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Master's thesis

Modeling of passive and active optical periodic structures

Modelování pasivních a aktivních optických periodických struktur

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Periodic systems and nanostructures find wide applications in optics, photonics, and also in the field of semiconductor light sources and lasers. Optical behavior of passive periodic structures can be modeled by Fourier modal methods. Due to progress in spin-lasers and light emitting diodes, there is a need for development of models for description of periodic structures with active sources. The main targets of the Master thesis are:

1. Understanding of the Rigorous Coupled Wave Analysis (RCWA) method and its application in passive one-dimensional (1D) grating structures.
2. Modeling of reflection, transmission, polarization properties, and diffraction from the periodic grating structures with anisotropic materials.
3. Calculation of optical response from active multilayers with active dipole sources.

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T. Fördös, et al, Eigenmodes of spin vertical-cavity surface-emitting lasers with local linear birefringence and gain dichroism, Phys. Rev. A 96, 043828 (2017).

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Abstrakt

Tato diplomová práce se zabývá vývojem nových přístupů k modelování anisotropních vrstevnatých struktur obsahující aktivní vrstvy a periodické laterální 1D mřížky. K modelování periodických mřížek je použita metody vázaných vidů (RCWA) a modely zdrojových vrstev vycházejí ze 4×4 maticového formalismu vhodného k modelování spin-polarizovaných elektroluminiscenčních diod (spin-LEDs) a spinových laserů s vertikální uspořádáním (spin-VCSELs). Pro umožnění kombinace těchto dvou přístupů je vyvinut nový formalismus k modelování šíření nekoherentního světla v periodických strukturách založený na koherenčních/Muellerových maticích, který je demonstrován na struktuře flexibilních difrakčních komponent obsahující tlusté vrstvy. Modely zdrojových struktur jsou poté vyjádřeny pomocí stejného formalismu, který zahrnuje nekoherentní procesy a umožňuje integraci periodických i zdrojových vrstev v rámci jednoho modelu.

Klíčová slova: RCWA, aktivní vrstvy, spin-LED, spin-VCSEL, periodické mřížky, nekoherentní šíření, koherenční matice, Muellerovy matice

Abstract

This thesis deals with the development of new approaches for modelling of multilayers with active dipole layers and 1D lamellar gratings. The rigorous coupled wave algorithm (RCWA) is used for modelling of periodic gratings and models of active dipole layers are based upon 4×4 matrix formalism suitable for modelling of spin-polarized light emitting diodes (spin-LEDs) and vertical-cavity surface-emitting lasers (spin-VCSELs). To enable the combination of these two approaches a new formalism for modelling of incoherent propagation in periodic structures based on coherence/Mueller matrices is introduced and it is demonstrated on the structure of flexible diffraction components that include thick layers. Models of active dipole layers are then expressed using the same formalism that enables the integration of both periodic and active layers in the same model.

Keywords: RCWA, active layers, spin-LED, spin-VCSEL, lamellar gratings, incoherent propagation, coherence matrix, Mueller matrix

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List of symbols and abbreviations

VCSELs	Vertical-cavity surface-emitting lasers
spin-LEDs	Spin-polarized light emitting diodes
spin-VCSELs	Spin-polarized vertical-cavity surface-emitting lasers
HCG	High contrast gratings
RCWA	Rigorous coupled wave analysis
MEs	Maxwell equations
$\mathbf{E}(\mathbf{r}, t)$	Electric field intensity vector
$\mathbf{H}(\mathbf{r}, t)$	Magnetic field intensity vector
$\mathbf{D}(\mathbf{r}, t)$	Electric displacement vector
$\mathbf{B}(\mathbf{r}, t)$	Magnetic flux density vector
$\rho(\mathbf{r}, t)$	Charge density
$\mathbf{j}(\mathbf{r}, t)$	Current density vector
ε_0	Permittivity of free space
μ_0	Permeability of free space
$\hat{\varepsilon}_0$	Relative permittivity tensor
$\hat{\chi}$	Electric susceptibility tensor
$\mathbf{P}(\mathbf{r}, t)$	Polarization density vector
$\mathbf{M}(\mathbf{r}, t)$	Magnetization density vector
$\mathbf{I}$	Identity matrix of proper dimension
$\hat{\sigma}$	Electric conductivity tensor
ω	Angular frequency
i	Imaginary unit
$\hat{\varepsilon}_R$	Complex permittivity tensor
ε	Permittivity tensor
E_0	Complex electric field amplitude
H_0	Complex magnetic field amplitude
$\mathbf{e}$	Electric field polarization vector
$\mathbf{h}$	Magnetic field polarization vector

$\mathbf{k}$	Wave vector
k_0	Free space wave vectro amplitude
n	Index of refraction
$\mathbf{r}$	Position vector
φ	Incidence angle
θ	Azimuth angle of the incidence plane
$\mathbf{E}'(\mathbf{r}, t)$	Normalized electric field intensity vector
$\mathbf{H}'(\mathbf{r}, t)$	Normalized magnetic field intensity vector
E'_0	Normalized complex electric field amplitude
H'_0	Normalized complex magnetic field amplitude
$\mathbf{e}'$	Normalized electric field polarization vector
$\mathbf{h}'$	Normalized magnetic field polarization vector
c	Speed of light
$\nabla \times$	curl operator
N_i	i-th part of index of refraction (see Eq. (2.22a))
$\mathbf{f}(z)$	Vector of the tangential components of the field vectors
$\mathbf{C}$	Matrix of the eigenvalue problem
λ_i	Eigenvalue of a matrix
$\mathbf{v}_i$	Eigenvector of a matrix
$\alpha, \beta, \gamma, \delta$	Coefficients of linear combination
$\mathbf{D}$	Eigenvalue matrix
$\mathbf{A}$	Amplitude of propagating eigenmodes
$\mathbf{P}$	Propagation matrix of a layer
d	Width of a layer
$\mathbf{n}$	Normal vector of the interface
$\mathbf{J}$	Surface current density
$\mathbf{M}$	Total transfer matrix
r_{ij}	Reflection coefficients
t_{ij}	Transmission coefficients
T_{ij}	Transmittance
R_{ij}	Reflectivity
$\mathbf{S}(\mathbf{r}, t)$	Poynting vector, S-matrix
T	Period

$\Re$	Real part
$\Im$	Imaginary part
c_{ij}	Fourier coefficient
$\hat{c}_i$	Tensor of i-th order Fourier coefficients of permittivity tensor
$\tilde{\cdot}$	Vector or matrix consisting of many fourier harmonic modes
E_{ij}	Toeplitz matrix of Fourier coefficients
$\ \cdot\ $	Operation of creating oeplitz matrix from Fourier coefficients
$\dot{\mathbf{t}}, \dot{\mathbf{r}}, \dots$	Backward coefficients
$\mathbf{J}_c$	Coherence matrix
$\mathbf{J}$	Coherence vector
$\mathcal{T}, \mathcal{J}, \mathcal{R}, \mathcal{P}, \mathcal{G}$	Coherence-transforming matrices of corresponding quantities
$\mathbf{B}$	Propagation transforming matrix
$\mathbf{A}^d$	Amplitude source vector
$\mathbf{T}$	Source matrix

1. Introduction

Vertical-cavity surface-emitting lasers (VCSELs) are important part of many technologies today. They dominate the light source market for data communication such as Gigabit Ethernet and Fiber Channel. They are ideal light sources in data centers, high-performance computers, optical interconnects, automotive networks, optical mice and high definition displays [1–8]. The high popularity of VCSEL lasers is due to its advantages, such as low operating current and power consumption, high fiber coupling efficiency and high modulation bandwidth. They are also ideal for 2D laser arrays due to their size. Their advantages lie also in the economical side of things because they are cheap and easily manufactured by the same processes as the traditional integrated parts. Furthermore, a new generation of spin-polarized light sources is approaching due to advances in the field of spintronics. The recombination of spin-polarized carriers in spin-polarized light sources leads to emission of polarized light and gives us a better control over the polarization of emitted light. Spin-polarized light-emitting diodes (spin-LEDs) [9–11] are already used in the experimental spintronics and spin-VCSELs [12,13] promise lower threshold [14], better polarization control [15] and faster modulation dynamics [16]. For future applications of spin-VCSELs, a precise modelling of light emission and its polarization is required and some models have already been presented [17,18]. This model is based on the combination of 4×4 Yeh's matrix formalism [19,20] and the description of active dipole layers done by Benisty [21] and the model has already been successfully used to model spin-VCSELs structures.

Another important trend in further development of VCSELs is the research of periodic structures, such as gratings or photonic crystals, in VCSEL structures. Photonic crystals are used for controlling of a single transverse mode operation and low far field divergence angle of output beam of VCSEL lasers, that is important for efficient coupling into optical fibers [22–24]. Photonic crystals can also be used for polarization control of VCSELs [25]. By designing photonic crystals with non-cylindrical holes, dichroism can be introduced and polarization control achieved. Besides photonic crystals, high contrast gratings can be also used to improve existing VCSELs designs [26,27]. High-contrast gratings (HCG) act as a high reflectivity monolayer and

can replace top distributed Bragg reflectors (DBR) in VCSELs. They are considerably thinner than conventional DBR and have high polarization dependence. They also suppress higher order transverse modes and operate in single mode. Another benefit of using HCGs in VCSEL designs is that they can be etched in post-epitaxial fabrication process. As the phase of reflected light of the HCG depends on grating parameters, by changing the grating parameters we can change the resonance wavelength. This enables the fabrication of the multi-wavelength VCSEL arrays [28]. The modelling of periodic structures can be done by several methods. In this thesis, we are adopting the rigorous coupled wave analysis (RCWA) for its good applicability in modelling of far field scattering. It is a semi-analytical Fourier-space method first developed by Moharam et. al. [29] and then further developed by the important work of Li [30–32] and Nevière and Popov [33–35]. The algorithm of RCWA is still being developed further for more arbitrary dielectric profiles and is now also being used for aperiodic structures [36,37].

There has already been done some work to combine models of periodic and active layers [38], however, these models do not address coherence of emission processes. As spontaneous emission inside active layers is an incoherent process, the model also needs to incorporate the incoherent effects during propagation through multilayers. This is usually done by averaging over random phase factor. This is, however, computationally highly demanding and not practical for application in grating structures that need to include sufficient number of harmonic modes to converge properly and the number of parameters for averaging rapidly increases. The alternative to modelling of incoherent effects by averaging over random phase is the use of intensity-based approaches, like the coherence matrix and Mueller matrix formalisms. Coherence and Mueller matrices are often used for modelling of incoherent propagation in the layered structures [39] and they have also already been used for modelling of incoherent propagation in periodic systems by Antoš et. al. [40]. Nevertheless, their approach does not treat higher diffraction modes rigorously and rigorous treatment of incoherent propagation needs to be developed.

1.1 Objective of this work

The goal of this thesis is to develop a general formalism for description of incoherent effects in active layers and layers with lateral periodicity in order to efficiently model light emission from spin-VCSELs with periodic layers (1D lamellar gratings, photonic crystals) for possible future applications. This is done in two steps. First, by combining RCWA (only 1D gratings for simplicity) with the coherence matrix methods to model incoherent propagation in multilayers containing thick layers, and second, by expressing the existing multilayer models of spin-polarized

emission developed by Fördös *et. al.* [17, 18] using the coherence matrix formalism to avoid averaging over a random phase factor.

1.2 Organization of the thesis

The thesis is organized into four chapters. Chapter 2 deals with the basic theory of light propagation in multilayer structures. Maxwell equations, that are used in the rest of the thesis, are formulated and all the assumption made in this thesis are stated. Then the solution of Maxwell equations for layered structures is derived. The chapter ends with description of experimental observables of layered structures.

Chapter 3 is devoted to modelling of 1D gratings by RCWA. First, the eigenmodes propagating in periodic layers are found. Then the boundary conditions are applied using scattering matrix algorithm (S-matrix). Fourier factorization is also discussed and the chapter ends with description of experimental observables in grating structures.

Chapter 4 introduces a new approach of modelling incoherent light propagation in layered structures by combining the intensity-based coherence matrix algorithms with RCWA. First, the partial wave summation method and coherence matrix formalism for modelling of incoherent propagation in thick layers are described. Then they are generalized for periodic layers. The results of the algorithm are then described on numerical models of flexible diffractive components.

Chapter 5 is devoted to modelling of emission from active multilayers. Previous models developed by Fördös *et. al.* [17], Postava *et. al.* [38] and the details of incoherent processes relevant for integration with RCWA are described. Then the models are expressed using coherence matrix formalism and the the new approach is compared with the original in numerical models of a simple LED structure.

Chapter 6 concludes by summarizing main original results of the thesis and presents perspectives for the future research.

2. Propagation of light in a layered media

The aim of this section is to mathematically describe how light propagates in layered media without any lateral periodicity, so it can be later generalized for 1D gratings. First the basic relations, describing propagation of light, and formulation of Maxwell equations (MEs) is introduced. Then all assumptions are stated and relations, on which optical models are based, are derived from MEs and the concept of the polarization is briefly introduced. In the section 2.2 the solution of the Maxwell equations in layered media is described and in Section 2.2.1 the solution for a special case of isotropic media is derived. Section 2.2.2 deals with solutions in separate layers and layers are connected by boundary conditions. Then the relations of calculated quantities with experimental observables are described.

