The direct extinction method within the Monte Carlo algorithm

When dealing with light propagation problems, the MC method constitutes a well-established numerical alternative to the analytical solutions of the radiative transfer equation \[95, 97, 98, 99\]. The main idea is to stochastically model the light propagation with individual photon paths similar to random walks. A single photon path is composed of successive ray segments, each of which is defined by (i) a starting point, (ii) a propagation direction, (iii) and a segment length. Since abundant documentation can be found on the matter \[95, 96, 100\], we do not repeat the successive steps needed to generate such paths; instead, we emphasize the novelty of our approach. Traditionally, the initial starting point of the very first ray segment is chosen at the position of the illuminating source, or on the surface of the sample, from where the illumination is performed. Here, we propose an alternative method where the initial starting point of the rays coincides to a “target position”. This position is sampled from a probability distribution independently calculated with the ASPW method and which corresponds to the probability that the ray has not yet interacted (by scattering or absorption) with the sample yet. We confine the first subsection to absorbing materials and the second subsection to scattering ones as a preliminary investigation.

In this section, we detail the calculation of the probability distribution for the incident beam and the inclusion of the absorption into the ASPW method. Further, we explain how our method
2.6 The direct extinction method

can be used to calculate the local Poynting vectors, as these can help modeling scattering processes at a later stage (future work which is not presented in this thesis). In all of these simulations, only the two-dimensional case is studied to simplify the computation and to be able to decouple the polarization of the light into two orthogonal components: parallel and perpendicular. Nevertheless, the consideration of the two-dimensional case is beyond a mere simplification of the three-dimensional one. “In fact, both the analysis and the final results are sufficiently different in the two cases to call for separate treatments” [101]. Furthermore, the 3-D case is shown using only an analytical formalism which is more efficient and gives comparable results to Maxwell’s solution under certain conditions.

2.6.2 Modeling the absorption

Consider the beam propagating in an absorbing material with a refractive index \( n = n + j \kappa \), such that its absorption coefficient is defined by \( \mu_a = 2k\kappa \).

If we denote the fields of a single plane wave in vacuo by \( \hat{E}_z(\theta) \), the corresponding expression of the fields in the absorbing material is \( \hat{E}_e^e(\theta, \mu_a) \), where the superscript “e” refers to the extinction. The influence of the medium can be calculated by means of attenuating the plane waves [102] composing the beam, based on Beer-Lambert law’s exponential decay (the Fresnel reflection which occurs between the non-absorbing and the absorbing medium). The modified ASPW representation (from equation 2.9) is defined as

\[
E_e^e(x, y, \mu_a) = \int_{\theta_{\text{max}}}^{\theta_{\text{max}}} \hat{E}_e^e(\theta, \mu_a) a(x, y, x_0, y_0, \theta) \, d\theta, \tag{2.21}
\]

where the integrand introduces the Beer-Lambert law as

\[
\hat{E}_e^e(\theta, \mu_a) = \hat{E}_{z, \text{inc}} \exp \left( -\frac{1}{2} \mu_a \frac{x}{\cos(\theta)} \right), \tag{2.22}
\]

and \( a(x, y, \theta) \) is the propagator of the ASPW similar to what is found in the exponential in equation (2.9). The variables \( x_0 \) and \( y_0 \) are necessary here since for a focused beam the origin as defined in equation (2.9) is at the center of the beam while in this case the origin is at the surface of the medium. \( \hat{E}_{z, \text{inc}} \) controls the angular distribution of the incident beam as has been shown in equations (2.14) and (2.15). The link from the electric field to the geometrical approach of MC is performed by taking the power \( P_a(r) \propto E^e(r, \mu_a) \cdot E^{e*}(r, \mu_a) \) to calculate a probability
density function \( p_a(r) \) to find a photon at a position \( r \) (the symbol \( r \) here represents only two components \( x \) and \( y \).) before it gets absorbed in the sample:

\[
p_a(r) = \frac{P_a(r)}{\int_r P_a(r) \, dr}.
\]

(2.23)

This constitutes the essence of the “direct extinction method”, which can later be extended to include scattering processes. The main advantage of this approach is that the diffraction phenomena can be recovered from the sampled probability distribution, without having to implement the coherent interference between photon paths.

For simplicity, in the following part of the work, we shall use the term “beam” to refer to the beam which fulfills the assumptions described in this section and whose electric field is given by \( E(r) \) in vacuo and by \( E^e(r, \mu_a) \) in an absorbing medium.

2.6.3 Ray direction: The Poynting vector

As already mentioned in subsection 2.6.2, the MC simulations do not need to propagate the photon paths, and the sampling from the aforesaid probability distribution suffices. However, if scattering processes are to be modeled, another key information besides the first interaction point needs to be known: the propagation direction of the first path segment.

To this end, we may utilize the energy flow or the energy flux density given by the local time-averaged Poynting vector \( \mathbf{S}(r) \)

\[
\mathbf{S}(r) \propto \text{real} \left\{ \mathbf{E}^e(r) \times \mathbf{H}^e(r) \right\},
\]

(2.24)

where the magnetic field \( \mathbf{H}^e \) at a point \( r \) is calculated similarly to the electric field with the modified ASPW method to give

\[
\mathbf{H}^e(r, \mu_a) = \int_{-\theta_{\text{max}}}^{\theta_{\text{max}}} \hat{\mathbf{H}}^e(\theta, \mu_a) \, b(r, \theta) \, d\theta,
\]

(2.25)

where \( b \) denotes the propagator of the single plane waves and \( \hat{\mathbf{H}}^e \) is the extinction of the magnetic field of a single plane wave similar to equation 2.22. For the linearly polarized beam, we obtain

\[
b(r, \theta) = \hat{H} \begin{pmatrix} \sin \theta \\ \cos \theta \\ 0 \end{pmatrix} \, a(r, \theta).
\]

(2.26)
2.6 The direct extinction method

\( \hat{H} \) denotes the amplitude of the incident magnetic field. Note that for \( \mu_a = 0 \), the magnetic and electric fields \( \mathbf{E}^e \) and \( \mathbf{H}^e \) are reduced to the fields \( \mathbf{E} \) and \( \mathbf{H} \) in vacuo, respectively. Note that the magnetic field contrary to the electric field has two components in the chosen polarization.

2.6.4 Modeling the scattering

In the previous section, the modeling of absorption of a beam was introduced by using \( \mu_a \) in the Lambert-Beer law and by combining those items in the ASPW. By assuming relatively small scattering and low concentration of scatterers (to avoid dependent scattering), it is also possible to model the scattering using \( \mu_s \). In this section, the direct extinction method is generalized using the factor \( \mu_t \) which can either be used for absorption, as shown in section 4.6, or - under certain conditions - for scattering, as shown in section 4.2. This is different from the method that was proposed in the previous sections to use the Poynting vector to model scattering (which is still in work in progress).

The formalism here is done for the 3-D case since the 2-D case is identical for equation (2.22) while taking \( \mu_t \) instead of \( \mu_a \). Since we are dealing with the 3-D case, it is not possible to decouple the polarization. Therefore, it is necessary to have a model for all three components of the electric field to be able to fully control the polarization of the beam

\[
\mathbf{E}^e(\mathbf{r}, \mu_t) = \int_{0}^{\theta_{\text{max}}} \int_{-\pi}^{\pi} \hat{E}^e(\theta, \mu_t) \, a(\mathbf{r}, \mathbf{r}_0, \theta, \phi) \left( \begin{array}{c} \cos \psi \sin \phi - \sin \psi \cos \theta \cos \phi \\ - \cos \psi \cos \phi - \sin \psi \cos \theta \sin \phi \\ \sin \psi \sin \theta \end{array} \right) \sqrt{\cos \theta \sin \theta d\psi d\phi d\theta}. \tag{2.27} \]

As can be seen in equation (2.27) there is a high degree of similarity with equation (2.22) which was used for the 2-D absorption case. \( \hat{E}^e \) is the angular distribution of the incident beam combined with the Lambert-Beer exponential term to model the absorption and/or scattering. \( a(\mathbf{r}, \mathbf{r}_0, \theta, \phi) \) is the propagator of the beam similar to the imaginary exponential term in equation (2.8). The \( \sqrt{\cos \theta} \)-term is to ensure the conservation of energy as discussed before in subsection 2.1.1. And lastly, the array of trigonometric identities is to control the polarization of the different components of the electric field. It is based on the model used by Taflove [51] to project 1-D plane waves onto a 3-D grid in the FDTD method. The angle \( \psi \) is used to specify the orientation of the incident electric field (its polarization). This angle is between the reference direction \( \hat{k} \times \hat{z} \) and the plane containing the propagation direction \( \hat{k} \) and the polar direction \( \hat{z} \).
2. THEORY
Chapter 3

Numerical methods

3.1 Introduction to FDTD

After introducing the ASPW method in section 2.1 and applying it in the analytical solution of scattering by multiple cylinders in 2.3, we can see that there is a limitation of the solution regarding the modeling of the scatterers. This is due to the fact that most analytical solutions exploit the symmetry in the scattering problem. If there is no symmetry, it becomes quite difficult to solve the problem analytically. One way to overcome this problem is by using a numerical solution for the electromagnetic problem. For this, we use the finite-difference time-domain (FDTD) method, in combination with the ASPW to model the incident light as beams.

The FDTD method is a direct solution method for Maxwell’s curl equations. It is based on the volumetric sampling of the unknown electric and magnetic fields within and surrounding the structure of interest. The sampling in space is at sub-wavelength resolution. This resolution should be fine enough to both sample the near-field and to model the scattering structure. The sampling in time is selected to ensure the stability of the simulation. The FDTD method has been introduced by Yee’s pioneer work in 1966 [103].

The technique of FDTD works by marching the time forward while updating the fields (both electric and magnetic) from the previous time step. The modeling of the scatters is done by staircasing. In this method the surface of the structure is approximated to fit the grid of the FDTD.
3. NUMERICAL METHODS

In this chapter, we start from Maxwell’s equations until we reach the update equations which are used as the kernel of the FDTD. Several internal methods will be discussed, also concerning the boundaries of the grid, and we can extend the results to the far-field without the need to increase the simulation grid itself. Also the total-field/scattered-field method, which helps in the implementation of the ASPW method in the FDTD scheme will be discussed.

3.2 Discretization of Maxwell’s equations

The starting point is to write down Maxwell’s curl equations:

\[ \nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}, \]  
\[ (3.1) \]

\[ \nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t}. \]  
\[ (3.2) \]

These equations are discretized in both space and time. In this work the 2-D case will be the main objective. As such, the main concentration is set on the TM\textsubscript{z} case, however the TE\textsubscript{z} case will be identical (mainly from the numerical modeling perspective, since each of these modes can be associated with completely different phenomena). Therefore it follows that any differentiation in terms of \( z \) will be set to zero (\( \partial / \partial z = 0 \)).

The vector components of the TM\textsubscript{z} equations can then be written as:

\[ \varepsilon \frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}, \]
\[ \mu \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x}, \]
\[ \mu \frac{\partial H_x}{\partial t} = -\frac{\partial E_z}{\partial y}. \]  
\[ (3.3) \]

The system of the three coupled partial differential equations of (3.3) forms the building blocks of the FDTD algorithm. By using finite differences on the previous equations:

\[ \varepsilon \frac{E_z^{n+1}_{i,j} - E_z^n_{i,j}}{\Delta t} = \frac{H_y^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - H_y^{n+\frac{1}{2}}_{i-\frac{1}{2},j}}{\Delta x} - \frac{H_y^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - H_y^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}}{\Delta y}, \]
\[ \mu \frac{H_y^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - H_y^n_{i+\frac{1}{2},j}}{\Delta t} = \frac{E_z^n_{i+1,j} - E_z^n_{i,j}}{\Delta x}, \]
\[ \mu \frac{H_x^n_{i,j+\frac{1}{2}} - H_x^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}}{\Delta t} = -\frac{E_z^n_{i,j+1} - E_z^n_{i,j}}{\Delta y}, \]  
\[ (3.4) \]
where \( n \) is the index for time, \( i \) and \( j \) are the indices for the discrete spatial position in \( x \) and \( y \), respectively. The FDTD equations are updated numerically. First, both the \( H_y \) and the \( H_x \) can be updated using the equations \([3.4]\). After having the magnetic field components, the electric field component is updated using the magnetic field from the surrounding magnetic field components. This procedure is called leap-frog iteration. In these equations the conductivity was assumed to be zero.

### 3.3 Total-field/scattered-field technique

An important aspect to discuss about the FDTD method is how to introduce an incident field into the grid. There are several ways to do that, the simplest way is to introduce a hard source. This means initializing one edge or one point in the grid by e.g. a sine wave. Such a time function is independent of any interactions with the model at the point of emission.

This method, while it is easy to implement, will make the implementation suffer from some disadvantages. The first one is the fact that the code causes non-physical phenomena at the source-point due to the reflected waves from the scatterers. This is an inherent problem in the method since the source is initialized without taking the reflected waves into account. The second problem is that it is desirable to separate the scattered fields from the total fields. One way to overcome these two obstacles is to use the total-field/scattered-field method (TF/SF). In this method, the FDTD grid is divided into two regions (see Fig. 3.1). The inner region is the total-field region. The scatterers are placed in this region, and the field resulting from the interaction between the scatterer and the incident field is calculated. In the second region which surrounds the first one, only the scattered fields exists. The latter region is called the scattered-field region.

The next point is the introduction of the incident field without interfering with the outer region. This can be examined by looking at the 1-D case. For a normal Yee algorithm, the following equation is used to calculate the E-field \([103]\):

\[
E_z |_{i,i+1}^{n+1} = E_z |_{i,i+1}^{n} + \frac{\Delta t}{\varepsilon_0 \Delta x} (H_y |_{i+\frac{1}{2},i+\frac{1}{2}}^{n+1} - H_y |_{i-\frac{1}{2},i-\frac{1}{2}}^{n+1}),
\]

where \( n \) is the temporal step and \( i \) is the spatial step. The TF/SF intersection is at \( i = i_0 \), where the total-field \((E_{\text{total}})\) is separated into incident \((E_{\text{inc}})\) and scattered \((E_{\text{scat}})\) fields.
3. NUMERICAL METHODS

according to:

\[ E_{\text{total}} = E_{\text{inc}} + E_{\text{scat}}. \]  

(3.6)

Combining the previous two equations and with some mathematical manipulation \[51\], the following result is reached:

\[ E_{z,\text{total}} |_{n+1}^{i_0} = E_{z,\text{total}} |_{n}^{i_0} + \frac{\Delta t}{\varepsilon_0 \Delta x} (H_{y,\text{total}} |_{n+\frac{1}{2}}^{i_0} - H_{y,\text{total}} |_{n-\frac{1}{2}}^{i_0}) - \frac{\Delta t \mu_0}{\varepsilon_0 \Delta x} E_{z,\text{inc}} |_{n+\frac{1}{2}}^{i_0}. \]  

(3.7)

Applying the same concept to the magnetic field \( H_y \) yields

\[ H_{y,\text{scat}} |_{n+\frac{1}{2}}^{i_0} = H_{y,\text{scat}} |_{n-\frac{1}{2}}^{i_0} + \frac{\Delta t \mu_0}{\mu_0 \Delta x} (E_{z,\text{total}} |_{n}^{i_0} - E_{z,\text{total}} |_{i-1}^{n}) - \frac{\Delta t \mu_0}{\mu_0 \Delta x} E_{z,\text{inc}} |_{i}^{n}. \]  

(3.8)

These equations have to be modified when the wave is exiting the total-field region. By generalizing equations (3.7) and (3.8) of the 1-D case for the 2-D situation (assuming a square grid), it can be seen that the incident magnetic field components from the scattered-field region are needed in order to get the electric field components in the total-field region, and the incident electric field component in the total-field region is also needed in order to get the magnetic fields in the scattered-field region. This can be formulated in a set of updating equations that are used to correct the fields at the boundary between the two regions in each time step. The equations are written here for the case of a TM\(_z\) wave:

Front wall:

\[ E_z |_{L: M-L, L}^{n+1} = E_z |_{L: M-L, L}^{n+1} + \frac{\Delta t}{\varepsilon_0 \Delta x} H_{x,\text{inc}} |_{L: M-L, L-1}^{n+1/2}, \]

\[ H_x |_{L: M-L, L-1}^{n+1/2} = H_x |_{L: M-L, L-1}^{n+1/2} + \frac{\Delta t \mu_0}{\mu_0 \Delta x} E_{z,\text{inc}} |_{L: M-L, L}^{n}. \]  

(3.9)

Back wall:

\[ E_z |_{L: M-L-M, L}^{n+1} = E_z |_{L: M-L-M, L}^{n+1} - \frac{\Delta t}{\varepsilon_0 \Delta y} H_{y,\text{inc}} |_{L-1, L: M-L}^{n+1/2}, \]

\[ H_x |_{L: M-L-M, L}^{n+1/2} = H_x |_{L: M-L-M, L}^{n+1/2} - \frac{\Delta t \mu_0}{\mu_0 \Delta y} E_{z,\text{inc}} |_{L: M-L, L}^{n}. \]

Left wall:

\[ E_z |_{L, L: M-L}^{n+1} = E_z |_{L, L: M-L}^{n+1} - \frac{\Delta t}{\varepsilon_0 \Delta y} H_{y,\text{inc}} |_{L-1, L: M-L}^{n+1/2}, \]

\[ H_y |_{L-1, L: M-L}^{n+1/2} = H_y |_{L-1, L: M-L}^{n+1/2} - \frac{\Delta t \mu_0}{\mu_0 \Delta y} E_{z,\text{inc}} |_{L, L: M-L}^{n}. \]
3.3 Total-field/scattered-field technique

**Figure 3.1**: The 2-D FDTD grid with the TF/SF regions. The bold black letters on the side (L,M-L,...) are the indices used in the implementation.