2.1 Basic relations

2.1.1 Maxwell equations

The light propagating through a medium can be described by the Maxwell equations in terms of the electric and magnetic field intensities $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{H}(\mathbf{r}, t)$, the electric displacement $\mathbf{D}(\mathbf{r}, t)$ and the magnetic flux density $\mathbf{B}(\mathbf{r}, t)$ [41, 42]. They are in form

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = \rho(\mathbf{r}, t), \quad (2.1a)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0, \quad (2.1b)$$

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t}, \quad (2.1c)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} + \mathbf{j}(\mathbf{r}, t), \quad (2.1d)$$

where $\mathbf{j}(\mathbf{r}, t)$ is the current density and $\rho(\mathbf{r}, t)$ is the volume density of free charges. The electric and magnetic intensities are related to the electric displacement and the magnetic flux density

by the constitution relations as follows:

$$\mathbf{D}(\mathbf{r}, t) = \varepsilon_0 \mathbf{E}(\mathbf{r}, t) + \mathbf{P}(\mathbf{r}, t), \quad (2.2a)$$

$$\mathbf{B}(\mathbf{r}, t) = \mu_0 \mathbf{H}(\mathbf{r}, t) + \mu_0 \mathbf{M}(\mathbf{r}, t). \quad (2.2b)$$

μ_0 and ε_0 are the vacuum permeability and permittivity. $\mathbf{P}(\mathbf{r}, t)$ and $\mathbf{M}(\mathbf{r}, t)$ represent the polarization and the magnetization, respectively. In this work, we are dealing with optical frequencies, so we can assume

$$\mathbf{M}(\mathbf{r}, t) = 0. \quad (2.3)$$

In homogeneous non-dispersive medium the polarization vector can be expressed using the electric susceptibility tensor

$$\mathbf{P}(\mathbf{r}, t) = \varepsilon_0 \hat{\chi} \mathbf{E}(\mathbf{r}, t). \quad (2.4)$$

By using relative dielectric tensor $\hat{\varepsilon}_r$, expressed as

$$\hat{\varepsilon}_r = \mathbf{I} + \hat{\chi}, \quad (2.5)$$

where $\mathbf{I}$ is 3x3 identity matrix, and substituting 2.3 and (2.4) into (2.2a) and (2.2b) we get

$$\mathbf{D}(\mathbf{r}, t) = \varepsilon_0 \hat{\varepsilon}_r \mathbf{E}(\mathbf{r}, t), \quad (2.6a)$$

$$\mathbf{B}(\mathbf{r}, t) = \mu_0 \mathbf{H}(\mathbf{r}, t). \quad (2.6b)$$

Furthermore, we assume that there are no free charges in the medium.

$$\rho(\mathbf{r}, t) = 0 \quad (2.7)$$

Next, we can express the electric current density as a function of $\mathbf{E}(\mathbf{r}, t)$ and the electric conductivity tensor $\hat{\sigma}$.

$$\mathbf{j}(\mathbf{r}, t) = \hat{\sigma} \mathbf{E}(\mathbf{r}, t) \quad (2.8)$$

Using these expressions and assumptions, we get the Maxwell equations in the following form:

$$\nabla \cdot [\varepsilon_0 \hat{\varepsilon}_r \mathbf{E}(\mathbf{r}, t)] = \rho(\mathbf{r}, t), \quad (2.9a)$$

$$\nabla \cdot \mathbf{H}(\mathbf{r}, t) = 0, \quad (2.9b)$$

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t}, \quad (2.9c)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \varepsilon_0 \hat{\varepsilon}_r \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} + \hat{\sigma} \mathbf{E}(\mathbf{r}, t). \quad (2.9d)$$

In this thesis, we take into account only monochromatic waves. Under this assumption we can express the electric and magnetic field vectors as harmonic functions of time as follows:

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}) \exp(-i\omega t), \quad (2.10a)$$

$$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r}) \exp(-i\omega t). \quad (2.10b)$$

The use of this form of the electric and magnetic field vectors simplifies equations (2.9c) and (2.9d). Furthermore, by excluding the time dependence we get

$$\nabla \times \mathbf{E}(\mathbf{r}) = i\omega\mu_0\mathbf{H}(\mathbf{r}), \quad (2.11a)$$

$$\nabla \times \mathbf{H}(\mathbf{r}) = -i\omega\varepsilon_0\hat{\varepsilon}_r\mathbf{E}(\mathbf{r}) + \hat{\sigma}\mathbf{E}(\mathbf{r}). \quad (2.11b)$$

For more compact description of the media response, we can define the complex permittivity tensor as

$$\hat{\varepsilon} = \varepsilon_0\hat{\varepsilon}_r + \frac{i}{\omega}\hat{\sigma} = \varepsilon_0\hat{\varepsilon}_R \quad (2.12)$$

This definition simplifies the relation (2.11b) even more, so that

$$\nabla \times \mathbf{H}(\mathbf{r}) = -i\omega\hat{\varepsilon}\mathbf{E}(\mathbf{r}). \quad (2.13)$$

The complex permittivity tensor describes optical properties of any homogenous anisotropic medium including absorbing media, where absorption is described by the imaginary part of the complex permittivity tensor.

2.1.2 Polarization of light

In this work, we are describing far field processes like reflection and transmission by using several matrix methods. For this purpose it is useful to assume monochromatic plane wave solution, which corresponds to collimated light emitted from a far source [41,42]. We can describe such a wave by the complex representation of the field intensity vectors as follows:

$$\mathbf{E}(\mathbf{r}, t) = E_0\mathbf{e} \exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)], \quad (2.14a)$$

$$\mathbf{H}(\mathbf{r}, t) = H_0\mathbf{h} \exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)], \quad (2.14b)$$

where E_0 and H_0 denote the complex amplitudes of the field vectors. The vectors $\mathbf{e}$ and $\mathbf{h}$ represent the polarization state of the propagating wave, ω denotes the angular frequency of the wave and the vector $\mathbf{k}$ is the wave vector. Assuming a planar interface between two isotropic

media according to the Figure 2.1, we can describe the wave vector $\mathbf{k}$ as

$$\mathbf{k} = k_0 n \begin{bmatrix} \sin \phi \sin \varphi \\ \cos \phi \sin \varphi \\ \cos \varphi \end{bmatrix}. \quad (2.15)$$

The physical (measurable) electromagnetic field is then described as the real part of the field vectors (2.14a) and (2.14b).

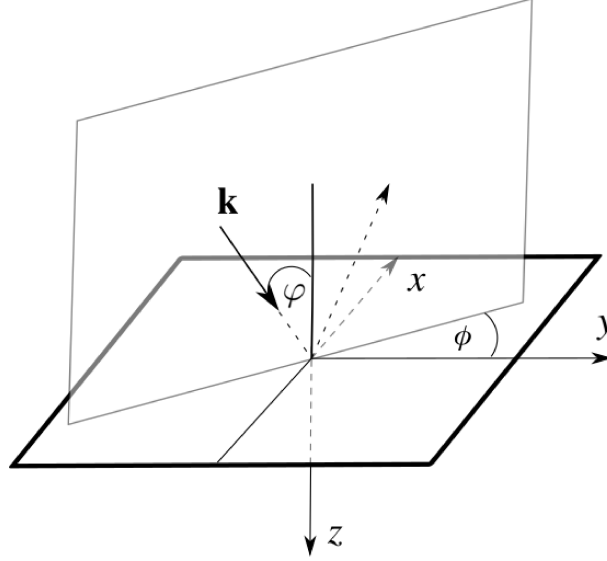


Figure 2.1: Light propagating on a boundary and the coordinate system used in the following sections

In any isotropic medium the field intensity vector $\mathbf{E}(\mathbf{r}, t)$ is always in the plane orthogonal to the propagation direction, but it can take different directions inside this plane. Vector components of $\mathbf{E}(\mathbf{r}, t)$ can have different amplitudes and phases. In the most general case, the endpoint of $\mathbf{E}(\mathbf{r}, t)$ traces an ellipse in the plane orthogonal to the direction of propagation. This elliptical polarization becomes circular for the same amplitudes and the phase difference $\pi/2$ and becomes linear when the components are in phase. Different polarizations behave differently when propagating through optical systems due to the boundary conditions at interfaces as we can see in Section 2.5. In the case of anisotropic media, there always exist four different linearly independent eigenmodes with different polarizations (two propagating forward and two backwards), which can be obtained by solving the Maxwell equations as discussed in Section 2.3. For the description of behaviour for different polarizations s- (TE, transversal electric) and p- (TM, transversal magnetic) polarizations are often used. For s-polarization the field vector is perpendicular to the plane of incidence, whereas for p-polarization the field vector lies in the

plane of incidence. According to Figure 2.1, normalized s- and p- polarization vectors can be described as

$$\mathbf{e}_s = \begin{bmatrix} \cos \phi \\ -\sin \phi \\ 0 \end{bmatrix}, \quad \mathbf{e}_p = \begin{bmatrix} \sin \phi \cos \varphi \\ \cos \phi \cos \varphi \\ -\sin \varphi \end{bmatrix}. \quad (2.16)$$

2.2 Solution of the Maxwell equations in layered medium

To understand the propagation of light through an anisotropic layered media, first we need to find a solution of the Maxwell equations in each individual layer. In this section, we introduce a matrix formalism developed by Berreman [44].

The electric and magnetic field vectors can be normalized in the following way:

$$\mathbf{E}'(\mathbf{r}) = \sqrt[4]{\mu_0^{-1}\varepsilon_0} \mathbf{E}(\mathbf{r}), \quad (2.17a)$$

$$\mathbf{H}'(\mathbf{r}) = \sqrt[4]{\mu_0\varepsilon_0^{-1}} \mathbf{H}(\mathbf{r}). \quad (2.17b)$$

Using the relations

$$k_0 = \frac{\omega}{c}, \quad (2.18a)$$

$$c = \frac{1}{\sqrt{\mu_0\varepsilon_0}}, \quad (2.18b)$$

and substituting relations (2.17a) and (2.17b) into (2.11a) and (2.13) we get a new form of the normalized Maxwell equations

$$\nabla \times \mathbf{E}'(\mathbf{r}) = ik_0 \mathbf{H}'(\mathbf{r}), \quad (2.19a)$$

$$\nabla \times \mathbf{H}'(\mathbf{r}) = -ik_0 \hat{\varepsilon}_R \mathbf{E}'(\mathbf{r}). \quad (2.19b)$$

This normalized form of Maxwell equations is later useful for obtaining a simple eigenvalue solution in a compact form, which is directly connected to the physical quantities and flows nicely into the boundary matrix methods. Using the matrix form of curl operator

$$\nabla \times \begin{bmatrix} H'_x(r) \\ H'_y(r) \\ H'_z(r) \end{bmatrix} = \begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{bmatrix} H'_x(r) \\ H'_y(r) \\ H'_z(r) \end{bmatrix}, \quad (2.20)$$

we can express the equations (2.19a) and (2.19b) as follows:

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{bmatrix} E'_x(r) \\ E'_y(r) \\ E'_z(r) \end{bmatrix} = ik_0 \begin{bmatrix} H'_x(r) \\ H'_y(r) \\ H'_z(r) \end{bmatrix}, \quad (2.21a)$$

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{bmatrix} H'_x(r) \\ H'_y(r) \\ H'_z(r) \end{bmatrix} = -ik_0 \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \begin{bmatrix} E'_x(r) \\ E'_y(r) \\ E'_z(r) \end{bmatrix}. \quad (2.21b)$$

Because the tangential components of the wave vectors are conserved quantity during propagation through layered media and because of the plane wave character of the solution, we can express the field vectors as

$$\mathbf{E}'(\mathbf{r}) = E'_0 \mathbf{e}'(z) \exp[ik_0(N_x x + N_y y)], \quad (2.22a)$$

$$\mathbf{H}'(\mathbf{r}) = H'_0 \mathbf{h}'(z) \exp[ik_0(N_x x + N_y y)]. \quad (2.22b)$$

After performing derivations and reducing the dependency of the field vectors on x - and y -coordinates, we get

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & ik_0 k_y \\ \frac{\partial}{\partial z} & 0 & -ik_0 k_x \\ -ik_0 k_y & ik_0 k_x & 0 \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \\ e'_z(z) \end{bmatrix} = ik_0 \begin{bmatrix} h'_x(z) \\ h'_y(z) \\ h'_z(z) \end{bmatrix}, \quad (2.23a)$$

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & ik_0 k_y \\ \frac{\partial}{\partial z} & 0 & -ik_0 k_x \\ -ik_0 k_y & ik_0 k_x & 0 \end{bmatrix} \begin{bmatrix} h'_x(z) \\ h'_y(z) \\ h'_z(z) \end{bmatrix} = -ik_0 \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \\ e'_z(z) \end{bmatrix}. \quad (2.23b)$$

Now we can extract z - components from equations (2.23a) and (2.23b)

$$e'_z(z) = \varepsilon_{zz}^{-1} [N_y h'_x(z) - N_x h'_y(z) - \varepsilon_{zx} e'_x(z) - \varepsilon_{zy} e'_y(z)], \quad (2.24a)$$

$$h'_z(z) = -N_y e'_x(z) + N_x e'_y(z), \quad (2.24b)$$

and substitute them back, so

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & 0 \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \end{bmatrix} + ik_0 \begin{bmatrix} N_y e'_z(z) \\ -N_x e'_z(z) \end{bmatrix} = ik_0 \begin{bmatrix} h'_x(z) \\ h'_z(z) \end{bmatrix}, \quad (2.25a)$$

$$\begin{aligned} & \begin{bmatrix} 0 & -\frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & 0 \end{bmatrix} \begin{bmatrix} h'_x(z) \\ h'_y(z) \end{bmatrix} + ik_0 \begin{bmatrix} N_y h'_z(z) \\ -N_x h'_z(z) \end{bmatrix} = \\ & -ik_0 \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{yx} & \varepsilon_{yy} \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \end{bmatrix} - ik_0 \begin{bmatrix} \varepsilon_{xz} e'_z(z) \\ \varepsilon_{yz} e'_z(z) \end{bmatrix}. \end{aligned} \quad (2.25b)$$