Right wall:

\[
E_z^{n+1}_{M-L,L:M-L} = E_z^{n+1}_{M-L,L:M-L} + \frac{\Delta t}{\varepsilon_0 \Delta y} H_y^{inc} \left[ H_z^{n+1/2}_{M-L,L:M-L} \right]
\]

\[
H_z^{n+1/2}_{M-L,L-1:M-L-1} = H_z^{n+1}_{M-L,L-1:M-L-1} + \frac{\Delta t}{\varepsilon_0 \Delta y} E_y^{inc} \left[ E_z^{n+1/2}_{M-L,L-1:M-L-1} \right]
\]

where M is the size of the grid and L is the position of the boundary of the TF/SF. The index system that was used here is different from the one used in [51]. The indexing here used whole numbers without fractions. This indexes the position of the cell under consideration and not the position of the individual field component. This does not decrease our accuracy however, since the positioning of the field components in relation to each other is still taken into consideration. This is shown in Fig. 3.1

From equations (3.9) it can be seen that the value of the incident field at the boundary between the two regions is needed to be able to make the algorithm work properly. As such it is necessary to calculate an incident field which is propagating in an arbitrary direction so that it can be used to update the boundary between the two regions.

This will be done by calculating a 1-D FDTD simulation for the incident field and then taking the projection of this field on the 2-D boundary in order to reach the values that are
3. NUMERICAL METHODS

Figure 3.2: Introduction of the incident field. (a) Generation of a 2-D incident field by the projection of a 1-D vector for $\phi$ less than 90°. (b) Generation of 2-D incident fields by the projection of a 1-D vector for $\phi$ more than 90°.

needed. In Fig. 3.1, the field components which are needed in 2-D for the calculation of the incident field are shown. Figure 3.2(a) emphasizes the projection of a 1-D wave vector on the 2-D grid. Special care should be taken at the four different corners since these are the first points that the incident wave reaches. This is shown in Fig. 3.2(b).

3.4 Modeling of beams in 2-D

The basic idea in this section is to use the angular spectrum method presented in section 2.1 to achieve the required incident field for a 2-D beam in the TF/SF. This is done by using equation 2.10. As such, an extra loop is initialized in the code. The extra loop is used for the different incident angles. At each angle a full 1-D FDTD simulation is performed, which consists of:

- The initialization of the 1-D wave,
- The projection of the 1-D wave on the 2-D grid to get the 2-D plane wave.

By the end of the incident angles loop, the following steps should be followed:

- Add up all the fields generated from all angles to get the complete incident field for the new time step,
- Use the initialized incident wave to update the total fields.
3.5 Numerical dispersion

Dispersion is the relation between the wave number and the frequency. The FDTD introduces additional dispersion numerically. This can be imagined as if the FDTD embeds an approximation of the material of interest in the simulation grid. This numerical difference produces some artifacts and can lead to complete instability in the simulation due to the accumulation of phase or delay errors for the waves and the artificial anisotropy of the material.

The general numerical dispersion relation of the Yee algorithm for the 2-D case is

\[
\left[ \frac{1}{c \Delta t} \sin \left( \frac{\omega \Delta t}{2} \right) \right]^2 = \left[ \frac{1}{\Delta x} \sin \left( \frac{\tilde{k}_x \Delta x}{2} \right) \right]^2 + \left[ \frac{1}{\Delta y} \sin \left( \frac{\tilde{k}_y \Delta y}{2} \right) \right]^2 ,
\]

(3.10)
where $\tilde{k}_x$ and $\tilde{k}_y$ are the $x$- and $y$- components of the numerical wave vector [51]. Considering the case under study of a square cell grid ($\Delta x = \Delta y$), and defining the Courant stability factor $S = c\Delta t/\Delta x$ and the grid sampling density $N_\lambda = \lambda_0/\Delta x$, equation (3.10) can be rewritten as:

$$\frac{1}{S^2} \sin^2 \left( \frac{\pi S \lambda}{N_\lambda} \right) = \sin^2 \left( \frac{\Delta x \tilde{k} \cos \theta}{2} \right) + \sin^2 \left( \frac{\Delta y \tilde{k} \sin \theta}{2} \right), \quad (3.11)$$

where $\theta$ is the propagation direction of the wave with respect to the $x$-axis. We can compare the numerical case in equation (3.10) to the ideal case that can be written as:

$$\left( \frac{\omega}{c} \right)^2 = k_x^2 + k_y^2. \quad (3.12)$$

It can be shown that the two cases are identical in the limit as $\Delta x$, $\Delta y$ and $\Delta t$ approach zero. This means that the numerical dispersion can be theoretically eliminated if we can keep using finer FDTD grid spacing.

From equation (3.11) we can conclude that the numerical dispersion is heavily dependent on the direction of the wave. To decrease this dependency, the work by Guiffaut and Mahdjoubi [104] has been implemented by using the equation of:

$$\Delta_{1D} = \Delta x^2 (\cos \theta)^4 + \Delta y^2 (\sin \theta)^4, \quad (3.13)$$

where $\Delta_{1D}$ is the resolution in the 1-D wave used in the TF/SF method. Using equation (3.13) allows us to artificially set the speed of the wave depending on the direction of propagation. Furthermore, this method is convenient since it uses the discretization of the 1-D wave used in TF/SF method. This means that we are able to decrease the mismatch between the 1-D and the 2-D numerical dispersion without the need to manipulate the resolution of the 2-D grid. This is important to keep the speed of the method as high as possible.

### 3.6 Absorbing boundary condition

After the scattered waves pass through the TF/SF boundary, there is a need to treat these waves at the grid boundary to prevent them from reflecting back. In an ideal case there would be an infinite grid where the waves can propagate to infinity. This would be an open space scattering problem. However, since computationally it is not possible to have an infinite grid, we make an absorbing layer around the grid to prevent the waves from reflecting back into the simulation region. This layer is adjacent to the main grid and is called the perfectly matched layer (PML) absorbing boundary condition (ABC).
There are several similar formulations of PML ABC. Berenger’s original formulation is called the split-field PML, because he artificially splits the wave solutions into a sum of two new artificial field components. Nowadays, a more common formulation is the uni-axial PML (UPML) which uses the standard Maxwell’s equations with a combination of artificial anisotropic absorbing materials [51].

The UPML was used since it is easier to be integrated into the scheme of Maxwell’s difference equations. The equations used for the TM\(_z\) case are shown here. The full derivation of the UPML and its enhancements is described elsewhere [105, 106].

Using the electric and magnetic fields will not be enough to describe the required artificial Maxwell’s equations. As such both the electric and magnetic flux densities (\(\mathbf{D}, \mathbf{B}\)) will be used. The updating scheme for the electric field density can be formulated as:

\[
D_{z}^{n+1}_{i,j} = \left( \frac{2\varepsilon_{0}\kappa_{x} - \sigma_{x} \Delta t}{2\varepsilon_{0}\kappa_{x} + \sigma_{x} \Delta t} \right) D_{z}^{n}_{i,j} + \left( \frac{2\varepsilon_{0}\Delta t}{2\varepsilon_{0}\kappa_{x} + \sigma_{x} \Delta t} \right) \cdot \left( \frac{H_{y}^{n+1/2}_{i+1/2,j} - H_{y}^{n+1/2}_{i-1/2,j}}{\Delta x} - \frac{H_{x}^{n+1/2}_{i,j+1/2} - H_{x}^{n+1/2}_{i,j-1/2}}{\Delta y} \right).
\]

(3.14)

After updating the electric flux density, the actual electric field can be found by:

\[
E_{z}^{n+1}_{i,j} = \left( \frac{2\varepsilon_{0}\kappa_{y} - \sigma_{y} \Delta t}{2\varepsilon_{0}\kappa_{y} + \sigma_{y} \Delta t} \right) E_{z}^{n}_{i,j} + \left( \frac{1}{2\varepsilon_{0}\kappa_{y} + \sigma_{y} \Delta t} \right) \cdot \left( \frac{2\varepsilon_{0}D_{z}^{n+1}_{i,j} - 2\varepsilon_{0}D_{z}^{n}_{i,j}}{\varepsilon} \right),
\]

(3.15)

where \(\sigma_{a}\) is the conductivity along the direction \(a\). It can be calculated according to:

\[
\sigma_{a}(x) = (x/d)^{m} \sigma_{a,max},
\]

(3.16)

where \(x\) is the distance to the inner PML interface and \(d\) is the thickness of the UPML layer. The constant \(m\) should be taken between 3 to 4 according to literature [51]. The maximum conductivity \(\sigma_{k,max}\) can be calculated as follows:

\[
\sigma_{k,max} = \frac{-(m+1)\varepsilon_{0}c \ln(R(0))}{2d},
\]

(3.17)

where \(R(0)\) is the desired maximum reflectivity when a wave with an incident angle of zero hits the UPML, this is usually in the range from \(e^{-5}\) to \(e^{-12}\). A similar two-step-procedure has to be performed to update the components of the magnetic field. First, the values of the magnetic...
3. NUMERICAL METHODS

Flux density are obtained as follows:

\[
B_x|_{i,j+1/2}^{n+3/2} = \left( \frac{2\varepsilon_0\kappa_y - \sigma_y\Delta t}{2\varepsilon_0\kappa_y + \sigma_y\Delta t} \right) \frac{B_x|_{i,j+1/2}^{n+1/2}}{} - \left( \frac{2\varepsilon_0\Delta t}{2\varepsilon_0\kappa_y + \sigma_y\Delta t} \right) \left( \frac{E_x|_{i,j+1/2}^{n+1} - E_x|_{i,j}^{n+1}}{\Delta y} \right),
\]

(3.18)

\[
B_y|_{i+1/2,j}^{n+3/2} = B_y|_{i+1/2,j}^{n+1/2} + \left( \frac{\Delta t}{\Delta x} \right) \left( \frac{E_z|_{i+1,j}^{n+1} - E_z|_{i,j}^{n+1}}{\Delta y} \right),
\]

(3.19)

The next step is to calculate the magnetic fields from the previously acquired magnetic flux:

\[
H_x|_{i,j+1/2}^{n+3/2} = H_x|_{i,j+1/2}^{n+1/2} + \frac{1}{2\varepsilon_0\mu} [(2\varepsilon_0\kappa_x + \sigma_x\Delta t)B_x|_{i,j+1/2}^{n+3/2} - (2\varepsilon_0\kappa_x - \sigma_x\Delta t)B_x|_{i,j+1/2}^{n+1/2}],
\]

(3.20)

\[
H_y|_{i+1/2,j}^{n+3/2} = \left( \frac{2\varepsilon_0\kappa_x - \sigma_x\Delta t}{2\varepsilon_0\kappa_x + \sigma_x\Delta t} \right) H_y|_{i+1/2,j}^{n+1/2} + \frac{1}{(2\varepsilon_0\kappa_x + \sigma_x\Delta t)\mu} \left( \frac{1}{\Delta t} \right) \left( \frac{E_z|_{i+1,j}^{n+1} - E_z|_{i,j}^{n+1}}{\Delta y} \right) - \left( \frac{1}{(2\varepsilon_0\kappa_y + \sigma_y\Delta t)\mu} \right) \left( \frac{1}{\Delta t} \right) \left( \frac{E_z|_{i,j+1}^{n+1} - E_z|_{i,j}^{n+1}}{\Delta y} \right),
\]

(3.21)

3.7 Near- to far-field transformation

The calculations of the fields in the FDTD method are performed in the near-field close to the scatterer. However, in many applications it is interesting to get the fields in the far-field. To achieve that, the FDTD grid can be theoretically extended so that the fields can be examined far away from the scatterer. This is practically not advisable due to the extra computation needed. The other option is to use the so called near- to far-field transformation (NFFF).

The basic theory of the NFFF comes from the fact that, if the tangential fields are known for a closed surface around the scatterer, then the far-field can be calculated by a surface integral. This applies not only for the FDTD but in general \[51\]. Since the grid in the FDTD is Cartesian in this work, the logical geometry to be used for the surface integration is a cube in the 3-D case or a rectangle in the 2-D case. The integration surface needs to be placed in the scattered-field region so that only the scattered fields would be examined. This can be seen in Fig. \[3.4\] where the \( E_z \) components are taken at the NFFF integration surface (since they are tangential to the integration surface).
3.8 Verification

The field components do not fit exactly on the integration boundary. In that case the fields have to be averaged according to their arithmetic mean \[107\]. This can be seen in Fig. 3.4 where the $H_x$ and the $H_y$ components are being averaged onto the point in the middle of these components. The average is marked as a cross between the closest points to it. On both the right and left sides, the $H_y$ components are averaged while on the top and bottom boundaries, the $H_x$ components are averaged.

For the verification of the implemented FDTD code and the ASPW method, both near- and far-fields of the light scattered by a single cylinder are investigated. First, we present the near-fields for the scattering of a plane wave by a cylinder in comparison to the corresponding analytical solution \[20\]. The wavelength of the incident plane wave is 1 $\mu$m and the refractive index of the cylinder is 1.33, surrounded by air ($n = 1$). The spatial resolution used in the FDTD simulation is equal to $\lambda/80$. In Fig. 3.5 it can be seen that the agreement between the numerical (Fig. 3.5(a)) and analytical (Fig. 3.5(b)) results is good. The relative difference between both methods (Fig. 3.5(c)) is below 1.8%. 160 plane waves were used to model the beam.

\[1\]The results and the conclusions in this section were already published \[22, 82, 87\].
3. NUMERICAL METHODS

Figure 3.5: Comparison of the normalized intensity of the $E_z$-component of the electric field for scattering by a cylinder of diameter 1 µm for an incident plane wave: (a) FDTD simulation, (b) analytical solution, (c) the relative difference between the first two figures. Figures (a) and (b) are normalized to the maximum of the intensity for each case, and the cylinder is located at $x/\lambda = y/\lambda = 0$.

Figure 3.6: The differential scattering cross section of a cylinder with a diameter of 1 µm for an incident plane wave and a focused beam. The focused beam has a maximum divergence angle of 45 degrees while both the focused beam and the plane wave have the wavelength of 1 µm. The refractive index of the cylinder is 1.33 surrounded by air ($n = 1$) in both cases. The spatial resolution in the FDTD simulation is equal to $\lambda/80$. 

40
3.8 Verification

Figure 3.7: Comparison between the grid sizes of FDTD and MC.

Next, the far-field results are verified for several cases. A FDTD simulation was performed for a normally incident plane wave scattered by a cylinder and was compared to the analytical solution [20]. Fig. 3.6 shows the differential scattering cross section for both cases indicating a good agreement. The maximum and the average relative differences are 7.5% and 1.2%, respectively. Fig. 3.6 shows, in addition, the comparison between the FDTD simulation for an incident focused beam and the analytical solution. The analytical solution is derived by applying a similar approach as the Fourier Lorenz-Mie Theory [21], where the ASPW method is utilized in the Mie theory to derive an analytical solution of the scattering of a Gaussian beam by a sphere. We used the same technique for an incident focused beam (i.e. a sinc-function in the focus) while having a cylindrical scatterer (this solution will be called the Fourier cylinder theory in this work). Again a good agreement between the FDTD results and the analytical solution is obtained, as can be seen in Fig. 3.6. The maximum and the average relative differences are 14.3% and 2.4%, respectively. We note that these results can be further improved by increasing the spatial resolution of the FDTD grid. In Fig. 3.6 it can also be seen that the difference between the scattering of light using a plane wave and a focused beam is significant.

In the FDTD simulations, the absorption of the sample is taken into account by increasing the imaginary part of the refractive index, while the scattering occurs due to the difference between the refractive index of the medium and the scatterer. The grid spacing is preserved, but the overall dimensions of the simulation grid need to be modified to model the wave propagation at oblique angles. This is shown in Fig. 3.7. In the case of larger divergence angles $\theta_{\text{max}}$, the
inclusion of absorption (and/or scattering) in the medium where the beam propagates requires an adjustment of the finite FDTD simulation grid. In the figure, the darker region corresponds to the area of interest. $x_{ph}$ indicates the position of the focal plane. The FDTD grid needs to be wide enough, so that all plane waves start getting attenuated at $x = 0$; this primarily concerns plane waves incident on the focal plane with a highly oblique angle $\theta$. The dashed area corresponds to the extra computational space: the choice of the additional space naturally affects the outcome of the simulations. This is explained by the fact that the plane waves required by the ASPW model are - by definition - infinite. As such, the interaction between the incident waves and the absorbing medium also requires an infinite boundary. However, FDTD can only calculate finite volumes. This gives rise to numerical artifacts. While this difference does not play a role in vacuo, it becomes apparent when the sample is absorbing or scattering, especially for plane waves with a highly oblique incidence angle $\theta$. This problem can be minimized by increasing the size of the simulation grid.

An optimal grid size can be evaluated, as shown in Fig. 3.8. Here, a larger grid space in the FDTD simulations, compared with the grid of interest, are evaluated. We show here the power distribution obtained with three different FDTD grid sizes for the linearly polarized beam focused in an absorbing material with $\mu_a = (2\lambda)^{-1}$ in the $x$-direction. The grid size in the FDTD simulations needs to be large enough to provide correct results by accounting for the absorption of plane waves with wide angular incidence on the focal plane. The figure in the center and on the right reveal that the grid size needs to be above a certain threshold for the results to converge.

**Figure 3.8:** Three different FDTD grid sizes (from left to right: $y = 8\lambda$, $16\lambda$ and $32\lambda$) displayed in logarithmic scale over the range $8\lambda \times 8\lambda$ for the linearly polarized beam.
Chapter 4

Results and applications

Abstract

In chapter 2 the theory of modelling and manipulating light beams has been introduced, while in chapter 3 the numerical method used for applying the theory is discussed. In the current chapter, both theoretical and numerical methods are combined to investigate several scenarios. This is done to both show the importance of the current work and to try and solve current problems. This chapter is divided into mostly independent sections. Each of those uses the tools already developed in the previous chapters. The observations and conclusions of each section are also mostly independent of each other since the main common factor between them are the tools used and not the problems themselves.