Now we can introduce a vector of the tangential components of the field vectors

$$\mathbf{f}(z) = [e'_x(z), h'_y(z), e'_y(z), h'_x(z)]^T, \quad (2.26)$$

which leads to the compact matrix form

$$\left\{ \begin{bmatrix} 0 & -\frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial z} \\ 0 & 0 & -\frac{\partial}{\partial z} & 0 \\ \frac{\partial}{\partial z} & 0 & 0 & 0 \end{bmatrix} + ik_0 \begin{bmatrix} -N_y^2 & 0 & N_y N_x & 0 \\ N_x N_y & 0 & -N_x^2 & 0 \\ -N_y \varepsilon_{zz}^{-1} \varepsilon_{zx} & -N_y \varepsilon_{zz}^{-1} N_x & -N_y \varepsilon_{zz}^{-1} \varepsilon_{zy} & N_y \varepsilon_{zz}^{-1} N_y \\ N_x \varepsilon_{zz}^{-1} \varepsilon_{zx} & N_y \varepsilon_{zz}^{-1} N_x & N_x \varepsilon_{zz}^{-1} \varepsilon_{zy} & -N_x \varepsilon_{zz}^{-1} N_y \end{bmatrix} \right\} \mathbf{f}(z) =$$

$$ik_0 \left\{ \begin{bmatrix} -\varepsilon_{xx} & 0 & -\varepsilon_{xy} & 0 \\ -\varepsilon_{yx} & 0 & -\varepsilon_{yy} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} \varepsilon_{xz} \varepsilon_{zz}^{-1} \varepsilon_{zx} & \varepsilon_{xz} \varepsilon_{zz}^{-1} N_x & \varepsilon_{xz} \varepsilon_{zz}^{-1} \varepsilon_{zy} & -\varepsilon_{xz} \varepsilon_{zz}^{-1} N_y \\ \varepsilon_{yz} \varepsilon_{zz}^{-1} \varepsilon_{zx} & \varepsilon_{yz} \varepsilon_{zz}^{-1} N_x & \varepsilon_{yz} \varepsilon_{zz}^{-1} \varepsilon_{zy} & -\varepsilon_{yz} \varepsilon_{zz}^{-1} N_y \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \right\} \mathbf{f}(z) \quad (2.27)$$

or after some reordering to

$$\frac{\partial}{\partial z} \mathbf{f}(z) = ik_0 \mathbf{C} \mathbf{f}(z), \quad (2.28)$$

where $\mathbf{C}$ is

$$\mathbf{C} = \begin{bmatrix} -N_x \varepsilon_{zz}^{-1} \varepsilon_{zx} & 1 - N_x \varepsilon_{zz}^{-1} N_x & -N_x \varepsilon_{zz}^{-1} \varepsilon_{zy} & N_x \varepsilon_{zz}^{-1} N_y \\ \varepsilon_{xx} - N_y^2 - \varepsilon_{xz} \varepsilon_{zz}^{-1} & -\varepsilon_{xz} \varepsilon_{zz}^{-1} N_x & N_y N_x + \varepsilon_{xy} - \varepsilon_{xz} \varepsilon_{zz}^{-1} \varepsilon_{zy} & \varepsilon_{xz} \varepsilon_{zz}^{-1} N_y \\ -N_y \varepsilon_{zz}^{-1} \varepsilon_{zx} & -N_y \varepsilon_{zz}^{-1} N_x & -N_y \varepsilon_{zz}^{-1} \varepsilon_{zy} & N_y \varepsilon_{zz}^{-1} N_y - 1 \\ -N_x N_y - \varepsilon_{yx} + \varepsilon_{yz} \varepsilon_{zz}^{-1} \varepsilon_{zx} & \varepsilon_{yz} \varepsilon_{zz}^{-1} N_x & N_x^2 - \varepsilon_{yy} + \varepsilon_{yz} \varepsilon_{zz}^{-1} \varepsilon_{zy} & -\varepsilon_{yz} \varepsilon_{zz}^{-1} N_y \end{bmatrix}. \quad (2.29)$$

The most convenient way to solve this system of differential equations is using eigenvalue method [45]. The expected solution is in form

$$\mathbf{f}(z) = \alpha \mathbf{v}_1 \exp(ik_0 \lambda_1 z) + \beta \mathbf{v}_2 \exp(ik_0 \lambda_2 z) + \gamma \mathbf{v}_3 \exp(ik_0 \lambda_3 z) + \delta \mathbf{v}_4 \exp(ik_0 \lambda_4 z), \quad (2.30)$$

where $(\mathbf{v}_i)$ are eigenvectors of the matrix $\mathbf{C}$ and λ_i are corresponding eigenvalues of the matrix $\mathbf{C}$. We can show the solution's validity, for example by assuming only α is non-zero and substitute it back into equation (2.28). We get

$$\alpha ik_0 \exp(ik_0 \lambda_1 z) (\mathbf{C} \mathbf{v}_1 - \lambda_1 \mathbf{v}_1) = 0, \quad (2.31)$$

which can be rewritten as

$$(\mathbf{C} - \lambda_1 \mathbf{I}) \mathbf{v}_1 = 0. \quad (2.32)$$

Resulting expression is a basic eigenvalue equation and can be generalized for the general case.

Eigenvalues of the matrix $\mathbf{C}$ corresponds to the propagation constant N_z and eigenvectors represent the tangential components of the polarization vector of the propagating mode. We can see from the solution that there are four different linearly independent waves propagating through the medium with corresponding propagation constants. Two of those modes propagate upward (real part of N_z is negative) and two downward (real part of N_z is positive) and are in general elliptically polarized. In an isotropic medium, there exists a degeneracy in the solutions due to the nature of the problem and therefore any two orthogonal polarizations can represent eigenmodes of the medium. In this thesis, we use s- and p- polarizations to represent propagating waves in isotropic media.

2.2.1 Solutions in isotropic media

In this thesis, we are assuming that superstrate and substrate are always isotropic media, so it is useful to calculate eigenmodes for isotropic medium, which can be solved analytically. Assuming an isotropic medium (diagonal dielectric tensor $\hat{\varepsilon}_r$) and the plane of incidence parallel with the x -axis ($N_x = 0$), we get

$$\mathbf{C} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \varepsilon_R - N_y^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & N_y \varepsilon_R^{-1} N_y - 1 \\ 0 & 0 & -\varepsilon_R & 0 \end{bmatrix}. \quad (2.33)$$

Solving eigenvalue problem

$$(\mathbf{C} - k_z \mathbf{I}) \mathbf{f}(z) = \mathbf{0} \quad (2.34)$$

by assuming the determinant of the matrix equation $(\mathbf{C} - k_z \mathbf{I})$ zero, we get

$$(N_z^2 - N_y^2 - \varepsilon_R)^2 = 0. \quad (2.35)$$

This equation has four solutions:

$$N_{z,1} = N_{z,3} = \sqrt{\varepsilon_R - N_y^2}, \quad (2.36a)$$

$$N_{z,2} = N_{z,4} = -\sqrt{\varepsilon_R - N_y^2}. \quad (2.36b)$$

The solutions correspond to the four propagating modes. Two positive solutions are the downward propagating modes, while two negative solutions are the upward propagating modes. By

substituting the solutions into (2.34), we get

$$\left\{ \begin{bmatrix} -N_{z,i} & 1 & 0 & 0 \\ \varepsilon_R - N_y^2 & -N_{z,i} & 0 & 0 \\ 0 & 0 & -N_{z,i} & N_y \varepsilon_R^{-1} N_y - 1 \\ 0 & 0 & -\varepsilon_R & -N_{z,i} \end{bmatrix} \right\} \mathbf{f}(z) = 0 \quad (2.37)$$

hence

$$h'_{y,i} = N_{z,i} e'_{x,i}, \quad (2.38a)$$

$$h'_{x,i} = -\frac{\varepsilon_R}{N_{z,i}} e'_{y,i}. \quad (2.38b)$$

Equation (2.37) has 4 solutions, assuming $e_x = 0$ (p- polarization) or $e_x = 1$ (s- polarization), substituting backward and forward propagating N_z and normalizing vector of electric intensity $\mathbf{e}'$ as follows [e'_z can be expressed using (2.24a)]

$$||\mathbf{e}'|| = \sqrt{e'^2_x + e'^2_y + e'^2_z} = 1. \quad (2.39)$$

The normalization is important here, in the superstrate and substrate media, for proper definition of the transmission and reflection coefficients, more details are described in the Section 2.3. The eigenvectors can then be written in a compact matrix form as follows:

$$\mathbf{D}_{iso} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ \sqrt{\varepsilon_R - N_y^2} & -\sqrt{\varepsilon_R - N_y^2} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{\varepsilon_R - N_y^2}}{\sqrt{\varepsilon_R}} & \frac{\sqrt{\varepsilon_R - N_y^2}}{\sqrt{\varepsilon_R}} \\ 0 & 0 & -\sqrt{\varepsilon_R} & \sqrt{\varepsilon_R} \end{bmatrix}, \quad (2.40)$$

where eigenvectors are ordered as s-down, s-up, p-down, p-up. For superstrate with the index of refraction $n^{(0)}$ and the angle of incidence φ , we can express the wave vector $\mathbf{k}$ as

$$\mathbf{k} = k_0 \begin{bmatrix} 0 \\ n^{(0)} \sin \varphi \\ n^{(0)} \cos \varphi \end{bmatrix}. \quad (2.41)$$

Furthermore, assuming $\mu_r = 1$ for optical frequencies we can express $n^{(0)}$ as

$$n^{(0)} = \sqrt{\varepsilon_R^{(0)}}. \quad (2.42)$$

Substituting (2.41), (2.41) into (2.40), we get the compact matrix form of eigenvectors for the isotropic superstrate medium

$$\mathbf{D}^{(0)} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ n^{(0)} \cos \varphi & -n^{(0)} \cos \varphi & 0 & 0 \\ 0 & 0 & \cos \varphi & \cos \varphi \\ 0 & 0 & -n^{(0)} & n^{(0)} \end{bmatrix}. \quad (2.43)$$

2.2.2 Boundary conditions - M-matrix algorithm

In the last few sections, the eigenmodes propagating in an individual layer were obtained. The next step is to describe propagation through a boundaries between such layers [19, 20, 44]. To do this, well known boundary conditions resulting from the Maxwell equations need to be applied. According to the boundary conditions the tangential components of the electric and magnetic field vectors are conserved, according to

$$\mathbf{n} \times (\mathbf{E}^{(n)} - \mathbf{E}^{(n+1)}) = 0, \quad (2.44a)$$

$$\mathbf{n} \times (\mathbf{H}^{(n)} - \mathbf{H}^{(n+1)}) = \mathbf{J}, \quad (2.44b)$$

,where $\mathbf{J}$ is the surface current density, or in used coordinate system and assuming there are no surface currents,

$$E_x^{(n)} = E_x^{(n+1)}, E_y^{(n)} = E_y^{(n+1)}, \quad (2.45a)$$

$$H_x^{(n)} = H_x^{(n+1)}, H_y^{(n)} = H_y^{(n+1)}. \quad (2.45b)$$

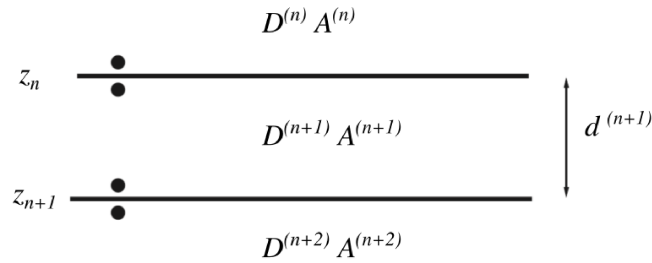


Figure 2.2: Interfaces between n -th, $(n+1)$ -th and $(n+2)$ -th media and corresponding matrices of each layer.

As was shown in the previous sections, the electric and magnetic field vectors in the n -th

medium can be written, excluding the time dependence as

$$\mathbf{E}^{(n)} = \exp[ik_0(N_x x + N_y y)] \sum_{i=1}^4 A_i^{(n)} \mathbf{e}_i^{(n)} \exp(ik_0 N_{z,i}^{(n)} z), \quad (2.46a)$$

$$\mathbf{H}^{(n)} = \exp[ik_0(N_x x + N_y y)] \sum_{i=1}^4 A_i^{(n)} \mathbf{h}_i^{(n)} \exp(ik_0 N_{z,i}^{(n)} z). \quad (2.46b)$$

Using expressions (2.46a) and (2.46b), the boundary conditions (2.45a), (2.45b) can then be written as

$$\sum_{i=1}^4 A_i^{(n)} \mathbf{e}_{x,i}^{(n)} = \sum_{i=1}^4 A_i^{(n+1)} \mathbf{e}_{x,i}^{(n)}, \quad (2.47a)$$

$$\sum_{i=1}^4 A_i^{(n)} \mathbf{e}_{y,i}^{(n)} = \sum_{i=1}^4 A_i^{(n+1)} \mathbf{e}_{y,i}^{(n)}, \quad (2.47b)$$

$$\sum_{i=1}^4 A_i^{(n)} \mathbf{h}_{x,i}^{(n)} = \sum_{i=1}^4 A_i^{(n+1)} \mathbf{h}_{x,i}^{(n)}, \quad (2.47c)$$

$$\sum_{i=1}^4 A_i^{(n)} \mathbf{h}_{y,i}^{(n)} = \sum_{i=1}^4 A_i^{(n+1)} \mathbf{h}_{y,i}^{(n)}, \quad (2.47d)$$

or in the compact matrix form

$$\mathbf{D}^{(n)} \mathbf{A}^{(n)} = \mathbf{D}^{(n+1)} \mathbf{A}^{(n+1)}, \quad (2.48a)$$

$$\mathbf{D}^{(n)} = \begin{bmatrix} e_{x,1}^{(n)} & e_{x,2}^{(n)} & e_{x,3}^{(n)} & e_{x,4}^{(n)} \\ h_{y,1}^{(n)} & h_{y,2}^{(n)} & e_{y,3}^{(n)} & e_{y,4}^{(n)} \\ e_{y,1}^{(n)} & e_{y,2}^{(n)} & e_{y,3}^{(n)} & e_{y,4}^{(n)} \\ h_{x,1}^{(n)} & h_{x,2}^{(n)} & h_{x,3}^{(n)} & h_{x,4}^{(n)} \end{bmatrix}, \quad (2.48b)$$

$$\mathbf{A}^{(n)} = [A_1^{(n)}, A_2^{(n)}, A_3^{(n)}, A_4^{(n)}]^T, \quad (2.48c)$$

where the matrix $\mathbf{D}^{(n)}$ is composed of the tangential components of polarization vectors $\mathbf{e}$ and $\mathbf{h}$, which are obtained by solving the Maxwell equations and consist of the eigenvectors of the matrix $\mathbf{C}^{(n)}$, and the vector $\mathbf{A}^{(n)}$ is a vector of eigenmode amplitudes. Next, to model propagation through a layer with a thickness $d^{(n)}$, the propagation matrix is defined as [19, 20, 44]

$$\mathbf{P}^{(n)} = \begin{bmatrix} \exp(ik_0 N_{z,1} d^{(n)}) & 0 & 0 & 0 \\ 0 & \exp(ik_0 N_{z,2} d^{(n)}) & 0 & 0 \\ 0 & 0 & \exp(ik_0 N_{z,3} d^{(n)}) & 0 \\ 0 & 0 & 0 & \exp(ik_0 N_{z,4} d^{(n)}) \end{bmatrix}. \quad (2.49)$$

Using the propagation matrix, we can now describe the transformation of the field vectors while travelling through the $(n+1)$ -th layer as follows,

$$\mathbf{A}^{(n)} = [\mathbf{D}^{(n)}]^{-1} \mathbf{D}^{(n+1)} \mathbf{P}^{(n+1)} [\mathbf{D}^{(n+1)}]^{-1} \mathbf{D}^{(n+2)} \mathbf{A}^{(n+2)}. \quad (2.50)$$

This approach can be then generalized for any system with N layers in the following way:

$$\mathbf{A}^{(0)} = [\mathbf{D}^{(0)}]^{-1} \prod_{i=1}^N \left(\mathbf{D}^{(i)} \mathbf{P}^{(i)} [\mathbf{D}^{(i)}]^{-1} \right) \mathbf{D}^{(N+1)} \mathbf{A}^{(N+1)} = \mathbf{M} \mathbf{A}^{(N+1)}, \quad (2.51)$$

where $\mathbf{M}$ denotes the transfer matrix of the whole system.