Section 4.1 shows the results of implementing the scanning method developed in section 2.2, while section 4.2 uses the same scanning technique to study the effect of using different beams to shine light deeply into a scattering medium. In section 4.3, the enhancement of the intensity inside scattering media by optimizing the phase of the incident light according to the theory developed in section 2.5 is shown. Section 4.4 deals with the time reversal method and how to use a dipole as a beacon to reach deeper inside scattering media.

In the last two sections, two problems that were faced on different projects are shown, where the developed tools proved to be advantageous. In section 4.5, a model for carbon fibers is introduced by using the analytical solution of electromagnetic scattering by multiple cylinders which was shown in section 2.3. Finally, section 4.6 shows the results of implementing the direct extinction method (introduced in section 2.6) in the Monte Carlo numerical solution, where the developed FDTD code was used as a verification tool. The resolution used in the
4. RESULTS AND APPLICATIONS

FDTD simulations is $\lambda/20$ in all sections unless stated otherwise.

4.1 Light beam scanning

Simulating microscopy techniques that use raster scanning such as laser scanning microscopes is important to further improve our understanding of such methods and to be able to enhance the resolution and the scanning efficiency. If the steady state of a beam is simulated as was discussed in section 2.2, it is possible to scan said beam without the need to repeat the simulation again for other focus positions as long as that beam has been modeled using the ASPW method (assuming enough plane waves are used according to equation (2.18)). Obviously, this is an advantage for simulating the scanning of the beam in a more efficient manner.

In this section, equation (2.17) is used for several scenarios to demonstrate the scanning capability. In Fig. 4.1a the shifting of the position of a focused beam is shown. The required position of the focus ($x_0, y_0$) is indicated in the caption of the figure. The intensity of the $E_z$ component is normalized to the maximum intensity at the beam focus while the maximum divergence angle of the incident beam is 45°.

In Fig. 4.1a it can be seen that there is a numerical error in the beam. Distorted images of the original beam are appearing at similar $x/\lambda$, but different $y/\lambda$ positions. These artifacts occur due to the insufficient sampling rate in the angular domain, as has been discussed in section 2.1. In this case, 11 plane waves are used to form the beam. However, according to equation (2.18), the minimum number of plane waves required to form the beam is 15 in this case. It is also interesting to note that it is sufficient to use a smaller number of plane waves when the beam is in the middle of the grid. This is because the distance between the focus and the more remote lateral boundary of the grid (at $|y/\lambda| = 5$) is smaller in comparison to the case when the beam is closer to one of the lateral boundaries. This can be seen in Fig. 4.1a(a) where only 8 plane waves are required according to equation (2.18) and therefore the 11 plane waves used in this case are sufficient (although there are some errors that appear near the edges of the grid since we are still using a low number of plane waves even if it is more than the minimum). When the same beam is shifted as in Fig. 4.1a(c), 13 plane waves are needed. And since only 11 are used, a distorted image of the beam appeared near a lateral boundary of the grid. In Fig. 4.1b the number of plane waves is doubled compared to the results in Fig. 4.1a. Due to this increase, all the numerical artifacts that were shown before have been suppressed.

1 The results from this section have been published in [22].
4.1 Light beam scanning

Figure 4.1: The normalized intensity of the $E_z$ component of the electric field at different positions of the focused beam. The desired focus positions in the figures (a) to (f) are at: $(x_0/\lambda = -4, y_0/\lambda = 0)$, $(x_0/\lambda = -4, y_0/\lambda = -4)$, $(x_0/\lambda = 0, y_0/\lambda = 0)$, $(x_0/\lambda = 0, y_0/\lambda = -4)$, $(x_0/\lambda = 3, y_0/\lambda = 3)$, and $(x_0/\lambda = 5, y_0/\lambda = 1)$. The intensity is normalized to the intensity of the non disturbed $E_z$ component at the focus of the beam. The maximum divergence angle is $45^\circ$ and the wavelength of the incident light is $1 \mu m$. The spatial resolution in the FDTD simulation is equal to $\lambda/20$ and $n_m = 1$.

In this following case, the medium is not homogeneous but consisted of parallel cylindrical scatterers ($r = 0.5 \mu m$) with refractive index of 1.45 suspended in water ($n_m = 1.33$) to model biological tissue. The volume concentration of the scatterers is 30%, which gave a mean free path of 6.9 $\mu m$ assuming independent scattering. The beam is first scanned in the $x$ direction to show the change in the focal shape and intensity in relation to the depth of the focus of the beam in the sample (Fig. 4.2). Then, a simulation is carried out for the scanning in the $y$-direction to show that the principle of scanning the beam by changing the phase works in this case as well (Fig. 4.3). The figures show the intensity of the sum of the incident and the scattered electric fields. This is mentioned because in Fig. 4.2 as expected, the focused beam is distorted after propagating through the scatterers. Remarkably, the beam is already distorted before it penetrates into the medium. This is because of the light scattered back from the cylinders. The intensity in Figs. 4.2 and 4.3 is normalized to the maximum intensity of the incident non-scattered focused beam. Interestingly, in Fig. 4.2(d) the intensity increased above one. This happens when the focus hits the exact position of a cylinder which then acts as a high NA lens. This is similar to finding jets of high intensity of light behind cylinders. Also it is interesting to note that the supposed position of the focus diverged from the actual position of the focus.
4. RESULTS AND APPLICATIONS

Figure 4.2: The normalized intensity of the $E_z$ component of the electric field for axial scanning ($x$ direction) at $y_0 = 0$. The normalization is relative to the maximum intensity of the incident non-scattered focused beam. Figure (a) shows the scatterers in red, while they are omitted in the latter pictures for better visibility of the beam shape. The figures from (a) to (f) show focus positions at: $y_0/\lambda = 0$ and $x_0/\lambda = (-8, -6, -2, 2, 4, 9)$. 21 plane waves are used to form the beam. The refractive indices are $n_s = 1.45$ and $n_m = 1.33$, the radius of the cylinders is $0.5 \mu m$, the wavelength of the incident light is $1 \mu m$, and $\theta_{\text{max}} = 45^\circ$. The spatial resolution in the FDTD simulation is equal to $\lambda/20$.

especially for the deeper foci. This displacement is caused partly by the different speeds of the light inside and outside the scatterers since the expected focus positions are calculated under the assumption of no scattering. By examining Fig. 4.2 it becomes apparent that the deeper the light propagated through the sample the more the intensity of the focus decreased and the more its shape is distorted. More precisely, the relative width of the beam is enlarged and, in addition, further unintentional ‘foci’ due to interference of scattered light appeared at larger depths of the focus position. We note that to reach these conclusions, it is necessary to run the simulation for more realizations of positions of the scatterers (as will be shown in the figures in section 4.2).

The simulations presented in Fig. 4.2 are allocated a memory of 47.3 Mbyte, compared to
4.2 Depth profile study for multiple beams

Figure 4.3: The normalized intensity of the $E_z$ component of the electric field for lateral scanning ($y$ direction) at $x_0 = 0$. The normalization is relative to the maximum intensity of the incident non-scattered focused beam. Figure (a) shows the scatterers in red, while they are omitted in the latter pictures for better visibility of the beam shape. The figures from (a) to (f) show focus positions at: $x_0/\lambda = -10$ and $y_0/\lambda = 2$, and then $x_0/\lambda = 0$ and $y_0/\lambda = (−8, 4, 0, −4, 8)$. 21 plane waves are used to form the beam. The refractive indices are $n_s = 1.45$ and $n_m = 1.33$, $r = 0.5 \mu m$, the wavelength of the incident light is $1 \mu m$, and $\theta_{max} = 45^\circ$. The spatial resolution in the FDTD simulation is equal to $\lambda/20$.

2.25 Mbyte which would have been needed to save the data in a classical FDTD simulation (i.e., saving the sum of all the plane waves without saving the fields from the individual plane waves). In return, the simulation took approximately 40 minutes compared to 14 hours which is the time needed for a classical FDTD simulation in case of scanning the focus in the depth direction.

4.2 Depth profile study for multiple beams

The main point of interest here is the deterioration of a focused beam while said beam is depth scanned through the scattering medium. The scanning of the beam is performed with help of the ASPW method as discussed in sections 2.2 and 4.1. Another advantage of modeling beams

\footnote{The results from this section have been published in [82].}
4. RESULTS AND APPLICATIONS

using the ASPW method (beside the scanning capability that was introduced in section 4.1) is the ability to simulate several types of beams using the same simulation data set as will be shown in this section.

4.2.1 Scattering media

The scattering medium is modeled as an ensemble of parallel cylindrical scatterers which are randomly distributed in a matrix. The cylinders had a diameter of 1 µm and are suspended in the matrix with a volume concentration of 30%. FDTD simulations are carried out for three samples which differed in the refractive index of the scatterers \( n_s = 1.4, 1.45 \) and 1.5, while the refractive index of the matrix is kept constant at \( n_m = 1.33 \). To get an estimation of how much scattering occurred in each sample, the mean free path \( \rho \) is examined for each case \( \rho = 21.98 \mu\text{m}, 7.53 \mu\text{m}, \) and 3.84 µm) by assuming only independent scattering, homogeneous distribution of the cylinders, and ignoring coherence effects. In addition, for all samples the absorption of both the scatterers and the surrounding media is set to zero.

4.2.2 The illumination

Three types of beams are simulated as the illumination source: a focused beam (from section 2.1.2), a Gaussian beam, and a quasi-Bessel beam (from section 2.1.3). Due to the fact that all beams are formed using the ASPW method, it is possible to reuse the intermediate results of a beam to calculate the respective ASPW solution of other beams. This is achieved by choosing the plane waves that correspond to the range of angles relevant to the beam of interest. For the focused beam, the maximum divergence angle amounted to \( \theta_{\text{max}} = 15^\circ, 25^\circ, 45^\circ \). These values are substituted in equation (2.9) and equation (2.14), while taking the beam waist to be much smaller than the wavelength.

The Gaussian beam is simulated by choosing a beam waist of FWHM = 0.86 µm which corresponds to an angle of 25° for the angular beam waist. For the quasi-Bessel beam, equation (2.15) is used with equation (2.9) while taking \( \Delta \theta = 20^\circ \) and \( \theta_{\text{max}} = 45^\circ \) according to the definitions of these parameters from section 2.1.3.

In all five cases, the wavelength \( \lambda \) is taken to be equal to 1 µm. The number of plane waves used to form the beams is 161 in the range from 45° to −45°. Each of the beams is defined by the range of angles that it had in the angular domain. Thus, a focused beam with a maximum...
4.2 Depth profile study for multiple beams

divergence angle of 45° consisted of plane waves in the range from −45° to 45°. This will be abbreviated as \(|\theta| = [0° : 45°]|\).

4.2.3 Results

![Figure 4.4: The intensity (W/m²) of a focused beam at different focus positions for an incident beam of 1 W/m power (|\theta| = [0° : 45°])](image)
The upper left picture shows the scatterers in blue while they are omitted in the latter pictures for better visibility of the beam shape. The origin in the longitudinal direction is placed at the starting point of the scatterers. The refractive indices are \(n_m = 1.33\) and \(n_s = 1.5\). \(x_0\) is the focal position.

The intensity of a focused beam (|\theta| = [0° : 45°]) at different focus positions is shown in Fig. 4.4 In Fig. 4.5 the same is shown for the quasi-Bessel beam case (|\theta| = [25° : 45°]). The two figures are normalized to an incident differential power of 1 Watt/m. In both cases, the scatterers had \(n_s = 1.5\).

It can be observed that certain transmission channels occur in the medium [110]. This was a problem since it was not possible to get a quantitative comparison between the simulated beams.
Figure 4.5: The intensity (W/m$^2$) of a quasi-Bessel beam at different focus positions for an incident beam of 1 W/m power (|θ| = [25° : 45°]). The upper left picture shows the scatterers in blue while they are omitted in the latter pictures for better visibility of the beam shape. The origin in the longitudinal direction is placed at the starting point of the scatterers. The refractive indices are $n_m = 1.33$ and $n_s = 1.5$. $x_0$ is the focal position.

while propagating through the different scattering media. Averaging over multiple randomly chosen distributions of scatterers is one possible solution (which is also used in this work, but not for too many realizations). However, this would have increased the simulation time. A more efficient solution is to use the information stored while using the ASPW method. The focus is scanned in the lateral direction ($±20 \mu m$). Then the intensity from all of these lateral scans is added up incoherently to obtain the averaged intensity for each depth. As an example, the averaging of the intensity in Fig. 4.4 and Fig. 4.5 can be seen in Fig. 4.6 and Fig. 4.7 respectively. In order to further improve the averaged results, 10 different realizations are used in addition to the usage of the beam scanning.

For a given distribution of the scatterers, the penetration depth depends mainly on the optical
4.2 Depth profile study for multiple beams

Figure 4.6: The intensity (W/m²) for the focused beam in Fig. 4.4, averaged over a lateral range of ±20 µm. $x_0$ is the focal position.

Figure 4.7: The intensity (W/m²) for the quasi-Bessel beam in Fig. 4.5, averaged over a lateral range of ±20 µm. $x_0$ is the focal position.

properties of the scattering medium. However, it is interesting to note that the rate of change of the transmission channels seen in Fig. 4.4 and 4.5 depends heavily on the type of beam. For the focused beam (Fig. 4.4), a shift of 1 µm in the position of the focus ($x_{sh} = 1 \mu m$) is enough to change the transmission channels considerably. In the case of the quasi-Bessel beam on the other hand (Fig. 4.5), the focus can be shifted by 10 µm and it still retains mostly the same transmission channels. After the incoherent averaging (in Fig. 4.6 and 4.7), it is easier to study the decrease of the beam intensity versus depth, since the characteristics of the beam become more apparent, e.g. the beam waist of the coherent peak and the ground level of the multiple scattering become visible. Furthermore, the channels that could be seen before in Fig. 4.4 and 4.5 disappear. This indicates that such channels depend on the individual distribution of
4. RESULTS AND APPLICATIONS

In Fig. 4.8 the on-axis intensity is shown for all of the beams after being depth-scanned through the scattering medium \( n_s = 1.5 \). It should be noted that the position of the maximum of the beam \( x_0 \) is different from the position without scatterers \( \hat{x}_0 \) since the original beam was intended to go through a homogeneous medium of refractive index of 1.33. Thus, a correction term considering the refractive indices of both the scatterers and the surrounding medium is used \([111]\) to get the approximate new position of the focus:

\[
x_0 = \hat{x}_0 \frac{n_mC_m + n_sC_s}{n_m},
\]

(4.1)

where the factors used in the correction term \( C_s \) and \( C_m \) are the fractional area of the scatterers and the surrounding medium, respectively. Fig. 4.9 shows the lateral intensity of each beam at different depths to see the deterioration of the beam profile.

By adding the intensities of the two beams corresponding to the angular ranges of \(|\theta| = [0^\circ : 25^\circ]\) and \(|\theta| = [25^\circ : 45^\circ]\) in Fig. 4.8, we observe that they are approximately equal to the intensity of the beam in the range of \(|\theta| = [0^\circ : 45^\circ]\) at the surface of the sample. This is due to the fact that each beam is normalized to the same incident differential power. For the beam in the range of \(|\theta| = [0^\circ : 45^\circ]\) we get about double the intensity of the arithmetic mean of the two
4.2 Depth profile study for multiple beams

Figure 4.9: The lateral profile of the beams at different depths for \( n_m = 1.33 \) and \( n_s = 1.5 \). The differential power of each beam is equal to 1 Watt/m. The first three focused beams have \( \theta_{max} = 45^\circ \) (blue), \( 25^\circ \) (green), \( 15^\circ \) (red). The quasi-Bessel beam has \( |\theta| = [25^\circ : 45^\circ] \), while the Gaussian beam has a FWHM = 0.86 \( \mu m \).

beams in the ranges of \( |\theta| = [0^\circ : 25^\circ] \) and \( |\theta| = [25^\circ : 45^\circ] \) because of the coherent addition of the plane waves. By going deeper into the sample (after 35 \( \mu m \) in the example in Fig. 4.8), the light experiences more scattering interactions and less constructive interference occurs in the focal region due to the decreasing non-scattered part of the light. As a result, we find that the intensity of the beam in the range of \( |\theta| = [0^\circ : 45^\circ] \) equals the arithmetic mean (non-coherent addition) of the intensities of the two beams in the ranges of \( |\theta| = [0^\circ : 25^\circ] \) and \( |\theta| = [25^\circ : 45^\circ] \).

Usually, a beam with a larger maximum divergence angle has a tighter focus. Therefore, since all the simulated beams have the same differential power, the more focused beam has a higher intensity at the focus. This can be seen \textit{e.g.} in Fig. 4.9 at a depth of \(-2.5 \mu m\). This changes when the beams propagate through the scattering medium. At higher depths, the high NA beams lose to some extent their advantage of having higher intensity at the focus. This can be visualized by looking at the propagation path of the individual plane waves that make up these beams. For the focused beam with \( \theta_{max} = 45^\circ \), the most divergent plane waves propagate...
4. RESULTS AND APPLICATIONS

![Graph showing the on-axis intensity for beams with different angular ranges.](image)

**Figure 4.10:** The on-axis intensity for the beams while using two sizes of cylindrical scatterers (solid lines for Dia. = 1 \( \mu \)m and dashed lines for 2 \( \mu \)m) while \( n_s \) is kept equal to 1.45 and \( n_m = 1.33 \).