2.3 Experimental observables

In the last section, the transfer matrix of the layered system was obtained. This matrix can then be used to calculate the reflection and trasmission coefficients of the propagating wave. These coefficients are in turn connected to the measurable intensities of the reflected and transmitted waves.

2.3.1 Reflection and transmission coefficients

The reflection and transmission coefficients are defined as the complex ratios between the complex amplitudes of individual propagating eigenmodes. Assuming $A_1^{(0)}$ and $A_3^{(0)}$ are downward propagating waves and $A_2^{(0)}$ and $A_4^{(0)}$ are upward propagating waves, see Figure 2.3, we can write them as

$$r_{ij}^{(kl)} = \frac{A_j^{(k)}}{A_i^{(k)}}, \quad (2.52)$$

where $i \in \{1, 3\}$ and $j \in \{2, 4\}$ and

$$t_{ij}^{(kl)} = \frac{A_j^{(l)}}{A_i^{(k)}}, \quad (2.53)$$

where $i \in \{1, 3\}$ and $j \in \{1, 3\}$. Now, let's assume the light comes only from superstrate, $A_2^{(N+1)} = 0$ and $A_4^{(N+1)} = 0$. The system is now described by the transformation [20]

$$\begin{bmatrix} A_1^{(0)} \\ A_2^{(0)} \\ A_3^{(0)} \\ A_4^{(0)} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \begin{bmatrix} A_1^{(N+1)} \\ 0 \\ A_3^{(N+1)} \\ 0 \end{bmatrix}. \quad (2.54)$$

It is now straightforward to the obtain reflection and transmission coefficients by combining

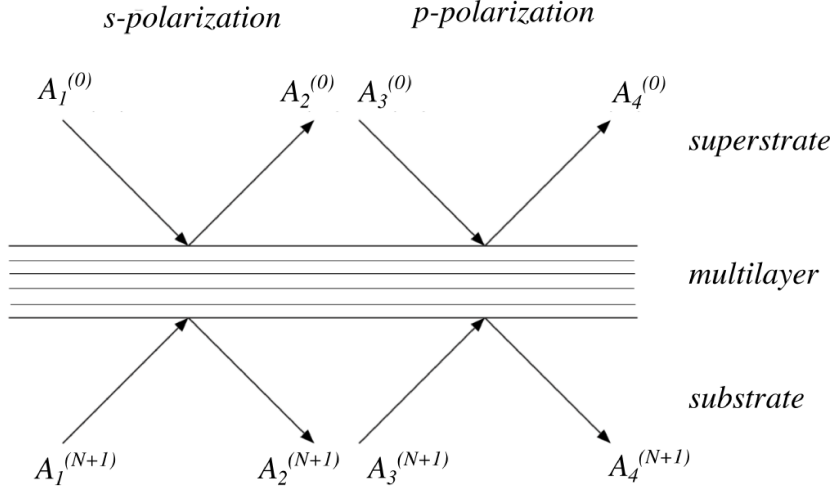


Figure 2.3: Propagating modes entering and leaving the system of layered media.

the expressions (2.52) and (2.53) so the reflection coefficients will take form

$$r_{12} = \frac{M_{21}M_{33} - M_{23}M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.55a)$$

$$r_{14} = \frac{M_{41}M_{33} - M_{43}M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.55b)$$

$$r_{32} = \frac{M_{11}M_{23} - M_{21}M_{13}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.55c)$$

$$r_{34} = \frac{M_{11}M_{43} - M_{41}M_{13}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.55d)$$

and the transmission coefficients

$$t_{11} = \frac{M_{33}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.56a)$$

$$t_{13} = \frac{-M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.56b)$$

$$t_{31} = \frac{-M_{13}}{M_{11}M_{33} - M_{13}M_{31}}, \quad (2.56c)$$

$$t_{33} = \frac{M_{11}}{M_{11}M_{33} - M_{13}M_{31}}. \quad (2.56d)$$

It is important to note that these coefficients can represent a transformation between various polarizations, for example s- and p- to left-hand and right-hand circular polarizations, dependent on the choice of eigenmode basis in the superstrate and substrate media. In this thesis, as was stated in Section 2.2.1, the eigenmodes in superstrate and substrate are chosen as s- and p-polarizations, so the transmission and reflection coefficients describe the transformation of s- and p- polarizations.

2.3.2 Reflectance and transmittance

Most of the experimental configurations don't allow to directly measure the field vectors, so it is more useful to describe the transformation of propagating waves in the term of intensities. The optical intensity can be defined using the Poynting vector as

$$I = | \langle \mathbf{S}(\mathbf{r}, t) \rangle |, \quad (2.57)$$

where $\langle \mathbf{S}(\mathbf{r}, t) \rangle$ is the time of average value of $\mathbf{S}(\mathbf{r}, t)$ determined by

$$\langle \mathbf{S}(\mathbf{r}, t) \rangle = \frac{1}{T} \int_0^T \mathbf{S}(\mathbf{r}, t) dt. \quad (2.58)$$

The Poynting vector represents the directional energy flux of the propagating wave and is expressed as [41, 42]

$$\mathbf{S}(\mathbf{r}, t) = \Re[\mathbf{E}(\mathbf{r}, t)] \times \Re[\mathbf{H}(\mathbf{r}, t)], \quad (2.59)$$

where

$$\Re[\mathbf{E}(\mathbf{r}, t)] = \frac{1}{2} [\mathbf{E}(\mathbf{r}) \exp(-i\omega t) + \mathbf{E}^*(\mathbf{r}) \exp(i\omega t)], \quad (2.60a)$$

$$\Re[\mathbf{H}(\mathbf{r}, t)] = \frac{1}{2} [\mathbf{H}(\mathbf{r}) \exp(-i\omega t) + \mathbf{H}^*(\mathbf{r}) \exp(i\omega t)]. \quad (2.60b)$$

Equation (2.58) will then take form

$$\begin{aligned} \langle \mathbf{S}(\mathbf{r}, t) \rangle &= \frac{1}{4T} \int_0^T [\mathbf{E}(\mathbf{r}) \times \mathbf{H}(\mathbf{r}) \exp(-2i\omega t) + \mathbf{E}(\mathbf{r}) \times \mathbf{H}^*(\mathbf{r}) + \\ &\mathbf{E}^*(\mathbf{r}) \times \mathbf{H}(\mathbf{r}) + \mathbf{E}^*(\mathbf{r}) \times \mathbf{H}^*(\mathbf{r}) \exp(2i\omega t)] dt = \frac{1}{2} \Re[\mathbf{E}(\mathbf{r}) \times \mathbf{H}^*(\mathbf{r})]. \end{aligned} \quad (2.61)$$

The reflectance $R_{ij}^{(kl)}$ and transmittance $T_{ij}^{(kl)}$ are defined as the ratio of the normal components of the intensities of the incident and reflected, or transmitted, waves,

$$R_{ij}^{(kl)} = \left| \frac{\langle \mathbf{S}_j^{(k)}(\mathbf{r}, t) \rangle_z}{\langle \mathbf{S}_i^{(k)}(\mathbf{r}, t) \rangle_z} \right|, \quad (2.62a)$$

$$T_{ij}^{(kl)} = \left| \frac{\langle \mathbf{S}_j^{(l)}(\mathbf{r}, t) \rangle_z}{\langle \mathbf{S}_i^{(k)}(\mathbf{r}, t) \rangle_z} \right|. \quad (2.62b)$$

Expressing the field vectors of j -th eigenmode in the k -th medium according to the (2.46a) and (2.46b) as

$$\mathbf{E}_j^{(k)}(\mathbf{r}) = A_j^{(k)} \mathbf{e}_j^{(k)} \exp(ik_0(N_x x + N_y y + N_{z,j}^{(k)} z)), \quad (2.63a)$$

$$\mathbf{H}_j^{(k)*}(\mathbf{r}) = A_j^{(k)*} \mathbf{h}_j^{(k)*} \exp(ik_0(N_x x + N_y y + M_{z,j}^{(k)} z)), \quad (2.63b)$$

we get

$$\langle \mathbf{S}_j^{(k)}(\mathbf{r}, t) \rangle_z = \frac{1}{2} \Re[A_j^{(k)} A_j^{(k)*} (\mathbf{e}_j^{(k)} \times \mathbf{h}_j^{(k)*})]_z. \quad (2.64)$$

In this thesis, it is assumed that superstrate and substrate media are always isotropic, so we can substitute the components of the polarization vectors $\mathbf{e}_j^{(k)}$ and $\mathbf{h}_j^{(k)*}$ by the elements of the $\mathbf{D}_{iso}$ matrix (2.43) and get

$$\langle \mathbf{S}_j^{(k)}(\mathbf{r}, t) \rangle_z = \frac{1}{2} \Re[A_j^{(k)} A_j^{(k)*} k_{z,j}^{(k)}]. \quad (2.65)$$

Substituting (2.65) into the equations (2.62a) and (2.62b) the reflectance and trasmittance take the following forms:

$$R_{ij}^{(kl)} = \left| \frac{\Re[A_j^{(k)} A_j^{(k)*} N_{z,j}^{(k)}]}{\Re[A_i^{(k)} A_i^{(k)*} N_{z,i}^{(k)}]} \right| = \left| \frac{A_j^{(k)}}{A_i^{(k)}} \right|^2 = |r_{ij}^{(kl)}|^2, \quad (2.66a)$$

$$T_{ij}^{(kl)} = \left| \frac{\Re[A_j^{(l)} A_j^{(l)*} N_{z,j}^{(l)}]}{\Re[A_i^{(k)} A_i^{(k)*} N_{z,i}^{(k)}]} \right| = \left| \frac{A_j^{(l)}}{A_i^{(k)}} \right|^2 \left| \frac{\Re[k_{z,j}^{(l)}]}{\Re[k_{z,i}^{(k)}]} \right| = |t_{ij}^{(kl)}|^2 \left| \frac{\Re[k_{z,j}^{(l)}]}{\Re[k_{z,i}^{(k)}]} \right|. \quad (2.66b)$$

3. Theory of gratings

In this chapter, we deal with modelling of layers with 1D lateral periodicity, like lamellar gratings as show in Figure (3.1). Because of the periodicity of the system, the field-vectors become distributed among infinite number of harmonic modes, which leads to a new phenomena, like diffraction, and gives engineers new tools for designing optical systems with the desired parameters.

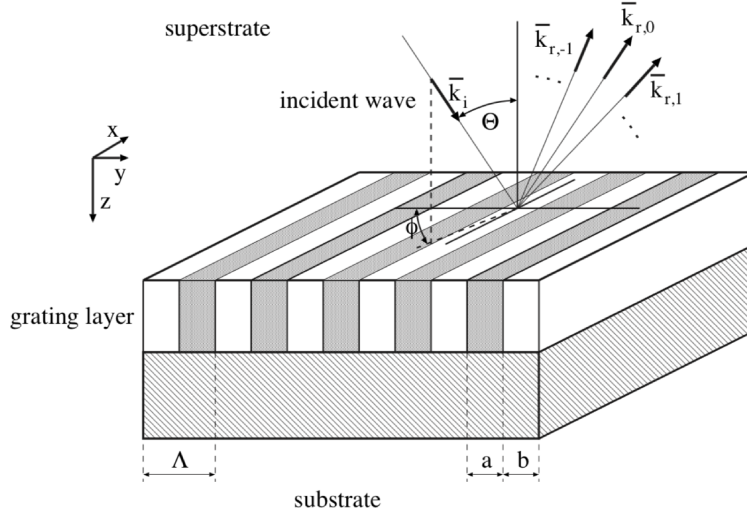


Figure 3.1: Layered system with a 1D lamellar grating [43]

In this chapter, we first introduce the rigorous coupled wave analysis (RCWA) [29, 32, 34], which describes propagating waves using truncated Fourier series. Then we describe the S-matrix algorithm needed for numerical stability of the problem and we derive the solution for isotropic media, which are used as superstrate and substrate. After that, the method of Fourier factorization for 1D lamellar gratings is briefly described to achieve faster convergence. In the last section, the relations between the calculated quantities and experimental observables are described.