A longer distance in the scattering medium due to their more oblique propagation directions. Therefore, they are more attenuated compared to the plane waves which are incident at smaller angles. This also explains the good performance of the Gaussian beam which has most of its power in the small angles, while the quasi-Bessel beam shows a disadvantage in this case since relatively large angles are applied. In addition, using low NA beams proves more efficient because it avoids unnecessary illumination of the sample with light coming from the large incident angles, which prevents e.g. bleaching in biological samples. Also, it is not common to have a Bessel beam which is focused, since the most attractive feature of such a beam is the large depth of field [112]. However, our purpose here is to examine the basics of the propagation of such a beam. Also, since we are only simulating in 2-D, we do not have the option of simulating a Bessel beam since it will simply appear as a sinusoidal wave (where a quasi-Bessel beam can be generated by blocking opposite sections of the angular spectrum of the beam [112]).

As can be seen in Fig. 4.9 the intensity at lateral points outside the beam focus area keeps increasing at different rates for each of the simulated beams when the focus depth is shifted deeper. This 'background' intensity is caused by multiply scattered light. Thus, it also affects the decrease rate of the curves in Fig. 4.8 making it difficult to judge where and if the intensity curves of the different beams, which are only due to the non-scattered light, intersect.
4.2 Depth profile study for multiple beams

Figure 4.11: Beam profiles at three different depths using the analytical solution for the non-scattered light ($\rho = 3.4 \ \mu m$).

As a rule of thumb, the scattering cross section increases with the size of the scatterers [20]. This can be seen in Fig. 4.10 where the on-axis intensity for the larger scatterers (Dia. = 2 $\mu$m) decreases at a higher rate than in the case of smaller scatterers (Dia. = 1 $\mu$m). This also agrees with the analytical solution of the scattering of a plane wave by a cylinder [20] since we obtain for the bigger cylinder (Dia. = 2 $\mu$m) a scattering cross section $C_{scat}$ of 2.7 $\mu$m, while for the smaller cylinder (Dia. = 1 $\mu$m), $C_{scat}$ amounts to 0.39 $\mu$m. There is a degradation in the quality of the intensity curves for the 2 $\mu$m particle. This is mainly because the averaging using lateral scanning is not as efficient compared to the averaging for the 1 $\mu$m particle since the beam has a higher correlation after being scanned laterally.

In order to study only the non-scattered contribution to the intensity at the focus area versus depth, the analytical equation (2.21) (or equation (2.27) for the 3-D case) found in section 2.6.2 is applied while using $\mu_t = \mu_s$ since we are dealing with scattering (and assuming negligible absorption). In equation (2.21), a Beer-Lambert exponential term is added to the ASPW expression of equation (2.9) to take into account the decrease in intensity due to scattering in a medium with a certain $\mu_s$. 

55
This model is validated by comparing its results to those obtained with the FDTD method (to be found later in this section in Fig. 4.14). Three more FDTD simulations are run ($n_s = 1.4$, $1.5$ and $1.9$ in $n_m = 1.33$ corresponding to $\rho = 117 \, \mu m$, $19.8 \, \mu m$ and $3.4 \, \mu m$ respectively) using a lower volume concentration of $5\%$ for cylinders with diameter of $1 \, \mu m$. This is done to decrease the influence of dependent scattering. The analytical model showed good agreement to the FDTD simulations at low scattering ($\rho = 117 \, \mu m$ and $19.8 \, \mu m$). For higher scattering ($\rho = 3.4 \, \mu m$), the curves started showing significant differences due to dependent scattering. This is discussed in more detail at the end of this section.

The profiles of the beams can be seen in Fig. 4.11 at three different depths calculated with equation (2.21) for similar scattering parameters as in Fig. 4.9 ($\rho = 3.84 \, \mu m$), but for lower concentration (conc. $= 5\%$). As an advantage of using this model, we can investigate the focus due to the non-scattered light much deeper in the scattering medium than it is possible with the FDTD method, compare Fig. 4.9. From Fig. 4.11 it can be noted that the deeper the focus depth is, the more the beams are broadening and the more the profiles of the different beams approach each other as expected from Fig. 4.9. This is due to the smaller contribution of the
4.2 Depth profile study for multiple beams

Figure 4.13: The intensity of the focused beam ($\theta_{\text{max}} = 45^\circ$) from the FDTD (dashed lines) while being scanned through scattering media for different concentrations of scatterers. The intensity is compared with the Beer-Lambert law using the direct extinction method (solid lines with squares).

plane waves incident at larger angles.

Fig. 4.12 shows the intensity ratio of the beams with $\theta_{\text{max}}$ of 25° to $\theta_{\text{max}}$ of 45° for the same scattering medium. It can be seen that for depths larger than 25.7 $\mu$m the intensity of the beam with lower NA is larger than the intensity of the beam with higher NA. Thus, at large depths, not only the total intensity at the focus position is larger for smaller $\theta_{\text{max}}$ compared to larger $\theta_{\text{max}}$, but also the intensity due to non-scattered light. Fig. 4.12 shows, in addition, the intensity ratio of the focused beams with $\theta_{\text{max}} = 35^\circ$ to $\theta_{\text{max}} = 70^\circ$. In this case, the non-scattered intensity of the low NA beam for depths larger than about 8 $\mu$m is larger than that of the high NA beam. We note that a maximal incident angle of 70° corresponds to a very high numerical aperture objective which is used in practice.

Due to the large hardware resources needed for the FDTD method, we simulated the light propagation only in a relatively small area. Therefore, we used scattering objects which have large scattering coefficients. This restriction can be relaxed when the analytical formula is used, allowing the use of more realistic optical properties for biological tissue. Thus, using a typical scattering coefficient which is approximately 10 times lower than applied in Fig. 4.12 (i.e. $\rho_s$ is 10 times larger), it follows that the shown curves are stretched to the right by a factor of 10.
(due to the exponential term in equation (2.27)). Furthermore, it follows that the intensity of
the non-scattered light of a relatively low NA beam with $\theta_{\text{max}}$ of 35° is larger than that of a
high NA beam with $\theta_{\text{max}}$ of 70° for depths larger than about 80 $\mu$m. However, we note that
also the depth where the lateral profiles of the beams approach each other is increased (in the
above case the depth is about 800 $\mu$m).

In Fig. 4.13 two different concentrations are simulated. In the second concentration case (conc.
= 5%), the refractive index of the scatterers is modified to get a theoretical mean free path that
is similar to the first concentration (conc. = 30%). From these curves we can reach a series of
conclusions:

- Having a high concentration sample leads to deviations from the Beer-Lambert law which
is based on the rules of geometrical optics. This is mainly due to the high dependent
scattering \[113\, \text{114}\] as can be seen in the red curves where the simulated curve is much
higher than the predicted Beer-Lambert law.

- Increasing the refractive index mismatch while maintaining a high concentration makes
the gap between the simulation and the prediction of geometrical optics even bigger as can
be seen in the blue curves.

- Decreasing both the refractive index mismatch and the concentration of the scatterers
removes - to a large extent - the influence of dependent scattering. This is shown in the
green curves where the simulation results agree with the Beer-Lambert law.

- Increasing the refractive index mismatch while keeping the concentration of the scatterers
low gives good agreement between both the simulation and the curves predicted by geo-
metrical optics. However, this conclusion is only valid to a certain depth, after which the
focus is too blurred and the beam enters the multiple scattering regime. This can be seen
in the case of the black curves.

In all of the previous comparisons in Fig. 4.13, the Beer-Lambert law results are obtained
by integrating an exponential function over the range of angles that constitutes the beam under
test (by using equation (2.27) from subsection 2.6.4). The exponent corresponds in each case
to the scattering parameters of the medium to be tested and the depth for each incident angle
(assuming a single scattering effect as was explained in the case of absorption in section 2.6, but
using $\mu_s$ instead of $\mu_a$). The assumptions taken into account while using this method (the direct
extinction method) become invalid for higher concentrations (as shown in Fig. 4.13) and for
4.3 Phase optimization

In section 2.5 it was already explained how the phase optimization works in principle and how important it is to build a tool capable of showing the different effects and phenomena that

Figure 4.14: Comparing the validity of the Beer-Lambert law using the direct extinction method compared to FDTD for different scattering parameters and for the same incident focused beam and volume concentration ($\theta_{\text{max}} = 45^\circ$, conc. = 5%). The tilde sign in the legend of the last curve is to show the range excluded from the interpolation. This is done to avoid taking the main peak, thus, taking only the multiple scattering contribution.

This is true even for relatively low concentration (5% in the case of this study in the solid red line in Fig. 4.14). The deviation in case of high scattering and low concentration samples comes mainly from multiple scattering. By looking at the solid red curve in Fig. 4.14 it can be shown that if the signal ground level is estimated (by interpolating the lateral focal plane after removing the forward scattering peak) such that we can have an approximation of the contribution of the multiple scattered light, we can in essence subtract that estimation from the overall beam. This is shown as plus symbols in the graph. Such a curve shows a tendency to follow the direct extinction method in that case. This would not have worked if the concentration is higher since there will be a dependent scattering effect as well.
are associated with such a technique. In this section we discuss some of the findings of these investigations.

![Graph](image)

(b) Phase optimization with averaging.

**Figure 4.15:** The effect of using lateral scanning to average over several incoherent intensities. The refractive indices are $n_s = 1.5$ and $n_m = 1.33$. In both cases, the intensity of the focus is shown after being scanned in depth direction. The wavelength is $\lambda = 1 \, \mu m$.

It was shown in section 4.2.3 that due to the fact that we have an exact solution of the scattering by a specific distribution of scatterers, we get a lot of information about the channels (defined in section 4.2.3) inside the medium. This information does not allow us to see the overall performance of the beam propagating through the medium. In Fig. 4.15a it is shown that this problem appears also while investigating phase optimization which causes a lot of fluctuations in the graphs. This is not a result of the phase optimization. Rather, it is a property of light scattering through a specific distribution of scatterers. As such, a modified version of the method of lateral scanning that was explained in section 4.2.3 is used here to get the average of several realizations to suppress the noise. The effect of this averaging is shown in Fig. 4.15b. Interestingly, the optimization of the phase enhances the intensity even before the focus enters into the scattering medium (as can be seen in Fig. 4.15b). This is due to the enhancement of the back-scattered light at these points.

The lateral scanning method needed to be modified for usage with phase optimization since after each lateral shift, the beam encounters a different distribution of scatterers. This means
4.3 Phase optimization

that the phase that was modified for the original distribution is not valid anymore. To solve this
problem, the phases need to be optimized for each different lateral shift. Since we are scanning
the beam by manipulating the phase of the individual plane waves, there is no need for any
further simulations. This procedure is illustrated with the help of the diagram in Fig. 4.16. It is
important to note that the phase optimization itself is a coherent process (since the optimization
is done for the phase), while the averaging process (over intensity) is by definition an incoherent
process.

There are independent parameters when dealing with phase optimization techniques in this
work. These are the number of segments used and the range of phase differences between the
segments (the amplitude of the light through the segments is assumed to be constant in all
cases). In section 2.5 we have seen the relation between the intensity enhancement and the
number of segments.

At this point it is necessary to both better understand the process of phase optimization and to
see if it is feasible to achieve the maximum possible enhancement. By looking at the proof by
Vellekoop [58] where he showed the maximum enhancement ratio (assuming the optimization of
only the phase), we can see that the basic problem that phase optimization tries to solve is the
loss of constructive interference in the focus of the incident light. As a result, the best possible
enhancement is reached in a situation where light is scattered without the loss of constructive
interference of the light. To examine such a situation, two different simulations are combined.
In the first one, a beam propagates without any scatterers in its path \(n_m = 1.33\) while in the
second, the medium contains scatterers. And since the ASPW-description of the beam is used,
the information about the individual plane waves is stored as well. Combining both simulations
means that - per plane wave - we take the amplitude of the scattered wave and combine it with
the phase of the non-scattered wave (where we assume no scattering medium). The result of such
a combination of simulations is shown in Fig. 4.17 for two different materials \(n_s = 1.5,\) conc.
\(= 30\%\) and \(n_s = 1.9,\) conc. \(= 5\%).\) In both cases we get a comparable mean free path \(\rho = 3.7\)
and 3.4 \(\mu m\) respectively) assuming independent scattering (which is a wrong assumption in the
high concentration case as was explained in section 4.2.3).

From the results in Fig. 4.17 we conclude that the model used here agrees with the phase
optimized beam when the phase difference ranges from 0 to \(2\pi\). Using only a maximum value
of \(\pi\) is not enough to achieve the maximum possible enhancement. The physical interpretation
of this is the following. To get an optimized focus at the point of interest, we need to have as
much destructive interference as possible in the rest of the focal plane. To achieve that, each
4. RESULTS AND APPLICATIONS

Figure 4.16: The procedure to analyze the effect of phase optimization on the enhancement of intensity. In the first column, the incident light is scattered. By shifting the beam laterally, the beam interacts with different configurations of the scatterers. In the second column, the phase of the beam is optimized. All the results from the second column are averaged by adding them incoherently to reach the desired focal plane in the third column. This procedure is repeated after going to the following depth point by shifting the focus of the beam in the longitudinal direction. The main advantage of this method is the usage of one set of simulation data to get the optimization of several realizations.
4.3 Phase optimization

Figure 4.17: FDTD simulations to show the effect of phase optimization. Two samples with two different concentrations are investigated while keeping the mean free path as close as possible while assuming single scattering. The dashed lines are the FDTD simulations without optimization. The circle symbols show the optimized case with a range of $2\pi$ for the phase, while the square symbols show the optimized case with a range of $\pi$. The solid lines show the combination of FDTD simulations for a homogenous medium (to have the information about the non-disturbed focus) and the FDTD simulations with scatterers, but without phase optimization. The agreement between the dashed lines and the circle curves shows that the optimization process merely corrects the phase of the focus which was disturbed due to the scattering process.

Two interfering plane waves need to have a phase shift of $180^\circ$. However, if the first plane wave already has a phase shift higher than zero then it is necessary to have a phase higher than $180^\circ$ in the second plane wave to be able to reach the destructive interference state.

Despite the fact that the two samples had comparable theoretical mean free paths, the sample with higher concentration had a higher intensity both before and after the enhancement in comparison to the respective low concentration case (when looking deep enough in the medium). This is due to dependent scattering as was shown in section 4.2.3. The optimization process showed approximately a fivefold increase in intensity compared to the non-optimized case.

In Fig. 4.18 a collection of stitched images of the focal planes of scanning beams in the depth direction is shown for several types of beams (two focused beams of $\theta_{\text{max}} = 25^\circ$ and $45^\circ$, a
4. RESULTS AND APPLICATIONS

Figure 4.18: A combined image of the intensity [W/m²] in focal planes after depth scanning through a scattering medium of \(n_m = 1.33\) and \(n_s = 1.5\). In each subfigure the normal propagation of the beam is shown, followed by the phase optimized propagation. The combination was done according to the scheme shown in Fig. 4.16 and \(\lambda = 1\ \mu m\).
4.4 Time reversal and phase conjugation

Bessel beam, and a Gaussian beam). This comparison shows that the amount of enhancement is independent of the type of beam used. The only difference in this case is the different number of segments (plane waves) used to shape the different beams according to equation (2.20). Also, the distribution of the beam becomes almost identical across all beams from a certain depth on. The only difference is the lower intensity for the enhanced beams with high NA (e.g. the Bessel beam) compared to the lower NA beams (e.g. Gaussian beams). This is due to the smaller distance traveled by light for the low NA beams as was shown in section 4.2.

By looking at the near fields after optimization at a single depth (Fig. 4.19), it can be seen that the intensity becomes more confined to a single region rather than being spread out through the entire focal plane as was the case for the non-optimized case. This can be explained by considering the following phenomenon. As was mentioned in section 4.2 for the light near the surface of the sample, the aperture is defined by the lens and its degree of focusing. However, deep inside the scattering media (Fig. 4.19b), the effective aperture is defined by the medium itself. As such, high spatial frequencies that were not available before become available due to the scattering of the medium [115, 116]. This phenomenon of efficiently using the effective high numerical aperture has been demonstrated recently in an experimental setup which uses a scattering material as a lens to resolve nanoparticles at 97 nm optical resolution using visible light wavelengths [116] and in other studies using scattering materials to focus light on fluorophores [117]. In Fig. 4.19c, the figures were rescaled to be oversaturated at the focus to see that away from said focus we get less light in the optimized case.

4.4 Time reversal and phase conjugation

Usage of optical instruments is usually limited to shallow depth applications due to the opacity of the subject under test. This is mainly a result of scattering which prevents transparency [118]. This opacity or blurring of imaging can be explained as the amplitude and the phase becoming distorted. This is mainly due to multiple scattering. One way to counter these effects is to use optical phase conjugation (OPC) which suppresses the effects of scattering. The general theoretical foundation of OPC was studied in different works [26]. Subsequently, a theoretical model of a phase conjugation mirror was proposed for OPC [27, 28]. This model is based on the paraxial wave equation, which made this model applicable in cases of thin random media where light propagation within the random medium is ignored. After that, a more general model was made based on Maxwell’s equations using the PSTD tool. This model can deal with random
4. RESULTS AND APPLICATIONS

Figure 4.19: Comparing the near field intensity [W/m²] for the optimized and non-optimized cases for two different depths and for a focused beam with $\theta_{max} = 45^\circ$. The refractive indices were $n_m = 1.33$ and $n_s = 1.5$. The wavelength was 1 $\mu$m. Fig. (c) is identical to Fig. (b) with the sole difference of keeping the same scale to better see and compare the low intensities away from the focus.
4.4 Time reversal and phase conjugation

media of arbitrary thickness [29, 30]. A great deal of work has been done to discover the limits of OPC and to find the best ways to utilize it, especially to suppress scattering, to enhance the intensity inside the medium [16, 119] and to achieve better focusing inside the scattering media [42, 120, 121].