3.1 RCWA method

This method is based on the normalized Maxwell equations (2.19a) and (2.19b). However, the permittivity is no longer a constant but it is a function of the position,

$$\nabla \times \mathbf{E}'(\mathbf{r}) = ik_0 \mathbf{H}'(\mathbf{r}), \quad (3.1a)$$

$$\nabla \times \mathbf{H}'(\mathbf{r}) = -ik_0 \hat{\varepsilon}_R(\mathbf{r}) \mathbf{E}'(\mathbf{r}). \quad (3.1b)$$

Assuming a lamellar grating as shown in figure 3.1, the permittivity is a periodic function of y (the coordinate system can be always rotated for 1D lamellar gratings so this holds) and can be expressed using the Fourier series as

$$\varepsilon_{ij}(y) = \sum_{n=-\infty}^{\infty} c_{ij,n} \exp\left(in \frac{2\pi}{\Lambda} y\right), \quad (3.2a)$$

$$c_{ij,n} = \frac{1}{\Lambda} \int_0^{\Lambda} \varepsilon_{ij}(y) \exp\left(-in \frac{2\pi}{\Lambda} y\right) dy, \quad (3.2b)$$

where Λ denotes the period of the grating. The solution of the periodic Maxwell equations is also periodic (Floquet's theorem, Bloch theorem in solid-state physics) and can be expanded as a series of plane waves with the same periodicity as follows:

$$\mathbf{E}'(\mathbf{r}) = E'_0 \sum_{n=-\infty}^{\infty} \mathbf{e}'_n(z) \exp(ik_0(N_x x + N_y y)) \exp\left(in \frac{2\pi}{\Lambda} y\right), \quad (3.3a)$$

$$\mathbf{H}'(\mathbf{r}) = H'_0 \sum_{n=-\infty}^{\infty} \mathbf{h}'_n(z) \exp(ik_0(N_x x + N_y y)) \exp\left(in \frac{2\pi}{\Lambda} y\right). \quad (3.3b)$$

By defining the wave vector of n -th order $N_{y,n}$ as

$$k_0 N_{y,n} = k_0 N_{y,0} + n \frac{2\pi}{\Lambda}, \quad (3.4a)$$

$$N_{y,n} = N_{y,0} + n \frac{\lambda}{\Lambda}, \quad (3.4b)$$

we can rewrite the field vectors as

$$\mathbf{E}'(\mathbf{r}) = E'_0 \sum_{n=-\infty}^{\infty} \mathbf{e}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)), \quad (3.5a)$$

$$\mathbf{H}'(\mathbf{r}) = H'_0 \sum_{n=-\infty}^{\infty} \mathbf{h}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)). \quad (3.5b)$$

Substituing (3.3a), (3.3b) and (3.2a) into (3.1a) and (3.1b), we get

$$\nabla \times \sum_{n=-\infty}^{\infty} \mathbf{e}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)) = ik_0 \sum_{n=-\infty}^{\infty} \mathbf{h}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)), \quad (3.6a)$$

$$\begin{aligned} \nabla \times \sum_{n=-\infty}^{\infty} \mathbf{h}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)) &= -ik_0 \sum_{m=-\infty}^{\infty} \hat{c}_m \exp\left(im \frac{2\pi}{\Lambda} y\right) \\ &\quad \sum_{n=-\infty}^{\infty} \mathbf{e}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)), \end{aligned} \quad (3.6b)$$

where $\hat{c}_m$ is tensor of Fourier coefficients $c_{ij,m}$ from (3.2b). We can multiply the Fourier series using Laurent rule

$$\sum_m \hat{c}_m \exp\left(im \frac{2\pi}{\Lambda} y\right) \sum_n \mathbf{e}'_n(z) \exp\left(in \frac{2\pi}{\Lambda} y\right) = \sum_n \sum_m \hat{c}_{n-m} \mathbf{e}'_m(z) \exp\left(in \frac{2\pi}{\Lambda} y\right), \quad (3.7)$$

therefore (3.6b) takes the form

$$\nabla \times \sum_{n=-\infty}^{\infty} \mathbf{h}'_n(z) \exp(ik_0(N_x x + N_{y,n} y)) = -ik_0 \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \hat{c}_{n-m} \mathbf{e}'_m(z) \exp(ik_0(N_x x + N_{y,n} y)). \quad (3.8)$$

This equation has to be fulfilled for every y and subsequently for every n (because $N_{y,n}$ is different for each mode). We can rewrite this equation in its reduced form as

$$\nabla \times \mathbf{h}'_n(z) = -ik_0 \sum_{m=-\infty}^{\infty} \hat{c}_{n-m} \mathbf{e}'_m(z). \quad (3.9)$$

For better insight into the problem, let's reduce the dimension of the problem to $N = M = 1$.

We get

$$\nabla \times \mathbf{h}'_{-1}(z) = -ik_0[\hat{c}_0 \mathbf{e}'_{-1}(z) + \hat{c}_{-1} \mathbf{e}'_0(z) + \hat{c}_{-2} \mathbf{e}'_1(z)], \quad (3.10a)$$

$$\nabla \times \mathbf{h}'_0(z) = -ik_0[\hat{c}_1 \mathbf{e}'_{-1}(z) + \hat{c}_0 \mathbf{e}'_0(z) + \hat{c}_{-1} \mathbf{e}'_1(z)], \quad (3.10b)$$

$$\nabla \times \mathbf{h}'_1(z) = -ik_0[\hat{c}_2 \mathbf{e}'_{-1}(z) + \hat{c}_1 \mathbf{e}'_0(z) + \hat{c}_0 \mathbf{e}'_1(z)]. \quad (3.10c)$$

or in the matrix form,

$$\begin{bmatrix} \nabla \times \mathbf{h}'_{-1}(z) \\ \nabla \times \mathbf{h}'_0(z) \\ \nabla \times \mathbf{h}'_1(z) \end{bmatrix} = \begin{bmatrix} \hat{c}_0 & \hat{c}_{-1} & \hat{c}_{-2} \\ \hat{c}_1 & \hat{c}_0 & \hat{c}_{-1} \\ \hat{c}_2 & \hat{c}_1 & \hat{c}_0 \end{bmatrix} \begin{bmatrix} \mathbf{e}'_{-1}(z) \\ \mathbf{e}'_0(z) \\ \mathbf{e}'_1(z) \end{bmatrix}. \quad (3.11)$$

Let's generalize the problem to N dimensions and define the vectors consisting of diffraction orders as follows:

$$\tilde{\mathbf{e}}_j = (e_{j,-N}, e_{j,-N+1}, \dots, e_{j,N})^T, \quad (3.12a)$$

$$\tilde{\mathbf{h}}_j = (h_{j,-N}, h_{j,-N+1}, \dots, h_{j,N})^T, \quad (3.12b)$$

$$\tilde{\mathbf{N}}_y = \text{diag}(N_{y,n}, n = -N, \dots, N), \dim(\tilde{\mathbf{N}}_y) = 2N + 1, \quad (3.12c)$$

$$\tilde{\mathbf{N}}_x = \text{diag}(N_x), \dim(\tilde{\mathbf{N}}_x) = 2N + 1, \quad (3.12d)$$

$$\tilde{\mathbf{E}}_{ij} = (c_{ij,nl}) = (c_{ij,n-l}), \dim(\tilde{\mathbf{E}}_{ij}) = (2N + 1) \times (2N + 1), \quad (3.12e)$$

where $\tilde{\mathbf{E}}_{ij}$ are so called Toeplitz matrices consisting of the Fourier series coefficients. By using the defined variables, the problem can be rewritten in the compact form

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & ik_0 \tilde{\mathbf{N}}_y \\ \frac{\partial}{\partial z} & 0 & -ik_0 \tilde{\mathbf{N}}_x \\ -ik_0 \tilde{\mathbf{N}}_y & ik_0 \tilde{\mathbf{N}}_x & 0 \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{e}}'_x(z) \\ \tilde{\mathbf{e}}'_y(z) \\ \tilde{\mathbf{e}}'_z(z) \end{bmatrix} = ik_0 \begin{bmatrix} \tilde{\mathbf{h}}'_x(z) \\ \tilde{\mathbf{h}}'_y(z) \\ \tilde{\mathbf{h}}'_z(z) \end{bmatrix}, \quad (3.13a)$$

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & ik_0 \tilde{\mathbf{N}}_y \\ \frac{\partial}{\partial z} & 0 & -ik_0 \tilde{\mathbf{N}}_x \\ -ik_0 \tilde{\mathbf{N}}_y & ik_0 \tilde{\mathbf{N}}_x & 0 \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{h}}'_x(z) \\ \tilde{\mathbf{h}}'_y(z) \\ \tilde{\mathbf{h}}'_z(z) \end{bmatrix} = -ik_0 \begin{bmatrix} \tilde{\mathbf{E}}_{xx} & \tilde{\mathbf{E}}_{xy} & \tilde{\mathbf{E}}_{xz} \\ \tilde{\mathbf{E}}_{yx} & \tilde{\mathbf{E}}_{yy} & \tilde{\mathbf{E}}_{yz} \\ \tilde{\mathbf{E}}_{zx} & \tilde{\mathbf{E}}_{zy} & \tilde{\mathbf{E}}_{zz} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{e}}'_x(z) \\ \tilde{\mathbf{e}}'_y(z) \\ \tilde{\mathbf{e}}'_z(z) \end{bmatrix}. \quad (3.13b)$$

This is a similar problem to the equations (2.23a) and (2.23b) and can be solved by the same approach. We can again introduce the vector

$$\tilde{\mathbf{f}}(z) = [\tilde{\mathbf{e}}'_x(z), \tilde{\mathbf{h}}'_y(z), \tilde{\mathbf{e}}'_y(z), \tilde{\mathbf{h}}'_x(z)]^T, \quad (3.14)$$

and obtain the equation

$$\frac{\partial}{\partial z} \tilde{\mathbf{f}}(z) = ik_0 \tilde{\mathbf{C}} \tilde{\mathbf{f}}(z), \quad (3.15)$$

where $\tilde{\mathbf{C}}$ takes a form

$$\tilde{\mathbf{C}} = \begin{bmatrix} -\tilde{\mathbf{N}}_x \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zx} & \mathbf{I} - \tilde{\mathbf{N}}_x \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_x & -\tilde{\mathbf{N}}_x \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zy} & \tilde{\mathbf{N}}_x \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_y \\ \tilde{\mathbf{E}}_{xx} - \tilde{\mathbf{N}}_y^2 - \tilde{\mathbf{E}}_{xz} \tilde{\mathbf{E}}_{zz}^{-1} & -\tilde{\mathbf{E}}_{xz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_x & \tilde{\mathbf{N}}_y \tilde{\mathbf{N}}_z + \tilde{\mathbf{E}}_{xy} - \tilde{\mathbf{E}}_{xz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zy} & \tilde{\mathbf{E}}_{xz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_y \\ -\tilde{\mathbf{N}}_y \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zx} & -\tilde{\mathbf{N}}_y \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_x & -\tilde{\mathbf{N}}_y \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zy} & \tilde{\mathbf{N}}_y \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_y - \mathbf{I} \\ -\tilde{\mathbf{N}}_x \tilde{\mathbf{N}}_y - \tilde{\mathbf{E}}_{yx} + \tilde{\mathbf{E}}_{yz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zx} & \tilde{\mathbf{E}}_{yz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_x & \tilde{\mathbf{N}}_x^2 - \tilde{\mathbf{E}}_{yy} + \tilde{\mathbf{E}}_{yz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{E}}_{zy} & -\tilde{\mathbf{E}}_{yz} \tilde{\mathbf{E}}_{zz}^{-1} \tilde{\mathbf{N}}_y \end{bmatrix}. \quad (3.16)$$

This equation again represents eigenvalue problem and the solution is in similar form as in (2.30), however now there are $4 \times (2N + 1)$ propagating modes, half of them upward and half downward. From the calculated eigenvectors the polarization matrix $\mathbf{D}^{(n)}$ can be obtained and then used in the boundary condition formulations.

3.2 S-matrix algorithm

In Sectin 2.2.2, we introduced the M-matrix algorithm as a boundary condition formulation, which works well for non-periodic layers. However, this algorithm is no longer applicable for the systems with lateral periodicity. Most of the propagating modes in a periodic layer are evanescent and decrease/increase exponentially. This leads to a huge gap between the smallest and the largest term of transfer matrices and it exceeds the numerical precision. To solve this problem, the scattering matrix algorithm (S-matrix) [32] was introduced. This algorithm rearranges the terms, so the transformation is only in the decreasing direction, and it avoids the numerical precision problem.

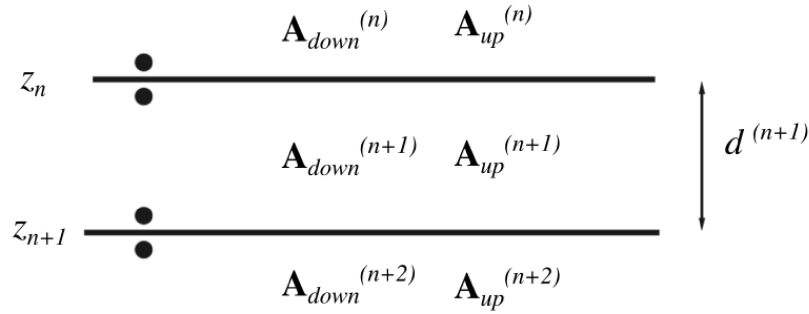


Figure 3.2: Propagating eigenmodes through a layer with the thickness $d^{(n+1)}$

The transformation of propagating waves on the boundary can be described similarly to (2.48a) as

$$\mathbf{A}^{(n+1)}(z_n) = \mathbf{c}^{(n)} \mathbf{A}^{(n)}(z_n), \quad (3.17)$$

however now the propagating modes are in this case sorted to upward and downward propagating modes (the direction of propagation of the evanescent modes can be decided on the basis of the imaginary part of their $N_{z,n}$ - the modes decay in the direction of propagation)

$$\begin{bmatrix} \mathbf{A}_{up}^{(n+1)}(z_n) \\ \mathbf{A}_{down}^{(n+1)}(z_n) \end{bmatrix} = \begin{bmatrix} \mathbf{c}_{uu}^{(n)} & \mathbf{c}_{ud}^{(n)} \\ \mathbf{c}_{du}^{(n)} & \mathbf{c}_{dd}^{(n)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(n)}(z_n) \\ \mathbf{A}_{down}^{(n)}(z_n) \end{bmatrix}. \quad (3.18)$$

Now we can swap the modes, so there are only modes which enter the boundary on the left side and the modes that leave the boundary on the right side,

$$\begin{bmatrix} \mathbf{A}_{up}^{(n)}(z_n) \\ \mathbf{A}_{down}^{(n+1)}(z_n) \end{bmatrix} = \mathbf{s}^{(n)} \begin{bmatrix} \mathbf{A}_{up}^{(n+1)}(z_n) \\ \mathbf{A}_{down}^{(n)}(z_n) \end{bmatrix}, \quad (3.19)$$

where

$$\mathbf{s}^{(n)} = \begin{bmatrix} \mathbf{t}_{uu}^{(n)} & \mathbf{r}_{ud}^{(n)} \\ \mathbf{r}_{du}^{(n)} & \mathbf{t}_{dd}^{(n)} \end{bmatrix} = \begin{bmatrix} \mathbf{c}_{uu}^{(n)-1} & -\mathbf{c}_{uu}^{(n)-1} \mathbf{c}_{ud}^{(n)} \\ \mathbf{c}_{du}^{(n)} \mathbf{c}_{uu}^{(n)-1} & \mathbf{c}_{dd}^{(n)} - \mathbf{c}_{du}^{(n)} \mathbf{c}_{uu}^{(n)-1} \mathbf{c}_{ud}^{(n)} \end{bmatrix}. \quad (3.20)$$

The propagation through a layer can be described as follows:

$$\mathbf{A}_{up}^{(n+1)}(z_n) = \mathbf{P}_{up}^{(n+1)} \mathbf{A}_{up}^{(n+1)}(z_{n+1}) \quad (3.21a)$$

$$\mathbf{A}_{down}^{(n+1)}(z_{n+1}) = \mathbf{P}_{down}^{(n+1)} \mathbf{A}_{down}^{(n+1)}(z_n) \quad (3.21b)$$

where $\mathbf{P}_{up}^{(n+1)}$ and $\mathbf{P}_{down}^{(n+1)}$ are the propagation matrices,

$$\mathbf{P}_{up}^{(n+1)} = \text{diag} \left[\exp(-ik_0 N_{z,n,up}^{(n+1)} d^{(n+1)}), n = -N, \dots, N \right], \quad (3.22a)$$

$$\mathbf{P}_{down}^{(n+1)} = \text{diag} \left[\exp(ik_0 N_{z,n,down}^{(n+1)} d^{(n+1)}), n = -N, \dots, N \right]. \quad (3.22b)$$

Substituting (3.21a) and (3.21b) into (3.20) leads to

$$\begin{bmatrix} \mathbf{A}_{up}^{(n)}(z_n) \\ \mathbf{P}_{down}^{(n+1)-1} \mathbf{A}_{down}^{(n+1)}(z_{n+1}) \end{bmatrix} = \begin{bmatrix} \mathbf{t}_{uu}^{(n)} & \mathbf{r}_{ud}^{(n)} \\ \mathbf{r}_{du}^{(n)} & \mathbf{t}_{dd}^{(n)} \end{bmatrix} \begin{bmatrix} \mathbf{P}_{up}^{(n+1)} \mathbf{A}_{up}^{(n+1)}(z_{n+1}) \\ \mathbf{A}_{down}^{(n)}(z_n) \end{bmatrix}. \quad (3.23)$$

After rearranging the terms, we get

$$\begin{bmatrix} \mathbf{A}_{up}^{(n)}(z_n) \\ \mathbf{A}_{down}^{(n+1)}(z_{n+1}) \end{bmatrix} = \tilde{\mathbf{s}}^{(n)} \begin{bmatrix} \mathbf{A}_{up}^{(n+1)}(z_{n+1}) \\ \mathbf{A}_{down}^{(n)}(z_n) \end{bmatrix}, \quad (3.24)$$

where

$$\tilde{\mathbf{s}}^{(n)} = \begin{bmatrix} \tilde{\mathbf{t}}_{uu}^{(n)} & \tilde{\mathbf{r}}_{ud}^{(n)} \\ \tilde{\mathbf{r}}_{du}^{(n)} & \tilde{\mathbf{t}}_{dd}^{(n)} \end{bmatrix} = \begin{bmatrix} \mathbf{t}_{uu}^{(n)} \mathbf{P}_{up}^{(n+1)} & \mathbf{r}_{ud}^{(n)} \\ \mathbf{P}_{down}^{(n+1)} \mathbf{r}_{du}^{(n)} \mathbf{P}_{up}^{(n+1)} & \mathbf{P}_{down}^{(n+1)} \mathbf{t}_{dd}^{(n)} \end{bmatrix}. \quad (3.25)$$

Let's assume we know the scattering matrix of the subsystem describing transformation

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)}(z_0) \\ \mathbf{A}_{down}^{(n)}(z_n) \end{bmatrix} = \mathbf{S}^{(n)} \begin{bmatrix} \mathbf{A}_{up}^{(n)}(z_n) \\ \mathbf{A}_{down}^{(0)}(z_0) \end{bmatrix}, \quad (3.26)$$

where

$$\mathbf{S}^{(n)} = \begin{bmatrix} \mathbf{T}_{uu}^{(n)} & \mathbf{R}_{ud}^{(n)} \\ \mathbf{R}_{du}^{(n)} & \mathbf{T}_{dd}^{(n)} \end{bmatrix}. \quad (3.27)$$

The next layer can then be included into the system using the recursive formulae

$$\mathbf{T}_{uu}^{(n+1)} = \mathbf{T}_{uu}^{(n)} \left[\mathbf{I} - \tilde{\mathbf{r}}_{ud}^{(n+1)} \mathbf{R}_{du}^{(n)} \right]^{-1} \tilde{\mathbf{t}}_{uu}^{(n+1)}, \quad (3.28a)$$

$$\mathbf{R}_{ud}^{(n+1)} = \mathbf{R}_{ud}^{(n)} + \mathbf{T}_{uu}^{(n)} \left[\mathbf{I} - \tilde{\mathbf{r}}_{ud}^{(n+1)} \mathbf{R}_{du}^{(n)} \right]^{-1} \tilde{\mathbf{r}}_{ud}^{(n+1)} \mathbf{T}_{dd}^{(n)}, \quad (3.28b)$$

$$\mathbf{R}_{du}^{(n+1)} = \tilde{\mathbf{r}}_{du}^{(n+1)} + \tilde{\mathbf{t}}_{dd}^{(n+1)} \left[\mathbf{I} - \mathbf{R}_{du}^{(n)} \tilde{\mathbf{r}}_{ud}^{(n+1)} \right]^{-1} \mathbf{R}_{du}^{(n)} \tilde{\mathbf{t}}_{uu}^{(n+1)}, \quad (3.28c)$$

$$\mathbf{T}_{dd}^{(n+1)} = \tilde{\mathbf{t}}_{dd}^{(n+1)} \left[\mathbf{I} - \mathbf{R}_{du}^{(n)} \tilde{\mathbf{r}}_{ud}^{(n+1)} \right]^{-1} \mathbf{T}_{dd}^{(n)}. \quad (3.28d)$$

3.3 Solutions in isotropic periodic media

In this section, the solution for isotropic media is derived. For the correct interpretation of calculated data, the modes in the superstrate and substrate layers must be properly sorted and the polarization vectors must be normalized. The matrix $\tilde{\mathbf{C}}$ in an isotropic medium takes the form

$$\tilde{\mathbf{C}} = \begin{bmatrix} 0 & \mathbf{I} & 0 & 0 \\ \tilde{\mathbf{E}}_R - \tilde{\mathbf{k}}_y^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \tilde{\mathbf{k}}_y \tilde{\mathbf{E}}_R^{-1} \tilde{\mathbf{k}}_y - I \\ 0 & 0 & -\tilde{\mathbf{E}}_R & 0 \end{bmatrix}, \quad (3.29)$$

where $\tilde{\mathbf{E}}_R$ and $\tilde{\mathbf{k}}_y$ are both diagonal matrices. Therefore there is no coupling between different modes. The Fourier coefficient matrix $\tilde{\mathbf{E}}_R$ is in the form

$$\tilde{\mathbf{E}}_R = \begin{bmatrix} c_0 & 0 & \dots & 0 \\ 0 & c_0 & & \\ \vdots & & \ddots & \\ 0 & & & c_0 \end{bmatrix}. \quad (3.30)$$

This problem is similar to the problem in Section 2.2.1 and the same approach is used to solve it. The eigenvalues of the matrix $\tilde{\mathbf{C}}$ will take form

$$N_{z,n,down} = \sqrt{\varepsilon_R - N_{y,n}^2}, \quad (3.31a)$$

$$N_{z,n,up} = -\sqrt{\varepsilon_R - N_{y,n}^2}, \quad (3.31b)$$

where

$$N_{y,n} = N_{y,0} + n \frac{\lambda}{\Lambda}, \quad (3.32)$$

and the matrix of the eigenvectors could be expressed as

$$\mathbf{D}_{iso} = \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \tilde{\mathbf{N}}_z & -\tilde{\mathbf{N}}_z & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{\sqrt{\varepsilon_r}} \tilde{\mathbf{N}}_z & \frac{1}{\sqrt{\varepsilon_R}} \tilde{\mathbf{N}}_z \\ \mathbf{0} & \mathbf{0} & -\sqrt{\varepsilon_r} \mathbf{I} & \sqrt{\varepsilon_R} \mathbf{I} \end{bmatrix}, \quad (3.33)$$

where

$$\tilde{\mathbf{k}}_z = \text{diag}(k_{z,n}, n = -N, \dots, N), \dim(\tilde{\mathbf{N}}_z) = 2N + 1. \quad (3.34)$$

Assuming the permittivity of the boundary medium $n^{(0)}$ and the angle of incidence φ

$$n^{(0)} = \sqrt{\varepsilon_R^{(0)}}. \quad (3.35a)$$

$$N_{y,0} = n^{(0)} \sin \varphi, \quad (3.35b)$$

the equation (3.33) will become

$$\mathbf{D}^{(0)} = \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \tilde{\mathbf{N}}_{\mathbf{z}} & -\tilde{\mathbf{N}}_{\mathbf{z}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{1}{n^{(0)}} \tilde{\mathbf{N}}_{\mathbf{z}} & \frac{1}{n^{(0)}} \tilde{\mathbf{N}}_{\mathbf{z}} \\ \mathbf{0} & \mathbf{0} & -n^{(0)} \mathbf{I} & n^{(0)} \mathbf{I} \end{bmatrix}. \quad (3.36)$$

In order to use the polarization matrix in the S-matrix algorithm, it is important to sort the matrix to upward and downward propagating modes:

$$\mathbf{D}^{(0)} = \begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{I} & \mathbf{0} \\ -\tilde{\mathbf{k}}_{\mathbf{z}} & \mathbf{0} & -\tilde{\mathbf{k}}_{\mathbf{z}} & \mathbf{0} \\ \mathbf{0} & \frac{1}{n^{(0)}} \tilde{\mathbf{k}}_{\mathbf{z}} & \mathbf{0} & \frac{1}{n^{(0)}} \tilde{\mathbf{k}}_{\mathbf{z}} \\ \mathbf{0} & n^{(0)} \mathbf{I} & \mathbf{0} & -n^{(0)} \mathbf{I} \end{bmatrix}. \quad (3.37)$$

3.4 Fourier factorization (FF) method

The expressions of the Maxwell equations (3.1a) and (3.1b) are in general valid, however by truncating the Fourier series we are introducing an error into the solution. The error depends on the dimension of the problem (the higher the better) and can be tested using the convergence tests. In Figure 3.3 we can see the convergence of the s- and p- reflectance of a lamellar grating. There is no problem with s- polarization, which is stable even for a few orders, however the p- polarization converges slowly and oscillates around the correct solution. This problem arises from the multiplication of Fourier series using the Laurent rule (3.7) of two functions with a concurrent discontinuity.

This behaviour is connected to the Gibbs phenomenon. The finite Fourier series has large oscillations near the discontinuities, which do not die out, but approach a finite limit [45], as seen in Figure 3.4. There is no problem with the convergence for s- polarization, because in the chosen coordinate system the field of s- polarized light is in x direction and is not influenced by the truncation of the Fourier series, whereas the p- polarization needs to obey the continuity of the D_y , where the Laurent rule applies.