4.4.1 Optical phase conjugation

From all of the previously shown studies about the topic of optical phase conjugation, it is apparent that we need a guiding star inside the medium in order to reverse the waves coming from that source to reach back to the point of origin (as can be seen in the sketch in Fig. 4.20). This is considered the main challenge for this method and especially for the field of biophotonics. One way to overcome this problem is the usage of nanoparticles [123, 124].

\[
\text{Figure 4.20: Schematic of time reversal of a point source. (a) An outgoing wave that gets scattered by an arbitrarily shaped scatterer which is drawn in gray. (b) The outgoing wave has been reversed and is directed back towards its original source.}
\]

Gold nanoparticles are commonly used as contrast and therapeutic agents because of their non-toxicity, their ease of bioconjugation with biomarkers for targeted delivery [5, 125], and their small size which allows for tunable resonance in the red and near infrared spectrum. That part of the spectrum is of particular interest due to the optical window that permits photon penetration into biological tissues with relatively high transmittance. Furthermore, due to the high absorption cross section of the particles, it is possible to achieve high absorption of pulsed light which leads to the production of sound waves (which serves as a good contrast agent for

\[1\text{The results in this section were published in [122].}\]
4. RESULTS AND APPLICATIONS

photoacoustic imaging [5, 6, 7, 8]) and heat (which is used in photothermal therapy [9, 10, 11, 12, 13, 14, 15]).

One of the most promising applications in the field of imaging is the photoacoustic imaging using time reversal [126, 127], specifically the technique of time-reversed ultrasound-encoded imaging both in its general case [30, 128, 129, 130] and its back-scattering mode [131]. The modeling of optical phase conjugation of ultrasonically encoded signals has also been done using FDTD simulations [132] by changing the permittivity and permeability of the material according to an ultrasound-modulated signal. The study of the usage of time reversal as a tool for thermal therapy is also a great topic of study [133]. The basic idea is to heat up the parts suspected of having tumorous tissue (using focused acoustic waves) after making sure that the nanoparticles have been bound to these tissues. Due to the high absorption cross section, gold particles heat up and the change in the surrounding refractive index can be used to modulate a light guiding signal. This signal can be detected and time-reversed to reach back into the tumorous tissue with more focused and higher energy beams compared to the non-optimized incident light. A similar approach is the bursting of microbubbles using ultrasound and then to use the nonlinear pressure-to-destruction response as the basis for time-reversal [134].

Simulating the usage of nanoparticles (or point sources in general) in the field of OPC has been done in several works using hard points as both sources and conjugation mirrors, meaning that the electric field at a certain point is excited as if there were a dipole at that point [42, 121]. In this section, the OPC is simulated in the FDTD scheme. The nanoparticle is assumed to be a hard source (the definition of such a source can be found in section 3.3). The fields are detected in the far-field, and the electric field component is flipped to get the effect of time reversal. Afterward, these time-reversed electric fields are reintroduced into the FDTD grid using the ASPW modeling method [122]. This way of modeling the time reversed fields is more intuitive when modeling the devices used in this process [135, 136, 137]. Most of these devices can be compared to the SLM (for phase modulation) \(^1\), DMD (for amplitude modulation) and in-plane switching liquid crystal display [139] (for polarization modulation) which can be modeled using ASPW as has been shown in section 2.5. Moreover, using the NFFF to get the far-field information is more efficient than simulating a bigger grid and propagating the wave for a larger

---

\(^1\)The usage of SLM as an efficient device in OPC has been shown in a recent study [138]. The setup has the advantage of being easy to build and alignment free. This method is nice since it uses wave-front optimization in order to achieve a optical time-reversal mirror
4.4 Time reversal and phase conjugation

distance to reach the far-field regime \([140]\). A theoretical comparison between the plane wave description used in this work and the multipole expansion used in \([121]\) can be found in \([141]\). A preliminary simulation is shown here to both validate the method by comparing the results to the literature and to have a better idea about how to proceed with researching this topic by using the developed tool. In Fig. \([4.21]\) we can see a random distribution of cylindrical scatterers \((n_s = 1.33)\) suspended in air. An area in the middle is without scatterers to have better visibility in the region of interest. The target of this simulation is to illuminate the simulation grid with a converging spherical wave (in 2-D) and to investigate the distribution of intensity and the quality of focusing. The maximum intensity possible is 1 W/m\(^2\) which is the value used for normalization. From Fig. \([4.21]\) it is obvious that we get only speckle patterns with no obvious structure of the intensity. This is an expected result due to the scattering of the incident light by the inhomogeneous medium.

Now we apply the phase conjugation method. We start by initializing a source point in the middle of the grid. This source acts as a guiding star later on to be able to home in onto that point. The guiding star wave is detected after it has propagated through the scattering medium and then it is transformed to the far-field using a near- to far-field transformer as mentioned before in section \([3.7]\). There are two reasons for this transformation to the far-field. The first one is, the fact that most devices that will be used in experiments interact with the light in the far-field. The second reason is that, a far-field description depends only on the detection angle. This coincides nicely with our ASPW description and will make utilizing the detected fields in the FDTD simulation much easier.

A phase shift of 180° is introduced to the detected electric far-fields. The magnetic fields on the other hand are not changed. This gives physically a time reversal effect of the wave. Subsequently, each plane wave around the grid is introduced into the simulation with the appropriate phase. The result of such a procedure is shown in Fig. \([4.22]\). It is apparent that the intensity has increased from the speckle level of around 0.05 that we have seen previously in Fig. \([4.21]\) to approximately 0.6 compared to an intensity of 1 in the case of no scatterers in the grid. The spot size on the other hand is 0.55 µm according to \(1/e^2\) times the maximum intensity value (1.699 times the full width at half maximum), which agrees with both previous simulations \([140]\) and theoretical predictions \([12, 132, 133]\). It is not possible using this setup to reach any better spatial resolution since the plane waves incident from opposite angles interfere constructively in a way similar to the behavior and limitations found in 4π-microscopy \([144]\). Other groups have reported reaching a subdiffraction limit resolution \([145]\). These kinds of simulations have
4. RESULTS AND APPLICATIONS

Figure 4.21: The normalized intensity [a.u.] of a converging radial wave. Assuming no scatterers, a dipole would have been formed in the middle of the grid with an intensity of 1. The refractive indices are $n_m = 1$, $n_s = 1.33$, and $\lambda = 1 \mu$m.

been carried out during the course of this work as well. However, this approach was not pursued further due to the fact that those results were reached mainly by the usage of a soft optical target that eliminates the incident light after reaching the focus position [146]. Such a setup assumes the introduction of an optical sink inside the scattering material. While those results are correct mathematically and numerically, it is the opinion of the author that such a model introduces extra information to the time-reversed wave (namely the position of the original focus, and the evanescent waves near the point of focus which could not have been detected before), making the model physically unrealistic.

Having a higher concentration of scatterers on the other hand and having the guiding dipole
4.4 Time reversal and phase conjugation

Figure 4.22: The normalized intensity [a.u.] of a converging radial wave after correcting the phases by detecting an outgoing dipole. The refractive indices are $n_m = 1$, $n_s = 1.33$, and $\lambda = 1 \, \mu m$.

near the scatterers would enhance the resolution significantly since the scatterers transform the evanescent waves to propagating waves. Consequently, more information can reach the detector in the far-field by ensuring that the distance between the scatterers and the dipole is less than the wavelength in all directions. Such a situation was simulated (the figure is not shown here), resulting in a spot size of 0.42 $\mu m$ (at $\lambda = 1 \, \mu m$). It is expected that the resolution can be further enhanced by choosing the positions of the scatterers such that they completely surround the dipole. As was mentioned before in section 2.1, an optical beam can be described as a summation of propagating plane waves and decaying evanescent waves. This is revisited...
4. RESULTS AND APPLICATIONS

here:

\[ p(x, y, z) = \frac{1}{4\pi^2} \int_{k_x} \int_{k_y} e^{i(k_xx + k_yy)} e^{jz(k^2_x-k^2_y)^{1/2}} \, dk_x \, dk_y. \] (4.2)

Equation (4.2) is the propagator from equation (2.1). The spatial frequency domain is originally infinite over both \( k_x \) and \( k_y \). However, since we deal only with propagating waves, the integration in equation (4.2) is limited over the range of \( k^2_x + k^2_y < k^2 \). Since we are dealing in this section with the modeling of dipoles, it is more convenient to rewrite our equations in polar coordinates [147]:

\[ p(\rho, \phi, z) = \frac{1}{2\pi} \int_{k_\rho} k_\rho J_0(k_\rho \rho \rho) e^{jz(k^2-k^2_\rho)^{1/2}} \, dk_\rho \] (4.3)

where \( \rho, \phi \), and \( z \) are the polar coordinates, \( k_\rho \) is the radial spatial frequency and \( J_0 \) is the Bessel function of the first kind of order zero. Equation (4.3) is the so called Hankel transform which acts as a radially symmetric Fourier transform. The condition for the propagating spherical waves is \( k^2_\rho < k^2 \). Since the dipole is placed in the middle of the scatterers, it is possible to convert many of the evanescent waves into propagating ones as long as the dipole is placed close to the scatterers. This is analogous to having a wide-angle lens placed extremely close to the object under test [148]. This in effect helps in capturing the high spatial frequency components and transform them to a smaller frequency range that can propagate.

It is worth mentioning that latency is a difficult obstacle that is being researched in the field of OPC. In recent work it has been shown that despite the dynamics of the sample under test it is possible to achieve a high intensity focus and to maintain that focus for approximately 200 ms for a system optimized to deal with this problem [149]. The authors of that work also suggest several possible additions and alterations to their setup that can enhance the overall performance even more.

4.4.2 Time reversal

The previous discussion is valid for the steady state-case. To enhance the focusing both in space and time, we need to take the time component into account. This is of particular interest in many fields where achieving high intensity by focusing light is only useful when done in time (e.g. two photon microscopy [2, 3], time-domain nonlinear spectroscopy [150], and coherent guiding of ions [151]). Other groups have investigated the focusing of light in both space and time experimentally [152]. In this section, this technique is simulated to have a more robust
way of testing further enhancements. There are two ways to simulate the effect of time reversal. The first is to generate results similar to the ones shown in Fig. 4.22 for multiple frequencies. Then, the time domain solution is obtained by mode-locking the steady-state results [76] as was explained in section 2.4. The disadvantage of this method is the numerical inefficiency considering the fact that we are using the FDTD method which already has the time-domain information. Therefore, using a Fourier transform to reach the steady-state and then going back to the time-domain after mode-locking is not the best way. The second method is to shape the input light before entering into the FDTD grid in the time-domain. This method is described here in more detail and some results are shown. We start by describing a pulse in time as

\[
\hat{E}_{z,inc}(t) = E_0 \exp\left(-\frac{(t-t_c)^2}{2\sigma^2}\right). \quad (4.4)
\]

Here \(\hat{E}_{z,inc}\) is the incident electric field in the angular domain with the same notation and definitions used in chapter 2 while \(t_c\) is a delay and \(\sigma\) is the standard deviation defined in this work as

\[
\sigma = \frac{\pi Z}{2\omega \sqrt{2 \log 2}}, \quad (4.5)
\]

where \(\omega\) is the angular frequency and \(Z\) is a parameter to control the temporal width of the beam. The information on how the pulse should look like is obtained from the far-field results of the outgoing dipole (similar to the experimental setup in [153] which uses the frequency-domain information for the time-domain pulse definition). The description of the pulse after being scattered is obtained by transforming the scattered near-fields to the far-field as explained in section 3.7. This method is used for a single frequency. We need to define the pulse in frequency-domain and shape that pulse. After that we transform the pulse back to the time-domain. The shaping of a time-domain pulse in the frequency-domain by applying a Fourier transformation is a well established method in linear filter theory which is commonly used in electrical engineering [154]. The time-domain pulse in equation (4.4) can be written in the frequency-domain as

\[
\hat{E}_{z,inc}(\omega) = \sigma \exp\left(-\frac{\sigma^2 \omega^2}{2}\right). \quad (4.6)
\]

If we use several plane waves incident with different angles with the time pulse in equation (4.6) after performing a Fourier transform, we get a lot of indistinguishable patterns due
to the interference of the plane waves, but we do not get a reversed dipole. This is due to the fact that the phases of the incident plane waves need to be corrected to take into account: 1. the position of the origin, 2. the prevention of sudden jumps in the differentiation of the electric field of the incident light (which is used to propagate the fields in the FDTD method), and 3. the phase disturbance caused by the scatterers. Several factors are introduced here to add these phase corrections. The first is

\[ C_n = \exp \left( -jk_n \frac{M \Delta}{2} \left( \frac{1}{\cos 45^\circ} - \frac{1}{\cos \theta} \right) \right), \quad (4.7) \]

where \( M \) is the number of cells in the total-field region in the FDTD grid in a single direction (assuming a square grid) and \( \Delta \) is the resolution. The factor \( C_n \) in equation (4.7) delays the incident plane wave such that all plane waves meet at the center of the grid. This transformation of the origin is important since the default origin in the FDTD is usually the corners of the grid.

When we transformed equation (4.4) from time to frequency domain in equation (4.6) we ignored the factor \( t_c \) to avoid having an imaginary part in the expression. However, this means that the resulting time domain pulse (after using inverse Fourier transform) in equation 4.6 would be centered around \( t = 0 \). This will cause an instability in the FDTD simulation since the fields near the edges of the grid will go from values of zero to the maximum possible value in the pulse. To avoid that, we introduce the factor \( D_n \) which causes a delay proportional to a constant \( D_e \):

\[ D_n = \exp \left( -jk_n D_e \right) \quad (4.8) \]

The larger \( D_e \) is, the later the pulse will be introduced into the grid. This will make the simulation run for a longer time but it will also preserve its stability. It is found that a good value for \( D_e \) is \( 20\sigma_0 c \). The final factor to be defined is

\[ E_n = \exp \left( -j\phi^*_n \left( \theta + 180^\circ \right) \right). \quad (4.9) \]

The factor \( E_n \) is the key element of this section. It introduces the conjugated phase \( \phi^* \) for each plane wave at a certain incident angle \( (\theta + 180^\circ) \). The addition of \( 180^\circ \) to the angle of incidence is necessary due to the reverse of the orientation of the axes between going out and then into the sample. Again, it should be noted that all the introduced factors are a function of
4.4 Time reversal and phase conjugation

frequency. The last step is to combine all these factors in equations (4.7), (4.8), and (4.9) into the Fourier transform:

\[
\hat{E}_{z,\text{inc}}(t, \theta) = \sum_{n} \hat{E}_{z,\text{inc}}(\omega_n, \theta) C_n D_n E_n \exp(j\omega_n t).
\]  

In Fig. 4.23 we can see a dipole at the point where we want to enhance the intensity. This source starts radiating a circular wave in time. Since the dipole is placed at an asymmetric position, the wave reaches the left edge of the grid earlier than the right one. These waves are detected with the NFFF from section 3.7 as was mentioned before. It should be noted that the wave-front on the left side shows less distortion compared to the right side. This is due to the shorter distance traveled in the scattering medium on the left side.

After time-reversing the fields in Fig. 4.24 we can see the waves entering first from the right-hand side since the wave-fronts need to travel a longer distance to reach the target point. In Fig 4.24e we can see the wave-fronts converging to the right spot both in space and time. It is interesting to see that the near-fields look perturbed on the right-hand side of the focus compared to the left-hand side. Again, this is mainly due to the necessity for much more spatial modulation of the wave-fronts coming from the right direction due to the larger distance traveled. The values used are \(n_m = 1, n_s = 1.33, r = 0.5 \mu m\) and \(\lambda = 1 \mu m\) which are identical to the parameters used in Fig. 4.23.

At certain points and at different times, it seems as if we get foci of high intensity away from the desired points. These are random speckles that appear mainly due to the scattering. This phenomenon is not related to the time reversal of the dipole, rather it is a characteristic of the geometry and distribution of the scatterers.

The speed of the developed code can be further enhanced by using a time-domain near- to far-field transformer [155]. Additionally, such a method has the advantage of having a continuous frequency spectrum which decreases the numerical errors. Also for simulating bigger grids, it is advantageous to use a pseudospectral time-domains (PSTD) solution. The time reversal of an ultrawideband signal has been studied recently using such a code [156]. On the other hand, the usage of the PSTD forces the usage of a Fourier transform followed by an inverse Fourier transform.
4. RESULTS AND APPLICATIONS

Figure 4.23: The intensity $[\text{W/m}^2]$ of a dipole propagating out of the point of interest to be detected using the NFFF. The parameters used are $n_m = 1$, $n_s = 1.33$, $r = 0.5 \text{ \mu m}$ and $\lambda = 1 \text{ \mu m}$.
4.4 Time reversal and phase conjugation

Figure 4.24: The intensity [W/m²] of a reversed dipole using the phase information from Fig. 4.23 trying to achieve focusing at the point $y = 0 \ \mu m$, $x = -4.75 \ \mu m$. In the case of $t = 75 \ \text{fs}$ we get the moment of best focus.
4. RESULTS AND APPLICATIONS

4.5 Carbon fiber

Carbon fiber-reinforced plastics (CFRP) are used in a strongly growing number of applications because of their high advantages in lightweight construction [157]. While their mechanical properties and their stability are very well studied in literature [158, 159], their optical properties are rather unknown.

The optical properties of CFRP will be of increasing interest in the near future because they are a prerequisite to better understand the interaction between an incident laser beam and the CFRP. This knowledge is very important for the optimization of laser processing of CFRP. Furthermore, the optical properties of CFRP are essential for design optimization.

A recent study of the polarization dependence of laser interaction with carbon fibers and CFRP has used a geometrical optics approach [160]. A variety of publications can be found about the index of refraction of different carbon structures [161]. Nevertheless, the refractive index was assessed only once for carbon fibers for a single wavelength in the visible range [162]. Dombrovskii calculated the absorption and scattering efficiencies for carbon fibers in the infrared [163]. Claybourn et al. found out that it is unsuitable to characterize carbon-fiber/polymer composites by specular reflectance [164].

In this work, we compare different methods of describing light propagation in carbon fiber assemblies and CFRP and compared the results of light propagation simulations with experiments. For the first time, solutions of the radiative transfer equation as well as of the exact Maxwell’s equations are implemented in this work for calculating the interaction of light with carbon fibers and CFRP. This study provided an interesting insight to the optical behavior of CFRP and revealed characteristics and details which had been unknown before. Furthermore, the comparison with experiments enabled an approximate assessment of the index of refraction of carbon fibers.

4.5.1 Comparison of different simulation models for light propagation in CFRP

The first goal of this study is to develop an appropriate simulation model for the calculation of light propagation and light reflection in carbon fiber structures since such a model did not

---

1. The multiple cylinder analytical code used in this section was programmed by Dr. Jan Schäfer for the purpose of simulating the scattering of a single incident plane wave by cylinders [55] and further developed and maintained for beams and scanning beams by the author.

2. The results from this section have been written to be submitted [49].

3. The reflectance measurements of polarized light were performed by my colleague Dr. Ansgar Hohmann.
exist yet. The high volume concentration of the fibers and the high imaginary part of the index of refraction are big challenges. For this purpose, the solution of the exact Maxwell theory is compared to a solution of the radiative transfer theory which is often an appropriate approximation to the Maxwell theory [165, 166]. Fig. 4.25 shows the investigated scattering scene for which light scattering is calculated by both methods for comparison. The scattering area (edge length $L = 40 \, \mu m$) is filled with scattering and absorbing cylinders corresponding to carbon fibers with a radius $r = 3.5 \, \mu m$ and an index of refraction of $n_{cyl} = 1.84 + 0.57j$. The volume fraction of the cylinders ($f_v$) is 0.61 which corresponds to a typical value for CFRP. The refractive index in the medium between the cylinders is set to $n_m = 1.0$ to simulate air around the carbon fibers after evaporation of the matrix. An incident Gaussian beam ($\lambda = 515 \, nm$) with a beam radius of $7.5 \, \mu m$ is modeled by both simulation methods (solution of Maxwell theory and solution of the radiative transfer theory). Two different polarizations of the incident beam are investigated. In the first case, the incident light is polarized parallel to the axes of the cylinders (TM case) while in the second case, the light is polarized perpendicular to the cylinders (TE case). The scattered light is detected for every scattering angle $\theta$.

![Figure 4.25: The setup of the carbon fiber simulations.](image)

The solution of the radiative transfer theory is solved using a Monte Carlo code \footnote{The Monte Carlo code was developed and maintained by Dr. Ansgar Hohmann.}. The principles of this method can be found in the literature [165]. In summary, the photons enter
on one side of the simulation volume according to a Gaussian distribution. They are scattered
or absorbed within the simulation volume with a specific probability depending on the Beer-
Lambert law (absorption coefficient and scattering coefficient) and the single cylinder phase
function resulting from Maxwell’s equations. An analytical solution of Maxwell’s equations for
the scattering of light by a single cylinder is used for calculation of the scattering coefficient $\mu_s$
and the absorption coefficient $\mu_a$ ($\mu_s = (C_{sca}f_v)/(\pi r^2)$, $\mu_a = (C_{ext} - C_{sca})f_v/(\pi r^2)$). $C_{sca}$ and
$C_{ext}$ denote the scattering and extinction cross sections respectively. The usage of the solution of
a plane wave incident on a single cylinder (Monte Carlo, PW on cyl.) is compared to the usage
of a single cylinder solution with a Gaussian beam incident on the cylinder (Monte Carlo, Gauss
on cyl.). The absorbed photons are registered together with their position within the medium
while the non-absorbed photons are registered in terms of angular resolution (see Fig. 4.25).
The analytical solution of the multiple cylinder theory is used to solve Maxwell’s equations
exactly [52, 55] as has been elaborated in section 2.3. Near-field as well as far-field solutions
are generated. The spatially dependent absorbed power density is calculated based on these
near-field and far-field solutions. In order to obtain realistic results for a comparison with the
experiments for the back-reflected part of the light in the far-field solution, a Gaussian beam
with a beam waist of 15 $\mu$m is used. The implementation of the Gaussian beam is necessary as
found out by comparisons with simulations with an incident plane wave. The deviations between
the two solutions (plane wave vs Gaussian beam) are shown in Fig. 2.7 in section 2.3.
The Gaussian beam is modeled with the ASPW method [33] as described in section 2.1. 31
plane waves are sufficient to model the beam appropriately. This number is relatively low due
to the small divergence angle of the beam used in this case ($\theta_{div} \approx 3^\circ$) and the large difference
between the beam waist and the wavelength which determines the minimum number of plane
waves needed according to equation (2.18). For a specific distribution of cylinders, the near-
fields exhibit pronounced speckles due to interference effects. In order to compare the results
to the measurements, 50 different spatial distributions of cylinders are generated and simulated
and the results are averaged. This approach corresponds to a simulation of an average CFRP.

4.5.2 Far-field results of the different simulation models and discussion

Fig. 2.7a and 2.7b in section 2.3 show the calculated differential scattering cross section of the
Gaussian beam incident on the scattering volume with a size of 40 $\mu$m by 40 $\mu$m for light
polarized parallel to the cylinder axis (Fig. 2.7a, TM case) and for light polarized perpendicular
to the cylinder axis (Fig. 2.7b, TE case). Large differences can be observed between the solution
4.5 Carbon fiber

of the radiative transfer theory and the solution of the Maxwell theory, especially if the scattering of a plane-wave on single-cylinder solution is used in the Monte Carlo solution of the radiative transfer theory. In the forward direction \((\theta = 0^\circ)\), a non-negligible fraction of the light is predicted to be transmitted through the carbon fiber sample (thickness: 40 \(\mu\)m) by the MC method. In contrast, according to Maxwell theory, almost no light is transmitted through the sample. In the backward direction \((\theta = 180^\circ)\), the remitted light determined by Maxwell theory exceeds the remitted light determined by the MC method using the plane-wave single-cylinder solution. These large differences show that taking into account interference effects is indispensable and hence, radiative transfer theory solved with a plane wave single cylinder solution is not appropriate for calculating the light propagation within carbon fiber structures or of the back-remission. The solution of the radiative transfer theory with an included Gaussian-beam single-cylinder solution gives better results in the backward direction, but the differences in the forward direction still exist.

A comparison of Fig. 2.7a and Fig. 2.7b shows that the differential scattering cross section in the backward direction is higher for light polarized parallel to the carbon fibers than for light polarized perpendicular to the carbon fibers. This means that more light is remitted in backward direction in the case of parallel polarization. The resulting scattering cross section is used to calculate the fraction of the remitted light in subsection 4.5.4.

4.5.3 Near-field results of the different simulation models and discussion

Fig. 4.26a shows the scattered light in a single realization of a carbon fiber sample \((n_m = 1.00, \: n_{cyl} = 1.84 + 0.57j)\). The position of the carbon fibers can be easily seen in the figure. It can be observed that only an extremely small part of the light enters the center of the carbon fibers and the part of the light which is not absorbed is scattered between the fibers.

The simulation results of the Maxwell method are averaged over 50 spatial distributions to get a model for a randomly distributed CFRP. Then the absorbed power in this average CFRP sample is calculated. Fig. 4.26b shows averaging for the scattered light while Fig. 4.27 shows the calculated absorbed power per unit volume in an average carbon fiber sample \((n_m = 1.00, \: n_{cyl} = 1.84 + 0.57j)\) as a function of the depth on a line below the incident point (which is defined as the point illuminated by the center of the Gaussian beam) for four different solution methods:
4. RESULTS AND APPLICATIONS

- Beer’s law for the absorption coefficient \( (\mu_a = 848.131 \text{ mm}^{-1}) \) calculated by standard Beer-Lambert law using the imaginary part of the index of refraction and the volume density of the carbon fibers \( \mu_a = 4\pi f_v \text{ Im}(n_{cyl})/\lambda \). This expression without the term \( f_v \) is often used for calculation of the absorption coefficient of homogeneous media in literature (labeled as “Lambert-Beer” in Fig. 4.27).

- Beer’s law for the absorption coefficient \( (\mu_a = 89.851 \text{ mm}^{-1}) \) calculated from the single cylinder absorption cross section and from the volume fraction by the following formula: \( \mu_a = (C_{ext} - C_{sca}) f_v / (\pi r^2) \). The light is assumed to hit the boundary of the simulation volume from one side and the internal decrease of power per unit volume is assumed to follow Beer’s law (labeled as “Lambert-Beer (Maxwell)” in Fig. 4.27).

- Radiative transfer theory: The light is assumed to hit the boundary of the simulation volume from one side with a Gaussian beam shape (Fig. 4.25). The MC technique is used to simulate light propagation within the simulation volume using an absorption coefficient of \( \mu_a = 89.851 \text{ mm}^{-1} \) and a scattering coefficient of \( \mu_s = 139.961 \text{ mm}^{-1} \) calculated from the single cylinder absorption and scattering cross sections by the formulas given above.

**Figure 4.26:** \( \log_{10} \) of the intensity of the scattered light [a.u.] in the 40 by 40 \( \mu \text{m} \) carbon fiber sample calculated by the Maxwell solution (polarization parallel to the carbon fibers) using 50 different realizations to average the results. The results are normalized by the intensity of the incident Gaussian beam.
4.5 Carbon fiber

Figure 4.27: Absorbed power density in the 40 by 40 µm carbon fiber sample according to four different simulation models (polarization parallel to the carbon fibers).

(labeled as “Monte Carlo” in Fig. 4.27).

- Maxwell theory: The analytical solution of the multiple cylinder theory is used to simulate light propagation within the simulation volume, assuming the Gaussian beam to hit the simulation volume (labeled as “Maxwell” in Fig. 4.27).

The Lambert-Beer (Maxwell) as well as the Monte Carlo model are also implemented and simulated using a Gaussian-beam single-cylinder solution instead of a plane-wave single-cylinder solution. A comparison between the usage of these different single-cylinder solution methods shows only very small differences of the power density within the material. Because of that, the Gaussian-beam single-cylinder solution has been omitted in Fig. 4.27 for clarity and readability.

This comparison between the four simulation models facilitates the assessment of the influence of the applied simulation model on the calculated absorbed power per unit volume in the carbon fiber sample. The Lambert-Beer model (green in Fig. 4.27) with the absorption coefficient determined by the standard Lambert-Beer law shows extremely strong absorption near the surface where the beam hits the sample. The comparison with the solution of the exact Maxwell
4. RESULTS AND APPLICATIONS

The MC model (blue in Fig. 4.27) shows that this model could therefore lead to misleading results if it is applied to calculation of the absorption coefficient in non-homogeneous media like carbon fiber composites. The MC model (dotted red in Fig. 4.27) and the Lambert-Beer (Maxwell) model (magenta in Fig. 4.27) give comparable results for the power density despite the fact that only the latter takes into account both the scattering and the absorption coefficients, while the first takes only the absorption coefficient into account. Nevertheless, the comparison of these two models with the Maxwell model shows that these two methods do not lead to correct results. The power density is underestimated near the surface while it is overestimated for higher penetration depths. While the light penetrates up to 15 µm in the medium according to the MC model, the exact Maxwell model demonstrates that almost no light is left at the same penetration depth. This is in agreement with the results shown in Fig. 2.7a and 2.7b (from section 2.3), where the MC model overestimates the light transmitted through the sample as well. These results show that the exact Maxwell solution cannot be approximated by common light propagation models such as the radiative transfer theory to calculate light propagation in carbon fiber structures. If light propagation and light absorption in CFRP or remission in the backward direction from CFRP is to be calculated, the Maxwell method has to be the method of choice. Because of that, the Maxwell method is chosen in the following subsection to calculate the remission of light from CFRP in backward direction.

A possible explanation for the discrepancy between the MC simulations which are based on the transport theory and the Maxwell solution is the dependence of the field intensity on the scatterers distribution. For low values of the imaginary numbers in the refractive index, usage of the MC method gives comparable results to the Maxwell solution as long as the proper phase function is used and if the other limitations of the MC method are taken into account (e.g. low concentration of scatterers). However, for high values of the imaginary part of the refractive index the light optimizes its own transmission channels through the medium to avoid the parts with reflections. This is done by avoiding the points of absorption, meaning the scatterers themselves. This results in a dependency of the field intensity on the distribution of the scatterers. Obviously, this is not possible in MC since the entire medium is homogeneous. This relation between absorption and the inhomogeneity of the medium has been shown in a recent study [50]. To show this effect, four samples with the same distribution of the scatterers are shown in Fig. 4.28. The comparison starts with low and high scattering scenarios in the absence of absorption in Fig. 4.28a and 4.28b, respectively. It can be seen in the first case that the light beam maintains most of its collimation through the first two cylinders. After that a
focus - or the so called jet - is formed due to the focusing effect of the scatterers which is in effect similar to having a lens. In the latter case, the collimation of the beam is lost almost immediately and the light focus is formed much earlier. This is due to the higher scattering. In Fig. 4.28c, the imaginary part of the refractive index is slightly increased. This absorption helps guiding the light in between the scatterers, which decreases the randomness in the Poynting vector directions shown in Fig. 4.28b. However, since the reflection of the light away from the scatterers is still small, it can be seen that there is still some power that goes through them. By increasing the reflection in Fig. 4.28d, no light goes through any of the scatterers. In this case, the positions of the scatterers can be estimated - even after removing the indicators of their positions - by looking at the points with no intensity. Furthermore, in Fig. 4.28d, the Poynting vectors are being guided through the direction with the least absorption, which guides the light to the backward direction. This explains why it is possible to get a higher intensity in the forward direction in the MC when compared to the Maxwell solution. This spatial relation between the Poynting vector direction and the position of the scatterers cannot be modeled in a method that depends on the homogeneity of the medium as is the case for the MC method.

Both Fig. 4.28c and 4.28d are shown again in Fig. 4.29 with an extended scale to show more of the details of the light propagation deep inside the sample. The minimum of the scale is at $10^{-16}$, so the light intensity is low enough that it can be neglected in an experiment. Nonetheless, by looking at how the light is avoiding the discrete positions of the scatterers in Fig. 4.29b, we get further proof that using the solution of Maxwell’s equations is necessary in this case.

4.5.4 Measurements of remitted light from CFRP in the backward direction

During laser processing of CFRP, the processing laser needs some time to remove the material which consists of carbon fibers surrounded by matrix material. The evaporation temperature of the matrix material is rather small (e.g. 800 °C) with respect to the evaporation temperature of carbon fibers (e.g. 3600 °C) [48]. Because of that, a laser-processed surface of a CFRP contains only the fibers as the matrix near the surface has already been evaporated. If a laser hits this surface, only the fibers and the surrounding air determine the remitted light from the surface. For investigation of this case, CFRP samples provided by the Institut für Strahlwerkzeuge at Stuttgart University (IFSW) are used. The type of carbon fibers contained in this CFRP sample is Tenax-E HTS40. These samples are processed by the IFSW with a laser so that the fibers at the surface are exposed as in common laser processing as described before. The samples are irradiated perpendicularly to the sample surface and the remitted light
4. RESULTS AND APPLICATIONS

(a) $n_s = 1.1$.

(b) $n_s = 1.84$.

(c) $n_s = 1.84 + 0.1j$.

(d) $n_s = 1.84 + 0.57j$.

Figure 4.28: A Gaussian beam with beam-waist of 15 $\mu$m illuminating a sample of parallel cylinders of diameter equal to 7 $\mu$m. The wavelength is 515 nm and the matrix containing the cylinders is vacuum ($n_m = 1$). The beam is incident from the left hand side of the sample. The color bar represents the logarithm to base 10 of the intensity of the light ($|E_z|^2$) while the blue arrows show the direction of the Poynting vector. The incident Gaussian beam is normalized to have a maximum intensity of 1 and a beam waist of 15 $\mu$m.

is detected angularly resolved in the backward half-space using a goniometric setup. A super-continuum light source is used to produce white light. An acoustic-optical tunable filter selected the wavelength of 515 nm from this light. A polarization filter is used to generate the incident light parallel (TM case) or perpendicular (TE case) to the carbon fibers in the sample. Before
4.5 Carbon fiber

(a) \( n_s = 1.84 + 0.1j \).

(b) \( n_s = 1.84 + 0.57j \).

Figure 4.29: The same intensity and Poynting vectors as in Fig. 4.28c and 4.28d but with an extended scale to show more details deep in the sample.

Each measurement, a reference measurement is performed with a spectralon sample with defined absorption (for the necessary normalization) to enable quantitative measurements. The resulting angularly resolved intensity of the back-remitted light is normalized such that the differential scattering cross section could be calculated by transforming the 3-D measurement results to a 2-D differential scattering cross section. Fig. 4.30a (Fig. 4.30b) shows the differential scattering cross section for light polarized parallel (perpendicular) to the carbon fibers calculated from the measurements. The plotted graphs in Fig. 4.30a and 4.30b correspond to the averaged value over 6 different single measurements each. These goniometric measurement results are used to determine the fraction of back-remitted light from the sample surface. For incident light polarized parallel to the fiber direction, the fraction of back-remitted light is \((6.05 \pm 0.38)\%\) while for light polarized perpendicular to the fiber direction, it is \((3.65 \pm 0.41)\%\). Integrating sphere measurements are performed to validate these measurements: The fraction of back-remitted light is observed to be \((5.98 \pm 0.28)\%\) for light polarized parallel to the fiber direction and \((3.77 \pm 0.17)\%\) for light polarized perpendicular to the fiber direction. These values are both within the standard deviations determined by the goniometric measurements. As stated before, the main purpose of this work is the investigation of laser processed carbon fiber samples with removed matrix. However, for comparison, the previous back-remission measurements using the integrating sphere setup are performed also on the unprocessed carbon fiber surface, where
the matrix covers the carbon fibers. The back-remission values are higher because of Fresnel reflection as integrating sphere measurements have shown: In this case, when the surface of the matrix is slightly polished, \((7.90 \pm 0.36)\%\) of the parallel polarized light is back-remitted, while \((6.11 \pm 0.28)\%\) of the perpendicular polarized light is back-remitted. The relatively small difference of only 2\% to the values for a laser processed surface for both polarizations could be explained by the different index of refraction mismatch between fibers and surrounding material and by the matrix-to-air boundary which also reflects a part of the light coming from inside the sample back into the material.