To solve this problem, the expression (2.6a) needs to be transformed, so there are no concurrent discontinuities, and then expanded into the Fourier series and finally transformed back

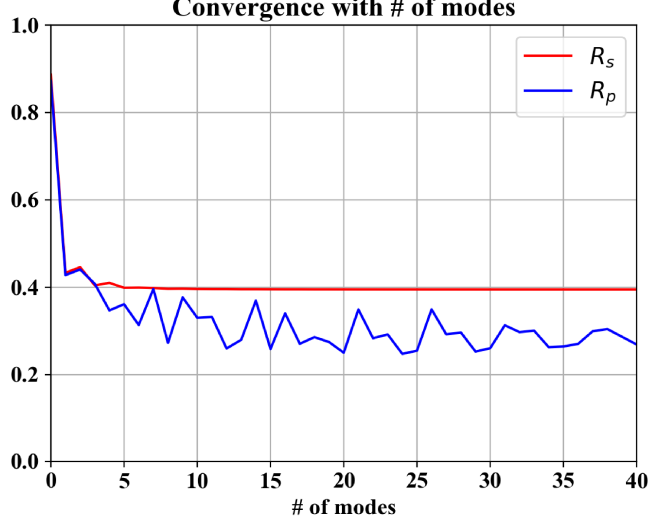


Figure 3.3: Coverage of zero diffraction orders in lamellar grating for 100 nm thick gold stripes, $\varepsilon_R = -11.753 + 1.2596i$ [49], on top of silicon substrate, $\varepsilon_R = 15.072 + 0.15210i$ [50]. The lamellar grating has period $2.5 \mu\text{m}$, fill factor $f = 0.4$ and the angle of incidence is 20 degrees. The algorithm for p- polarization converges slowly and oscillates around the limit value.

to its original form. In general, this is a complex problem and the research is still being conducted [46], [47], however in the case of 1D gratings with periodicity in y - direction, the solution is quite simple [30,31]. First, the relation (2.6a) is rearranged, so there are no two discontinuous functions being multiplied,

$$\begin{bmatrix} D_x \\ D_z \\ E_y \end{bmatrix} = \begin{bmatrix} \varepsilon_{xx} - \varepsilon_{xy}\varepsilon_{yy}^{-1}\varepsilon_{yx} & \varepsilon_{xz} - \varepsilon_{xy}\varepsilon_{yy}^{-1}\varepsilon_{yz} & \varepsilon_{xy}\varepsilon_{yy}^{-1} \\ \varepsilon_{zx} - \varepsilon_{zy}\varepsilon_{yy}^{-1}\varepsilon_{yx} & \varepsilon_{zz} - \varepsilon_{zy}\varepsilon_{yy}^{-1}\varepsilon_{yz} & \varepsilon_{zy}\varepsilon_{yy}^{-1} \\ -\varepsilon_{yy}^{-1}\varepsilon_{yx} & -\varepsilon_{yy}^{-1}\varepsilon_{yz} & \varepsilon_{yy}^{-1} \end{bmatrix} \begin{bmatrix} E_x \\ E_z \\ D_y \end{bmatrix}. \quad (3.38)$$

Now the functions are expanded to their Fourier series (symbol $\|...\|$ denotes the Toeplitz matrices of the Fourier coefficients of the expression inside the brackets)

$$\begin{bmatrix} \tilde{\mathbf{D}}_x \\ \tilde{\mathbf{D}}_z \\ \tilde{\mathbf{E}}_y \end{bmatrix} = \begin{bmatrix} \|\varepsilon_{xx} - \varepsilon_{xy}\varepsilon_{yy}^{-1}\varepsilon_{yx}\| & \|\varepsilon_{xz} - \varepsilon_{xy}\varepsilon_{yy}^{-1}\varepsilon_{yz}\| & \|\varepsilon_{xy}\varepsilon_{yy}^{-1}\| \\ \|\varepsilon_{zx} - \varepsilon_{zy}\varepsilon_{yy}^{-1}\varepsilon_{yx}\| & \|\varepsilon_{zz} - \varepsilon_{zy}\varepsilon_{yy}^{-1}\varepsilon_{yz}\| & \|\varepsilon_{zy}\varepsilon_{yy}^{-1}\| \\ \|\varepsilon_{yy}^{-1}\varepsilon_{yx}\| & \|\varepsilon_{yy}^{-1}\varepsilon_{yz}\| & \|\varepsilon_{yy}^{-1}\| \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{E}}_x \\ \tilde{\mathbf{E}}_z \\ \tilde{\mathbf{D}}_y \end{bmatrix}, \quad (3.39)$$

and then rearranged back to the original form

$$\begin{bmatrix} \tilde{\mathbf{D}}_x \\ \tilde{\mathbf{D}}_y \\ \tilde{\mathbf{D}}_z \end{bmatrix} = \mathbf{Q} \begin{bmatrix} \tilde{\mathbf{E}}_x \\ \tilde{\mathbf{E}}_y \\ \tilde{\mathbf{E}}_z \end{bmatrix}, \quad (3.40)$$

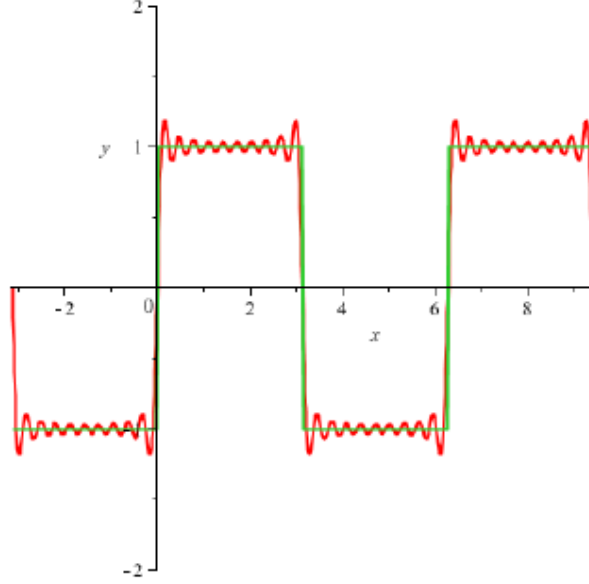


Figure 3.4: Gibbs phenomenon. The partial sums of Fourier series has large oscillations around discontinuities. This overshoot does not disappear with increasing number of terms, but approaches a finite limit. [48]

where the matrix $\mathbf{Q}$ is in the form

$$\mathbf{Q} = \begin{bmatrix} \|\varepsilon_{xx} - \varepsilon_{xy}\varepsilon_{yy}^{-1}\varepsilon_{yx}\| + \|\varepsilon_{xy}\varepsilon_{yy}^{-1}\| \|\varepsilon_{yy}^{-1}\|^{-1} \|\varepsilon_{yy}^{-1}\varepsilon_{yx}\| & \|\varepsilon_{xy}\varepsilon_{yy}^{-1}\| \|\varepsilon_{yy}^{-1}\|^{-1} & \vdots \\ \|\varepsilon_{yy}^{-1}\|^{-1} \|\varepsilon_{yy}^{-1}\varepsilon_{yx}\| & \|\varepsilon_{yy}^{-1}\|^{-1} & \vdots \\ \|\varepsilon_{zx} - \varepsilon_{zy}\varepsilon_{yy}^{-1}\varepsilon_{yx}\| + \|\varepsilon_{zy}\varepsilon_{yy}^{-1}\| \|\varepsilon_{yy}^{-1}\|^{-1} \|\varepsilon_{yy}^{-1}\varepsilon_{yx}\| & \|\varepsilon_{zy}\varepsilon_{yy}^{-1}\| \|\varepsilon_{yy}^{-1}\|^{-1} & \vdots \\ \vdots & \|\varepsilon_{xz} - \varepsilon_{xy}\varepsilon_{yy}^{-1}\varepsilon_{yz}\| + \|\varepsilon_{xy}\varepsilon_{yy}^{-1}\| \|\varepsilon_{yy}^{-1}\|^{-1} \|\varepsilon_{yy}^{-1}\varepsilon_{yz}\| & \vdots \\ \vdots & \|\varepsilon_{yy}^{-1}\|^{-1} \|\varepsilon_{yy}^{-1}\varepsilon_{yz}\| & \vdots \\ \vdots & \|\varepsilon_{zz} - \varepsilon_{zy}\varepsilon_{yy}^{-1}\varepsilon_{yz}\| + \|\varepsilon_{zy}\varepsilon_{yy}^{-1}\| \|\varepsilon_{yy}^{-1}\|^{-1} \|\varepsilon_{yy}^{-1}\varepsilon_{yz}\| & \vdots \end{bmatrix}.$$

The matrix $\mathbf{Q}$ then replaces the matrix of the Fourier coefficients $\tilde{\mathbf{E}}$ in the algorithm. It is good to notice, that in the case of non-periodic permittivity function, the matrix $\mathbf{Q}$ simplifies to the matrix $\tilde{\mathbf{E}}$. However, this is not true for the truncated Fourier expansion of the periodic permittivity function. The comparison between convergence of algorithm with and without FF can be seen in the figure 3.5. We can see that FF leads to faster and stable convergence of the algorithm.

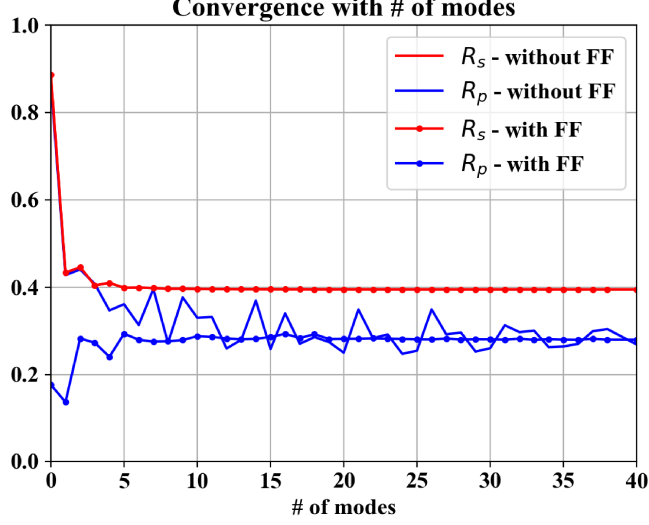


Figure 3.5: Comparison of the zero diffraction order with and without FF algorithm implemented for the same structure as in Figure 3.3. The FF algorithm converges even for small number of modes.

3.5 Experimental observables

The final S-matrix is composed of the reflection and transmission coefficients, but its structure depends on the ordering of the modes. Assuming the polarization matrices of the boundary layers are ordered according to (3.37), the transformation of the wave propagating through a layered system can be expressed as

$$\begin{bmatrix} \mathbf{A}_{up,s}^{(0)} \\ \mathbf{A}_{up,p}^{(0)} \\ \mathbf{A}_{down,s}^{(N)} \\ \mathbf{A}_{down,p}^{(N)} \end{bmatrix} = \mathbf{S} \begin{bmatrix} \mathbf{A}_{up,s}^{(N)} \\ \mathbf{A}_{up,p}^{(N)} \\ \mathbf{A}_{down,s}^{(0)} \\ \mathbf{A}_{down,p}^{(0)} \end{bmatrix}, \quad (3.41)$$

where the S-matrix is composed of the reflection and transmission coefficients

$$\mathbf{S} = \begin{bmatrix} \mathbf{t}_{ss} & \mathbf{t}_{ps} & \mathbf{r}_{ss} & \mathbf{r}_{ps} \\ \mathbf{t}_{sp} & \mathbf{t}_{pp} & \mathbf{r}_{sp} & \mathbf{r}_{pp} \\ \mathbf{\hat{r}}_{ss} & \mathbf{\hat{r}}_{ps} & \mathbf{t}_{ss} & \mathbf{t}_{ps} \\ \mathbf{\hat{r}}_{sp} & \mathbf{\hat{r}}_{pp} & \mathbf{t}_{sp} & \mathbf{t}_{pp} \end{bmatrix}. \quad (3.42)$$

$\mathbf{t}$ denotes the matrix of the transmission coefficients, $\mathbf{\hat{t}}$ denotes the matrix of the backward transmission coefficients, $\mathbf{r}$ denotes the matrix of the reflection coefficients and $\mathbf{\hat{r}}$ denotes the matrix of the backward reflection coefficients. We can define coefficients and diffraction efficiencies in

the same way as in (2.62a) and (2.62b), but we have to take into account the different k-vectors of the propagating modes. The reflectance and transmittance between the i -th mode of the m -th order in the k -th medium and the j -th mode of the n -th order in the l -th medium then take a form

$$R_{mn,ij}^{(kl)} = \left| \frac{\langle \mathbf{S}_{n,j}^{(k)}(\mathbf{r}, t) \rangle_z}{\langle \mathbf{S}_{m,i}^{(k)}(\mathbf{r}, t) \rangle_z} \right| = \left| \frac{\Re[A_{n,j}^{(k)} A_{n,j}^{(k)*} k_{z,n,j}^{(k)}]}{\Re[A_{m,i}^{(k)} A_{m,i}^{(k)*} k_{z,m,i}^{(k)}]} \right| = \left| \frac{A_{n,j}^{(k)}}{A_{m,i}^{(k)}} \right|^2 \left| \frac{\Re[k_{z,n,j}^{(k)}]}{\Re[k_{z,m,i}^{(k)}]} \right| = \quad (3.43a)$$

$$= \left| r_{mn,ij}^{(kl)} \right|^2 \left| \frac{\Re[k_{z,n,j}^{(k)}]}{\Re[k_{z,m,i}^{(k)}]} \right|,$$

$$T_{mn,ij}^{(kl)} = \left| \frac{\langle \mathbf{S}_{n,j}^{(l)}(\mathbf{r}, t) \rangle_z}{\langle \mathbf{S}_{m,i}^{(k)}(\mathbf{r}, t) \rangle_z} \right| = \left| \frac{\Re[A_{n,j}^{(l)} A_{n,j}^{(l)*} k_{z,n,j}^{(l)}]}{\Re[A_{m,i}^{(k)} A_{m,i}^{(k)*} k_{z,m,i}^{(k)}]} \right| = \left| \frac{A_{n,j}^{(l)}}{A_{m,i}^{(k)}} \right|^2 \left| \frac{\Re[k_{z,n,j}^{(l)}]}{\Re[k_{z,m,i}^{(k)}]} \right| = \quad (3.43b)$$

$$= \left| t_{mn,ij}^{(kl)} \right|^2 \left| \frac{\Re[k_{z,n,j}^{(l)}]}{\Re[k_{z,m,i}^{(k)}]} \right|.$$

4. Propagation of incoherent light in layered media

So far the methods presented dealt only with the coherent processes that can be described by the amplitude formalisms. This approach is sufficient for many applications, however a variety of processes in nature is more complicated and it also involves incoherent effects. In order to model such systems, statistical methods or methods based on transformation of intensities need to be used. The most straightforward approach is to include a random phase difference into the models and average the result over it. This method is relatively simple, but it is not feasible for computationally more demanding systems, such as periodic structures.

In this chapter, a new method based on transformation of intensities using coherence-transforming matrices is introduced and then it is generalized for periodic structures with many propagating modes. First, the concept of coherency of light is described. Then the partial wave summation method is introduced and generalized for incoherent propagation. After that, the procedure for calculating response of multilayer structures is described. In the last section, examples of numerical models are presented.

4.1 Coherence

The concept of coherence was first introduced in connection with the famous Thomas Young's double slit experiment. Coherence is an ideal property of waves, which describes the statistical similarity of a field (electromagnetic, quantum, acoustic, etc.) in two points in space or time [51–53]. Two perfectly coherent waves have constant phase difference, which enables stationary interference between them. Interference is an important physical effect that influences many practical areas of interest, in our case the light propagation through a layered media. Incoherency, the lack of correlation between propagating waves, leads to changing phase difference and can radically change the optical response of the system. It has also great effect in the systems

with active layers. The interference between various emitted waves can influence the profile of electric field in the active layer and alter the way the field is amplified. The coherence is also an important concept in the case of light sources with preferred polarization of emitted light, such as spin lasers, due to its effect on polarization. The incoherent summation of waves with different polarizations leads to the depolarization of light, which is unwanted effect and should be avoided.