Figure 4.30: Measurement and simulation of the differential scattering cross section of a carbon fiber sample irradiated by a Gaussian beam with a beam waist of 15 \(\mu\)m (\(\lambda = 515\) nm).

4.5.5 Results and discussion of the measurements and comparison with simulations

Fig. 4.30a and 4.30b show the angularly resolved differential scattering coefficient calculated by the analytical solution of Maxwell’s equations for three different refractive indices for the carbon fibers. Altogether, the calculations are performed for 11 different indices of refraction of the carbon fibers for each polarization and averaged over 50 realizations each. Thereby, the real part as well as the imaginary part of the refractive index of the carbon fibers are varied. Despite the high computational resources needed this method still proved more efficient than
4.5 Carbon fiber

using other numerical solutions of Maxwell’s equations such as the FDTD method. This is due to the high fiber volume concentration (which limits our usage of the MC method) and the high absorption (which limits our usage of the FDTD due to the shorter plasmon wavelength as was discussed in section 2.3). A selection of three results ($n_{cyl} = 1.84 + 0.57j$, $1.84 + 1.07j$ and $1.64 + 0.57j$) is shown in Fig. 4.30a and 4.30b for clarity’s sake. An assumed index of refraction of $n_{cyl} = 1.84 + 0.57j$ of the carbon fibers leads to the best agreement between the simulation and the experimental results. This refractive index corresponds to a fraction of the back-remitted light of 5.95% for light polarized parallel to the fiber direction and 3.97% for light polarized perpendicular to the fiber direction.

These values correspond best to the measured values of back-remitted light of (6.05 ± 0.38)% for incident light polarized parallel to the fiber direction and (3.65 ± 0.41)% for incident light polarized perpendicular to the fiber direction. This shows that an index of refraction of $n_{cyl} = 1.84 + 0.57j$ is a good approximation for the index of refraction of the carbon fibers used in this study. Ségur et al. [162] have measured the index of refraction of two types of carbon fibers. They found for an XN05 fiber (diameter: 10 µm) an index of refraction of $n_{cyl} = 1.9 + 0.7j$ and for a UMS40 fiber (diameter: 5 µm) an index of refraction of $n_{cyl} = 2.3 + 0.6j$ for a wavelength of 796 nm. The elastic modulus of their XN05 fiber corresponds best to the elastic modulus of the carbon fiber we used while their UMS40 fiber has a higher elastic modulus.

Therefore, we compare in the following our results to the results of their XN05 measurements. For amorphous carbon, the real part of the index of refraction is reported to be 1.96 for 796 nm and 1.82 for 515 nm (difference: 0.14) [167, 168, 169]. The imaginary part is reported to be 0.80j for 796 nm and 0.70j for 515 nm (difference: 0.10) [167, 168, 169]. It is assumed that these differences in the index of refraction approximately also hold true for carbon fiber structures which are not amorphous. Under this assumption and if these differences due to the different wavelengths are taken into account, the results of our assessment method of the index of refraction of the carbon fibers are not in contradiction to the measurements of Ségur et al. [162]. Pluchino et al. [170] reported for carbon particles with a radius between 3.1 µm and 4.7 µm and a wavelength of 488 nm for the real part of the index of refraction values between 1.6 and 1.8 and for the imaginary part of the index of refraction value between 0.5j and 0.8j. These numbers deviate from our results, but they still lie within the same range as our values for the index of refraction of carbon fibers.

Another application of the results of Maxwell simulations is the investigation of the effects of different incident angles or a different incident beam. In Fig. 4.31 the absorbed light is shown
for three different incident angles. It is vital to use a broader grid for the larger incident angle (30 µm by 80 µm compared to 40 µm by 40 µm in the other simulations) since otherwise the light would have entered from the side of the sample, making the traveled distance through the scattering material shorter. And that would make the comparison invalid when compared to the other tilting angles. It can be seen in Fig. 4.31a and 4.31b that for small tilting of the incident beam, the distribution of the absorbed energy is almost the same inside the grid. For larger angles, obviously the light does not get the chance to travel deep in the direction perpendicular to the surface, it rather moves in the lateral direction.

Fig. 4.32 shows the far-field results for the tilted beams compared to the non tilted beam and furthermore, the scattering by a radially polarized beam is also shown. Such a beam can be implemented using the equations introduced in section 2.1.4 in the scheme of the analytical solution found in section 2.3. It can be noticed that for the back-scattered light, tilting the beam has almost no effect (unless the angle is too large). For the radially polarized beam, we can see that the back-scattered light is weaker than in the case of the linearly polarized beam (≈ 1.58 times). This agrees with the enhanced penetration depth of such a beam which means less back-reflected light.

The sharp peaks found at the angles that correspond to the direction of each beam are numerical artifacts. They are not actual errors, rather they appear (despite the fact that we have no forward scattering) since we are here examining the scattered light. From the definition found in section 3.3, the scattered light is the total light minus the incident undisturbed light. We always find such a peak with a 180°-phase shift in the forward direction of the beam.
4.5 Carbon fiber

Figure 4.31: Absorbed light for a Gaussian beam rotated by $\theta_{\text{tilt}}$. 

(a) $\theta_{\text{tilt}} = -7.5^\circ$. 

(b) $\theta_{\text{tilt}} = -15^\circ$. 

(c) $\theta_{\text{tilt}} = -60^\circ$. 

Figure 4.32: Differential scattering cross section results [log_{10}(value)] for a Gaussian beam incident on a carbon fiber sample with different tilting directions. The radially polarized beam has a tilting angle of 0°.

4.6 The direct extinction method

4.6.1 Principle - *in vacuo*

The 2-D setup sketched in Fig. 2.2 is simulated: The focused beam (as described in section 2.1) propagating in the x-direction is focused by an aplanatic microscope objective so that the divergence angle is \( \theta_{\text{max}} = 65^\circ \), which lies beyond the paraxial limit. This corresponds to a numerical aperture of NA= 0.9 in air or NA= 1.2 in water and it is relatively common for modern confocal microscope objectives. As an example, we consider a monochromatic beam with a wavelength \( \lambda = 1 \mu m \). MC simulations are carried out in a square-shaped sample with a detection grid resolution of 200 grid points in the x- and y-directions with a grid spacing of \( \Delta x = \Delta y = \lambda/25 \). As in the ASPW model, Fresnel reflection at the sample interfaces is

\[�\text{The results from this section have been published in [57] except subsection 4.6.3.}\]
\[�\text{The MC simulations were performed by my colleague Arnd Brandes}\]
neglected, i.e. the refractive index of the sample is assumed to be equal to that of the surrounding medium \((n_{\text{sample}} = n_{\text{air}} = 1)\). Since we are dealing with non-scattering materials, the MC simulations are confined to sampling “target positions” from the normalized probability distribution \(p_v(r)\) calculated with the ASPW method where 41 plane waves are superimposed. In vacuo, \(p_v(r)\) simply expresses the probability of finding a photon at a position \(r\). The sampling is achieved with the rejection method. First, a pseudorandom position \(r_i\) is drawn. Pseudorandom numbers are generated with the Mersenne Twister algorithm [171]. The corresponding probability density \(p_v(r_i)\) at position \(r_i\) is compared with a pseudorandom number \(\xi \in (0, 1)\): If the number is such that \(\xi > p_v(r_i)\), the position is rejected and the sampling is repeated.

![Figure 4.33: Comparison of the probability distributions yielded by the MC simulations (the number of sampled “target positions” are \(10^6\) and \(10^9\) on the left and on the right, respectively) and the FDTD simulations for the linearly polarized beam focused in vacuo in the \(x\)-direction. These distributions are displayed here in logarithmic scale over the range \(8\lambda \times 8\lambda\). The MC simulations are shown for \(y/\lambda > 0\) and FDTD simulations for \(y/\lambda \leq 0\) for both figures. The blue curves are cross-sections of the probability profiles at the focal plane \(x = x_{ph} = 4\lambda\), while the green curves are cross-sections of the FDTD results.](image)

In order to assess the accuracy of our results, we conducted independent FDTD simulations. To remain consistent with the MC simulations, 41 plane-waves are propagated with incidence angles in the range of \([-\theta_{\text{max}}, +\theta_{\text{max}}]\). For a given incidence angle \(\theta\), an expression of the electric field at \(r_0\) is obtained from the ASPW calculations (e.g. from equation (2.14) in the case of linearly polarized waves). All FDTD simulations throughout this section are performed with a resolution of \(\lambda/25\) and \(\lambda = 1\ \mu\text{m}\).

Results obtained with MC and FDTD simulations for a linearly polarized beam propagating
4. RESULTS AND APPLICATIONS

Figure 4.34: Comparison of the probability distributions displayed here in logarithmic scale over the range $8\lambda \times 8\lambda$ and yielded by the MC simulations (with $10^9$ “target positions” sampled) and the FDTD simulations (grid size $8\lambda \times 32\lambda$) for the linearly polarized beam focused in the $x$-direction in increasingly absorbing media. From left to right and top to bottom: $\mu_a = (16\lambda)^{-1}$, $(8\lambda)^{-1}$, $(4\lambda)^{-1}$ and $(2\lambda)^{-1}$ (the corresponding values for the imaginary component $\kappa$ of the material’s refractive index are $(64\pi)^{-1}$, $(32\pi)^{-1}$, $(16\pi)^{-1}$, and $(8\pi)^{-1}$, respectively). The curves are cross-sections of the probability profiles at the focal plane $x = x_{ph}$ (MC in blue and FDTD in green).

In vacuo are shown in Fig. 4.33. In this section, all simulation results are displayed after normalization by the probability density value at the focal point $(x = x_{ph}, y = 0)$ of the simulation in vacuo, denoted by $p_{v,0}$ and $p'_{v,0}$ for the linearly and radially polarized beams, respectively. Both types of simulations are performed with the same grid dimensions. The agreement between the two sets of data serves as a verification to the implementation of both the MC and the FDTD algorithms.

Besides, as the FDTD method accounts for the near field interactions, we can verify here the formation of the Fraunhofer diffraction patterns in the vicinity of the focal plane. However, we stress here the main constraint inherent to the MC technique: the amount of sampling should be large enough to provide reasonable convergence.

4.6.2 In absorbing media

As a following step, we compare the MC and FDTD simulations in the presence of absorption. The MC simulations are performed with a square-shaped detection grid of dimensions $8\lambda \times 8\lambda$, such that the focal plane of the focused beam is located at $x_{ph} = 4\lambda$.

Four types of samples are considered with each sample having a different absorption coefficient.
4.6 The direct extinction method

$4.6 \text{ The direct extinction method}$

Figure 4.35: Quantitative representation of the results shown in Fig. 4.34. The probability profiles corresponding to the different absorbing materials are cross-sections close to the illumination face (left), at $x = 0.01\lambda$ and in the focal plane at $x = x_{ph} = 4\lambda$ (right).

$$(16\lambda)^{-1} \leq \mu_a \leq (2\lambda)^{-1}.$$ Note that despite the large absorption values, we omit re-emission here, heat transfer etc., since these do not contribute to the present study.

We proceed according to the extinction method by sampling “target positions” from $p_a(r)$ instead of $p_v(r)$. These “target positions” bear a slightly different significance when absorption is involved: $p_a(r)$ represents the probability to find a photon in the sample at position $r$ before it gets absorbed along its path (defined in section 2.6.2).

Simulation results obtained with the four types of samples are shown in Fig. 4.34 and more detailed profiles from the same results are shown in Fig. 4.35. It can be seen that good agreement is achieved between the MC and the FDTD simulations. Nonetheless, closer inspection reveals the appearance of discrepancies both close to the illumination surface of the sample and in the focal region (the latter case cannot be seen in the figures shown here, but it has been observed for instance in the case of beams focused with a divergence angle of $\theta_{max} = 25^\circ$). Since similar discrepancies have been observed, no matter which divergence angle $\theta_{max}$ taken for the beam, the most plausible explanation for the differences is the presence of Fresnel reflection in the FDTD simulations. In the FDTD model, the plane waves propagate from air into the sample whose refractive index has a non-zero imaginary component. However, as mentioned earlier, the MC simulations are implemented assuming that there is no refractive index mismatch along the
4. RESULTS AND APPLICATIONS

path of the plane waves. Another reason for the discrepancies could be numerical artifacts of the FDTD simulations, namely the projection of oblique waves to a rectangular grid and the finite resolution.

4.6.3 In scattering media

As mentioned before, scattering can also be modeled using the direct extinction method (section 2.6.4). This is further proven by comparing the results of equation 2.21 with FDTD simulations in section 4.2 after substituting for $\mu_t$ instead of $\mu_a$. It is shown then that this model works quite well assuming low concentration of scatterers and relatively low scattering. Under these assumptions the impact of multiple and dependent scattering is weak.

In this section, three examples for beams of different profiles and polarizations are shown. For each of those beams both the in-vacuo case is shown (Fig. 4.36) as well as the scattering case of $\rho_s = 10 \mu m$ (Fig. 4.37). The first scenario shown in Fig. 4.36a is a linearly polarized Gaussian beam with a beam waist of $\omega_o = 1 \mu m$. To get a beam which is linearly polarized in the $x$-direction the $\psi$-angle is substituted in equation (2.27) with the value of $\phi + 90^\circ$. Fig. 4.36d shows a beam with the same parameters like the previous one but polarized radially. To achieve such a polarization, $\psi$ is substituted in equation (2.27) with the value of $90^\circ$. Finally, a Bessel beam is shown in Fig. 4.36c. Such a beam is formed by taking an annular range of angles in the angular description as has been done in 2-D in section 2.1.3. In this simulation $\theta_{max} = 15^\circ$ while $\Delta \theta = 3^\circ$. The wavelength is $1 \mu m$ while the resolution is $0.3 \lambda$. Increasing the resolution does not affect the accuracy of the results since each pixel is completely independent of the rest of the medium which is one of the main advantages of the direct extinction method. A slice every $20 \mu m$ is taken in the depth direction and then the results are interpolated to get the images of the propagation. This is possible in the case of non-scattering media due to the high symmetry in the beams and the slow deviations in the intensity. Both the Gaussian and the ring beam show a great amount of focusing. The depth of field in both cases did not exceed $20 \mu m$. The Bessel beam on the other hand showed a much greater depth of field as expected.

For the scattering case shown in Fig. 4.37, $\rho$ is set to $10 \mu m$. In the case of the Bessel beam, the resolution is increased to $0.1 \lambda$ to enhance the visibility of the rings surrounding the main beam. In Fig. 4.37a we can see that the Gaussian beam has a very uniform distribution (compared to the other beams) away from the focus. A small gap appears in the center of the beam away from the focal plane. This is due to the fact that we look at a plane while the beam itself has a certain curvature due to its focusing. In Fig. 4.37c the radially polarized
4.6 The direct extinction method

- (a) Gaussian beam.
- (b) Focused beam.
- (c) Bessel beam.
- (d) Radially polarized beam.

**Figure 4.36:** The normalized intensity of the $E_x$-component for a Gaussian (a), a focused (b), and a Bessel (c) beam and the intensity of the lateral component of the electric field ($I_r = |E_x|^2 + |E_y|^2$) for a radially polarized beam (d). All beams are formed using equation (2.27) while propagating in a non-scattering medium ($n_m = 1$). For the Gaussian and the radially polarized beams, the beam waist is set to 1 μm. In each case the desired focus depth is 40 μm. All the beams are normalized to the maximum intensity for each individual case and the scale is logarithmic.
4. RESULTS AND APPLICATIONS

Figure 4.37: The normalized intensity of the $E_x$-component for a Gaussian (a), a focused (b), and a Bessel beam (c) and the normalized intensity of the lateral component of the electric field ($I_r = |E_x|^2 + |E_y|^2$) for a radially polarized beam (d). All beams are formed using equation (2.27) while propagating in a scattering medium of $\rho = 10 \mu m$. For the Gaussian and the radially polarized beams the beam waist is set to 1 $\mu m$. In each case the desired focus depth is 40 $\mu m$. All the beams are normalized to the maximum intensity for each individual case and the scale is logarithmic.
beam keeps its main property which is the null intensity in the middle of the beam, both before and after going through the focal plane. Contrary to the previous two beams, the Bessel beam in Fig. 4.37c keeps its structure almost entirely intact throughout its propagation. It suffers mainly from losing intensity due to scattering. In a full 3-D Maxwell solution of the Bessel beam it is expected that the drop in intensity will not be that dramatic due to the reconstruction capabilities which is still under investigation [172]. Comparing a high-NA focused beam (θ_{max} = 45°) in Fig. 4.37b to a smaller NA beam like the Gaussian beam in Fig. 4.37a confirms that we do get higher resolution in the former case. However, by comparing the two cases of small- and high-NA beams quantitatively it is found that the lower NA beams gives higher intensity at higher depths compared to the high-NA beams. This is in accordance with our 2-D results [82] in section 4.2 (Fig. 4.12). The only difference between the 2-D and the 3-D cases is the higher overall intensity found in 3-D since we are dealing then with a solid angle.

4.6.4 Direction of the Poynting vectors

In this section, the orientation of the Poynting vectors \( \mathbf{S}(r) \) is calculated with both MC and FDTD simulations. In the MC method, the Poynting vector is calculated according to Sec. 2.6.3, averaged over a bin of sub-wavelength size \( \Delta x \times \Delta y \). On the other hand, in the FDTD simulations the Poynting vector is determined from the resulting electric and magnetic fields at a certain grid point \( (x, y) \) at the end of the simulation, see equation (2.24).

The results obtained by focusing a linearly polarized beam is shown in Fig. 4.38. Again, very good quantitative agreement is achieved between the two data sets. However, differences can be seen in the vicinity of the focal plane, in particular in the darker regions of the probability distribution where destructive interferences occur. In those regions, the orientation of the Poynting vector varies considerably over a bin, in which case the averaging with the MC method does not yield results identical to the FDTD simulations. In other regions where discrepancies are not visible, the orientation of the Poynting vector remains relatively constant over a bin and thus, the averaging produces identical results to the FDTD simulations. Moreover, the effect of the aforementioned Fresnel reflection included in the FDTD calculations and neglected in the MC simulations should not be excluded in the interpretation of the differences.

Additionally, results yielded by the focusing of a radially polarized beam are shown in Fig. 4.39: The corresponding Fraunhofer diffraction pattern differs noticeably from that of the previous example. As for the Poynting vectors in Fig. 4.39 the remarks on Fig. 4.38 still hold true. Here however, the detected power distribution depends then on the resulting electric field from both
4. RESULTS AND APPLICATIONS

Figure 4.38: Direction of the normalized Poynting vectors $\mathbf{S}(r)$ plotted over probability distributions displayed here in logarithmic scale over the range $3\lambda \times 3\lambda$, and calculated with both MC simulations ($10^9$ “target positions” sampled) and FDTD simulations (grid size of $8\lambda \times 32\lambda$). Left: The linearly polarized beam is focused in vacuo. Right: The same beam is focused in an absorbing medium, where $\mu_a = (2\lambda)^{-1}$. In MC simulations, the binning size is kept at $\Delta x = \Delta y = \lambda/25$.

$E_x$ and $E_y$. Furthermore, the tight focusing of the radially polarized beam leads to a strong longitudinal electric field component in the $x$-direction in the focal region, and the Poynting vector vanishes (as can be seen from the FDTD simulations on the left of Fig. 4.39). 

[173, 174, 175]
4.6 The direct extinction method

Figure 4.39: A radially polarized beam is focused in vacuo. On the left: Distribution of the non-normalized Poynting vectors $\mathbf{S}(\mathbf{r})$ plotted over the probability distribution displayed here in logarithmic scale over the range $4\lambda \times 4\lambda$ and calculated with FDTD simulations (grid size of $8\lambda \times 32\lambda$). On the right: same distribution of the normalized Poynting vectors obtained with both MC simulations ($10^8$ “target positions” sampled) and the FDTD simulations plotted over the probability distribution displayed here in logarithmic scale over the range $8\lambda \times 8\lambda$. The Poynting vectors are normalized in the figure on the right to better show the results in regions with extremely small intensity (the points of destructive interference).
4. RESULTS AND APPLICATIONS
High-resolution microscopy has been an important research topic for a long time due to its applications in many fields in science, industry and in particular in biomedical optics. Many of the high resolution microscopy techniques like confocal microscopy [1], two photon microscopy [2, 3], and optical coherence tomography (OCT) [4] depend on focusing of the illumination light into a tight spot at the point of interest. The focusing of the beam has the advantage of increasing the resolution of the microscope but it increases the measurement time since it becomes necessary to scan the focus in order to get a full image of the considered sample. Accordingly, to simulate the interaction between a scattering sample and the incident scanning light beam, the simulation needs, in principle, to be run for every position of the scanned focus. This can be extremely time consuming. In this work, an efficient technique is introduced which models the scanning of a beam through a scattering medium using a numerical solution of Maxwell’s equations.

In a previous study, focused beams have been modeled with the finite-difference time-domain method (FDTD) using the angular spectrum of plane waves approach (ASPW) [18, 19]. This method has been used to study the scattering of a focused beam by biological tissue [176] and to investigate optical projection tomographic microscopy [177]. In this work, the ASPW method has been used to model the incident focused light as a summation of plane waves in two dimensions. The method of scanning the focused beam based on the addition of an extra phase to the calculated near-fields caused by each individual plane wave has been introduced. This method allows the beam to be shifted without the need to resimulate the beam propagation again. Thus, the calculation time is strongly reduced at the expense of larger memory requirements. The theoretical treatment of this method is introduced in section 2.2. By simulating a beam using this method (as shown in section 4.1) it can be seen that although the method works
5. DISCUSSION AND OUTLOOK

quite well for simulating the scanning of a focused beam, special care needs to be taken while trying to simulate a scattering medium that is infinite in a certain direction since an abrupt end to the scatterers before a certain limit will give erroneous results. This limit can be mainly decided upon by examining the maximum divergence angle and the wavelength of the incident beam.

The ASPW method is also used to simulate the scanning of several beam profiles through scattering media in section 4.2. The simulated beams are focused beams of varying types (Gaussian, Bessel, and sinc-like beams). For the latter beam, several maximum divergence angles are used. It is observed that for focusing light in scattering media, the focus intensity of a high-NA beam decreases faster versus depth than it is the case for a small-NA beam. The FDTD simulations demonstrate that at a certain depth in the scattering medium, the total intensity at the focus position (including both the non-scattered and the scattered light) is larger e.g. for the focused beam with \( \theta_{\text{max}} = 25^\circ \) compared to the focused beam with \( \theta_{\text{max}} = 45^\circ \). However, due to the high amount of the necessary calculation time (for large depths and thus, large simulation areas) the FDTD simulations do not show, whether this is also the case for the focus intensity of the non-scattered light at high depth which is the important quantity for many microscopical applications. Hereupon, we have used a simple mathematical model to calculate the intensity profile for the non-scattered light versus depth and lateral positions. It shows that for large depths, the focus intensity of the non-scattered light is larger for the low-NA beam that for the high-NA one, e.g. about twice as large for the focused beam with \( \theta_{\text{max}} = 25^\circ \) compared with the focused beam with \( \theta_{\text{max}} = 45^\circ \). In addition, we showed that for a large focus depth the lateral profile of the non-scattered intensity of the low-NA beams approaches that of the high-NA beams resulting in a similar resolution when used in a microscope. As such, it is better to use a less focused beam or a Gaussian beam since these beams avoid the unnecessary illumination of larger volume. Having a tool based on Maxwell’s equations means that it is possible to simulate wave phenomena like interference and dependent scattering.

Being able to study the effect of depth-scanning of the focus of beams facilitates the study of methods that can enhance the penetration depth of said beams. In section 2.5, the concept of phase optimization, where the wave-front of the incident light is spatially modulated is introduced. By simulating such a technique in section 4.3 we see that the phase optimization can be understood as the propagation of the plane waves that constitute the incident light while insuring the optimal constructive interference of those plane waves. Furthermore, it is shown that after scanning a beam deep enough inside a scattering medium and after optimizing the
phase of said beam, it does not matter what kind of beam is used since the optimization works mainly locally around the point of interest, meaning that all beams lose their defining features (their profiles) in the focal plane. Further studies are needed to overcome the most prominent problem that phase optimization faces, \textit{i.e.} speed. Investigations in the optimization algorithm show promising results, \textit{e.g.} by using a microgenetic optimization scheme \cite{[178]} that shows faster and more reliable results compared to the classic iterative algorithms \cite{[28]}.

Another method that is used to get the information about the proper phase needed to modulate the incident light is phase conjugation or the so-called time reversal technique where a source inside the scattering medium is used as a beacon to be detected outside of the medium after being scattered. The detected wave is then time-reversed by conjugating its phase, making the wave propagate back to its source point. The results from section \ref{section:4.4} show how valuable the ASPW is in modeling such techniques which can help in understanding the results from the experiments. The simulations are shown for both the steady-state case which is ideal for studying monochromatic light and for time-domain situations when a pulsed light is preferable. The developed code simulates the grid efficiently since there is no need to simulate a bigger grid just to reach the far-field regime. Rather, we use a combination of the ASPW method and the near- to far-field transformer (NFFF) to get the desired values to shape the time-revered pulse.

It is shown in section \ref{section:2.3} that despite contrary expectations, strong inaccuracies occur if light propagation in carbon fiber structures is modeled by the radiative transfer theory or other common approximation methods. To avoid these problems, light propagation in carbon fibers had to be modeled by solving the exact Maxwell’s equations in section \ref{section:4.5}. Furthermore, it could be shown by reflectance measurements of polarized light (performed by my colleague Dr. Ansgar Hohmann), that the reflectance agrees best with Maxwell’s simulations if an index of refraction of $1.84 + 0.57i$ is assumed for the carbon fibers. This is a reasonable value for carbon fibers at a wavelength of 515 nm. A further conclusion is that the amount of reflected light is strongly dependent on the polarization of the light incident on the carbon fiber sample.

The feasibility of modeling the tight focusing of beams with MC simulations based on the “direct extinction method” is investigated in section \ref{section:4.6} (The MC simulations are performed by my colleague Arnd Brandes), where “target positions” for the photon paths are sampled from probability distributions calculated separately with the ASPW technique. The simulations present an efficient tool to examine some of the wave properties of the light (\textit{e.g.} Fraunhofer diffraction pattern, polarization state, and the direction of the energy flow) in the focal region of
a high-aperture system. Unlike the FDTD simulations, the MC method presented here imposes much looser limitations on the dimensions of the observed sample.

Naturally, the accuracy of the results depends not only on the spatial resolution, but also on the number of sampled positions and the number of plane waves used. While the FDTD grid has to be fine enough to avoid numerical artifacts, the MC binning can be broadened to a limit given by the theorem of Nyquist-Shannon ($<\lambda/2$). Although the modeling of the focusing of a collimated beam with a uniform profile in the angular domain has been chosen here, more intricate beam profiles (Gaussian, Bessel, etc.) can easily be implemented as shown in section 4.2.

Likewise, it can be concluded from this proof of concept in vacuo and in absorbing media that the direct extinction method using attenuated plane waves yields a very good approximation when treating problems involving absorption. Certainly, including Fresnel reflection phenomena would be of particular importance in a next step. Another significant improvement would be the treatment of scattering processes within the medium in which the beam is focused. A preliminary investigation has been undertaken here by calculating the direction of the energy flow in the vicinity of the focal region. This highlights a meaningful advantage of this method. It is shown that this alternative MC approach can also account for waves that show longitudinal components (non transverse electromagnetic waves (TEM)). The modeling of such longitudinal components is part of the limitations of existing vectorial MC programs: this necessitates the development of new adequate models, as initiated by Azzam. The usage of the direct extinction method for a scattering medium is also possible, taking into account that there are restrictions on the extent of the scattering to avoid dependent scattering.

The current work helps in exploring several avenues for future investigations and developments. The entire protocol for the simulation of beam propagation and its scanning through scattering media needs to be further extended for the 3-D case. Other groups have already made steps in that regard (only for the modeling of 3-D beams, not for the simulation of the scanning of said beams) and also in this work in section some examples for 3-D beams have been given. However, in all these cases the simulation grid could not be made large enough to simulate a real situation since the computational resources needed by the FDTD are too much. There are three ways from the author’s perspective to tackle this problem. The first is the usage of other numerical methods that - for the most part - keep the advantages of the FDTD while having the ability to simulate bigger grids. A prime example for that is the pseudo-spectral time-domain method which has already shown great performance in simulating macroscopic dimensions of optical problems. The second way to simulate bigger grids (in
2-D or 3-D) is to use analytical solutions of light scattering. Such a solution is well-suited for a low volume concentration problem since in such a case, the run time depends mainly on the number of scatterers. A code developed by Mackowski and Mishchenko can already simulate large 3-D grids of spherical scatterers [180]. However, this solution has some limitations when dealing with beams. If a Gaussian beam is used, the beam waist cannot be comparable to the wavelength because then, the code fails to converge correctly ($k\omega_0$ must be larger or equal to 5, where $\omega_0$ is the beam waist). The third way is to use the direct extinction method for turbid media as shown in section 4.6.3. This solution obviously introduces some restrictions, mainly to avoid dependent scattering which cannot be modeled using this method.

The analytical solution used in section 4.5 proved to be highly useful when examining the intensity distributions of light incident on carbon fibers. It is also advantageous that the near field solution does not require a high resolution grid to converge. Nonetheless, the code should be developed further to have an adaptive resolution grid to have better visibility in the parts of greater interaction, e.g., in the vicinity of the fibers, and lower resolution in places of less importance, e.g., at the core of the fibers where the light does not reach in the first place.

The purpose of all of these suggestions is to enhance the already developed tools. However, there are several studies that can be made using these tools. Assuming the development of a faster way to simulate the ASPW description of a beam, it will be possible to repeat the study of the intensity of the beam focus versus depth that is performed in section 4.2 but for larger depths and in 3-D. This will give a more realistic model to be compared to biological tissue. It is also necessary to use the simulations of time-reversed dipole to further our understanding of the interactions occurring during this process and to apply these new ideas in real life experiments that can help in enhancing the field of microscopy. Integrating an acoustic model in the simulation would furthermore enable better modeling of photoacoustic systems.
5. DISCUSSION AND OUTLOOK
References


REFERENCES


REFERENCES


REFERENCES


114


REFERENCES


REFERENCES


31
REFERENCES


REFERENCES


120


REFERENCES


REFERENCES


REFERENCES


CURRICULUM VITAE

PERSONAL INFORMATION

Name
AHMED Elmaklizi

Address
2 Am Hochsträß
Ulm, 89081, Germany

Telephone
+49–1639287620

E-Mail
ahmed.desoki@gmail.com

Nationality
Egyptian

Date of birth
18 May 1987

LinkedIn profile
de.linkedin.com/in/AhmedElmaklizi

PROFESSION

▷ Period

◦ Employer

Laser Institute for Medicine and Meteorology – University of Ulm
12 Helmholtz, Ulm, 89081, Germany

◦ Position
PhD candidate / CAE engineer in the field of optics and electromagnetic

▷ Project May 2012 until December 2013

Main responsibilities

• The development of a finite-difference time-domain method code using Matlab
• Modeling focused beams
• Enhancing the speed of the simulation for raster scan microscopes

▷ Project May 2013 until September 2015

Simulation of shearing interferometry system

Main responsibilities

• Developing a Beer – Lambert model for focused beam
• Using the developed model to simulate Michelson interferometer illumination setup
• Simulating shearing interferometry for detection of fluorescent light

▷ Project July 2013 until February 2015

Study of light propagation in Carbon fibers
Main responsibilities

- Developing a Matlab to solve analytically light scattering by cylinders
- Deducing the refractive index of Carbon Fibers by comparing simulation results with experiments

February 2014 until September 2015

Main responsibilities

Enhancement of light intensity in scattering media

Simulating spatial light modulator devices (SLM) and MEMs to achieve wave front shaping to enhance the intensity inside scattering media. This is done by the optimization of the phase of the light incident on the media

EDUCATION

Period

April 2010–May 2012

Master of Science (M.Sc.) in Communication Engineering track of Microelectronics

Laser Institute for Medicine and Meteorology – University of Ulm

Analytical and Numerical Analysis of Electromagnetic Scattering using Gaussian and Focused Beams

RF and Microwave Engineering, Monolithic Microwave ICs in High-Speed Systems, Laser, Laser-Matter Interactions, Integrated Microwave Circuits, Numerical Methods in Microwave Techniques

1.8 out of 1

- The optimization of multiple resonance slot antenna using the tool HFSS as part of a student job
- Simulating a 60 GHz CMOS transceiver system using the tool ADS as part of the course of MMIC

Period

September 2005 – April 2010

Bachelor of Science (B.Sc.) in Information Engineering and Technology

Department of Microwave engineering – German University in Cairo

Enhancement of antennas using Metamaterials


1.67 out of 0.7

- Investigating Metamaterials for microwave applications (generic filters, couplers and antenna)
- The design, optimization, manufacture and measuring of an UWB antenna
TRAINING, INTERNSHIPS AND TEACHING

- **2012 – 2014**: Ulm University – laser Institute
  Two years teaching experience in a supplementary course on FDTD simulation method

- **2013**: University of Ulm and Max Plank Institute for plasma physics
  Two courses in plasma physics followed by a lab course

- **2011**: Ulm University – Laser Institute
  Six month student job in studying and simulating the Mie theory for light scattering

- **2010**: Ulm University – Microwave department
  Six month student job in antenna design and optimization

- **2009**: German University in Cairo
  Two month training in microstrip design, manufacturing and testing of antennas in the electromagnetic waves lab

- **2009**: Vodafone Egypt
  Three month training in the Network Management Center (NMC), GPRS team with “very good” cardinals and high recommendations of the team leader to join the company

- **2008**: German University in Cairo
  Two semesters of teaching electric circuits lab

- **2008**: German University in Cairo
  One semester of teaching an introduction to Matlab

- **2008**: Egyptian Company for Airports and Air Navigation
  Two month training in the communication engineering department

LANGUAGES

- **Mother tongue**: Arabic

- **First language**: English
  - **Certificate**: TOEFL score: 103/120

- **Second language**: German
  - **Certificate**: fair-B2 level

CONFERENCES
2014
International Conferences on Laser Applications in Life Sciences (LALS) in Ulm, Germany

2013
The 14th Electromagnetic and Light Scattering in Lille, France

2013
6th International Graduate summer school - Biophotonics ‘13 in Island of Ven, Sweden

ABILITIES

SOCIAL AND ORGANIZATIONAL SKILLS
Presentations, and communication skills, fast reader, experience with team working

TECHNICAL SKILLS

• Matlab/Simulink
• HFSS and HFSS designer
• ADS circuit designer
• CST
• Java
• Blender

PUBLICATIONS

Publication
Ahmed Elmaklizi, Dominik Reitzle, Arnd Brandes, and Alwin Kienle: *Penetration depth of focused beams in highly scattering media investigated with a numerical solution of Maxwell’s equations in two dimensions* Journal of Biomedical Optics, 2015

Publication
Ahmed Elmaklizi, Jan Schäfer, and Alwin Kienle: *Simulating the scanning of a focused beam through scattering media using a numerical solution of Maxwell’s equations* Journal of Biomedical Optics, 2014

Publication

Ulm, August 3, 2015

Ahmed, Elmaklizi