Incoherent propagation in multilayer structures can have many origins. In the case of our interest, it is the process of spontaneous emission in LED and laser structures. Another important cause is a propagation through a thick substrate, which is often the case for samples on transparent substrates in optical measurements. The measurements of multilayer structures are also influenced by the technical limitations of our instruments, such as finite spectral resolution of a monochromator. This leads to decrease of temporal coherence and interference phenomena in spectral domain are suppressed. Another case is the spam of incident angles in the measured beam, as the optical response of thicker films and resonant gratings usually strongly depends on the angle of incidence. The convergence of focused optical beam could cause incoherent averaging of responses for different angles. Another cause often seen while working with prepared structures is thickness inhomogeneity. Inhomogeneity of a layer thickness over the beam spot causes incoherent averaging of different polarimetric responses. To account for these effects also in structures with lateral periodicity, next sections deal with developing a new approach to modelling of such systems.

4.2 Coherent propagation

In the first chapter, the M-matrix method for modelling of light propagation in layered media was introduced. This method is convenient for modelling of thin films, but it isn't as easily generalized for incoherent propagation. In this section, we introduce another method, partial wave summation [39] that can be easily generalized for incoherent propagation using coherence-transforming matrices. This approach is based upon summation of partially reflected and transmitted waves which form a geometric series, see Figure 4.1, and it uses the Jones calculus as its mathematical apparatus.

4.2.1 Partial wave summation method

Jones vectors describe the electric field vector on the basis of two orthogonal polarizations, in our case s- and p- (for an anisotropic case of media the propagating eigenmodes need to be

used). The transformation of the state during the propagation through optical systems is then described using 2×2 Jones matrices. To describe the interaction of propagating waves with an interface, the reflection and transmission Jones matrices $\mathbf{R}$ and $\mathbf{T}$ of k -th and $k+1$ -th layer are defined as follows:

$$\begin{bmatrix} A_{s,down}^{(k)} \\ A_{p,down}^{(k)} \end{bmatrix} = \begin{bmatrix} r_{ss}^{(k)} & r_{sp}^{(k)} \\ r_{ps}^{(k)} & r_{pp}^{(k)} \end{bmatrix} \begin{bmatrix} A_{s,up}^{(k)} \\ A_{p,up}^{(k)} \end{bmatrix} = \mathbf{R}^{(k)} \begin{bmatrix} A_{s,up}^{(k)} \\ A_{p,up}^{(k)} \end{bmatrix}, \quad (4.1a)$$

$$\begin{bmatrix} A_{s,down}^{(k)} \\ A_{p,down}^{(k)} \end{bmatrix} = \begin{bmatrix} t_{ss}^{(k)} & t_{sp}^{(k)} \\ t_{ps}^{(k)} & t_{pp}^{(k)} \end{bmatrix} \begin{bmatrix} A_{s,down}^{(k+1)} \\ A_{p,down}^{(k+1)} \end{bmatrix} = \mathbf{T}^{(k)} \begin{bmatrix} A_{s,down}^{(k+1)} \\ A_{p,down}^{(k+1)} \end{bmatrix}, \quad (4.1b)$$

where the reflection and transmission coefficients that comprise the Jones matrices $\mathbf{R}$ and $\mathbf{T}$ can be obtained using the matrix methods described in Chapter 2. Similarly are defined backward-reflection and backward-transmission Jones matrices,

$$\dot{\mathbf{R}}^{(k)} = \begin{bmatrix} \dot{r}_{ss}^{(k)} & \dot{r}_{sp}^{(k)} \\ \dot{r}_{ps}^{(k)} & \dot{r}_{pp}^{(k)} \end{bmatrix}, \quad (4.2a)$$

$$\dot{\mathbf{T}}^{(k)} = \begin{bmatrix} \dot{t}_{ss}^{(k)} & \dot{t}_{sp}^{(k)} \\ \dot{t}_{ps}^{(k)} & \dot{t}_{pp}^{(k)} \end{bmatrix}. \quad (4.2b)$$

To describe the process of propagation through a layer, similar propagation Jones matrices, as in (2.49), are defined, but now they are separate for the forward and backward propagation,

$$\mathbf{P}_{down}^{(k+1)} = \begin{bmatrix} \exp(ik_0 k_{z,s}^{(k+1)} d^{(k+1)}) & 0 \\ 0 & \exp(ik_0 k_{z,p}^{(k+1)} d^{(k+1)}) \end{bmatrix} \quad (4.3a)$$

$$\dot{\mathbf{P}}_{up}^{(k+1)} = \begin{bmatrix} \exp(-ik_0 k_{z,s}^{(k+1)} d^{(k+1)}) & 0 \\ 0 & \exp(-ik_0 k_{z,p}^{(k+1)} d^{(k+1)}) \end{bmatrix} \quad (4.3b)$$

The process of propagation is quite complicated even through one layer, as can be seen in the Figure 4.1. The incident wave is partially reflected and partially transmitted. The transmitted part propagates through the layer and is again partially reflected/transmitted at the second interface. The reflected part again propagates through the layer to the first interface where it is in the case of thin layers coherently added to the first reflected wave. As we can see, this process repeats infinitely and the partial waves form a series. In the terms of Jones calculus, the first partial transmitted wave can be described as $\mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} \mathbf{T}^{(k)} \mathbf{E}_{down}^{(k)}$, the second wave can be described as $\mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} [\dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)}] \mathbf{T}^{(k)} \mathbf{E}_{down}^{(k)}$, the third wave can be described as $\mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} [\dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)} \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)}] \mathbf{T}^{(k)} \mathbf{E}_{down}^{(k)}$, etc. After summing

all of the terms up, we get the following expression for the transmission Jones matrix:

$$\begin{aligned} \mathbf{T}^{(k \rightarrow k+2)} &= \mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} [\mathbf{I} + \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)} + \\ &\dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)} \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)} + \dots] \mathbf{T}^{(k)}, \\ &= \mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} [\mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \mathbf{Q}^3 \dots] \mathbf{T}^{(k)} \end{aligned} \quad (4.4)$$

where

$$\mathbf{Q} = \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)}. \quad (4.5)$$

We get a geometric series with limit in zero (partial waves get weaker and weaker after each reflection) that sums up to

$$\mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \mathbf{Q}^3 \dots = (\mathbf{I} - \mathbf{Q})^{-1}. \quad (4.6)$$

Using this expression in (4.4) we get

$$\begin{aligned} \mathbf{T}^{(k \rightarrow k+2)} &= \mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} (\mathbf{I} - \mathbf{Q})^{-1} \mathbf{T}^{(k)} = \\ &\mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} (\mathbf{I} - \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)})^{-1} \mathbf{T}^{(k)}. \end{aligned} \quad (4.7)$$

Similar approach can be applied to the derivation of remaining Jones matrices:

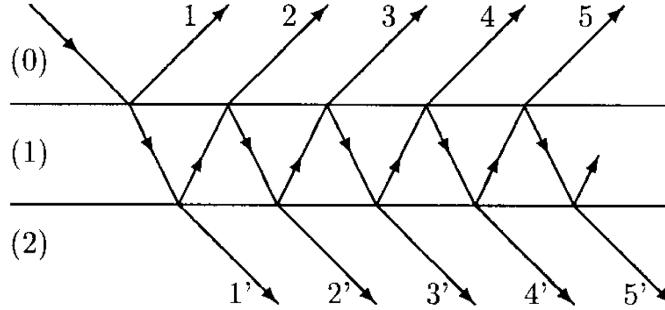


Figure 4.1: Partial waves reflected and trasmitted by a layer. The wave is partially reflected and trasmitted upon reaching any interface and bounces back and forth inside the layer. [39]

$$\mathbf{R}^{(k \rightarrow k+2)} = \mathbf{R}^{(k)} + \dot{\mathbf{T}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{up}^{(k+1)} (\mathbf{I} - \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)})^{-1} \mathbf{T}^{(k)}, \quad (4.8)$$

$$\dot{\mathbf{T}}^{(k \rightarrow k+2)} = \dot{\mathbf{T}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)} (\mathbf{I} - \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)} \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)})^{-1} \dot{\mathbf{T}}^{(k+1)}, \quad (4.9)$$

$$\dot{\mathbf{R}}^{(k \rightarrow k+2)} = \dot{\mathbf{R}}^{(k+1)} + \mathbf{T}^{(k+1)} \mathbf{P}_{down}^{(k+1)} \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{down}^{(k+1)} (\mathbf{I} - \mathbf{R}^{(k+1)} \mathbf{P}_{down}^{(k+1)} \dot{\mathbf{R}}^{(k)} \dot{\mathbf{P}}_{up}^{(k+1)})^{-1} \dot{\mathbf{T}}^{(k+1)} \quad (4.10)$$

4.2.2 Partial wave summation in layers with lateral periodicity

In the presence of periodic layers, the relations (4.7), (4.8), (4.9) and (4.10) still hold, however, there are many different propagating modes throughout the system and there exists a

coupling between individual modes which needs to be taken into account. As all the transformations are linear, the interaction of the propagating wave with an interface can be described as

$$\begin{bmatrix} \tilde{\mathbf{A}}_{s,down}^{(k)} \\ \tilde{\mathbf{A}}_{p,down}^{(k)} \end{bmatrix} = \begin{bmatrix} \mathbf{r}_{ss}^{(k)} & \mathbf{r}_{sp}^{(k)} \\ \mathbf{r}_{ps}^{(k)} & \mathbf{r}_{pp}^{(k)} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{A}}_{s,up}^{(k)} \\ \tilde{\mathbf{A}}_{p,up}^{(k)} \end{bmatrix} = \mathbf{R}^{(k)} \begin{bmatrix} \tilde{\mathbf{A}}_{s,up}^{(k)} \\ \tilde{\mathbf{A}}_{p,up}^{(k)} \end{bmatrix}, \quad (4.11a)$$

$$\begin{bmatrix} \tilde{\mathbf{A}}_{s,down}^{(k)} \\ \tilde{\mathbf{A}}_{p,down}^{(k)} \end{bmatrix} = \begin{bmatrix} \mathbf{t}_{ss}^{(k)} & \mathbf{t}_{sp}^{(k)} \\ \mathbf{t}_{ps}^{(k)} & \mathbf{t}_{pp}^{(k)} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{A}}_{s,down}^{(k+1)} \\ \tilde{\mathbf{A}}_{p,down}^{(k+1)} \end{bmatrix} = \mathbf{T}^{(n)} \begin{bmatrix} \tilde{\mathbf{A}}_{s,down}^{(k+1)} \\ \tilde{\mathbf{A}}_{p,down}^{(k+1)} \end{bmatrix}, \quad (4.11b)$$

where the vectors $\tilde{\mathbf{A}}_{s,down}^{(k)}$ and $\tilde{\mathbf{A}}_{p,down}^{(k)}$ consist of amplitudes of $(2N + 1)$ different propagating modes

$$\tilde{\mathbf{A}}_{s,down}^{(k)} = (A_{-N,s,down}^{(k)}, A_{-N+1,s,down}^{(k)}, \dots, A_{N,s,down}^{(k)})^T, \quad (4.12a)$$

$$\tilde{\mathbf{A}}_{p,down}^{(k)} = (A_{-N,p,down}^{(k)}, A_{-N+1,p,down}^{(k)}, \dots, A_{N,p,down}^{(k)})^T, \quad (4.12b)$$

and the reflection coefficient matrices are in the form of

$$\mathbf{r}_{ss}^{(k)} = \begin{bmatrix} r_{-N,-N,ss}^{(k)} & r_{-N,-N+1,ss}^{(k)} & \dots & r_{-N,N,ss}^{(k)} \\ r_{-N+1,-N,ss}^{(k)} & r_{-N+1,-N+1,ss}^{(k)} & & \vdots \\ \vdots & & \ddots & \\ r_{N,-N,ss}^{(k)} & & \dots & r_{N,N,ss}^{(k)} \end{bmatrix}, \quad (4.13a)$$

$$\mathbf{r}_{sp}^{(k)} = \begin{bmatrix} r_{-N,-N,sp}^{(k)} & r_{-N,-N+1,sp}^{(k)} & \dots & r_{-N,N,sp}^{(k)} \\ r_{-N+1,-N,sp}^{(k)} & r_{-N+1,-N+1,sp}^{(k)} & & \vdots \\ \vdots & & \ddots & \\ r_{N,-N,sp}^{(k)} & & \dots & r_{N,N,sp}^{(k)} \end{bmatrix}, \quad (4.13b)$$

etc. These matrices are the result of the application of S-matrix algorithm as seen from (3.42).

Similarly, we can define the backward reflection and transmission matrices

$$\dot{\mathbf{R}}^{(k)} = \begin{bmatrix} \dot{\mathbf{r}}_{ss}^{(k)} & \dot{\mathbf{r}}_{sp}^{(k)} \\ \dot{\mathbf{r}}_{ps}^{(k)} & \dot{\mathbf{r}}_{pp}^{(k)} \end{bmatrix}, \quad (4.14a)$$

$$\dot{\mathbf{T}}^{(k)} = \begin{bmatrix} \dot{\mathbf{t}}_{ss}^{(k)} & \dot{\mathbf{t}}_{sp}^{(k)} \\ \dot{\mathbf{t}}_{ps}^{(k)} & \dot{\mathbf{t}}_{pp}^{(k)} \end{bmatrix}. \quad (4.14b)$$

The matrices $\mathbf{R}$, $\mathbf{T}$, $\dot{\mathbf{R}}$ and $\dot{\mathbf{T}}$ behave in the same way as the Jones matrices used in the partial wave summation method and can be used in the Eq. (4.7), (4.8), (4.9) and (4.10) to obtain an optical response of a thin film.

4.3 Incoherent propagation

In the last section, the partial wave summation method was introduced as a way to describe optical response of thin films. In this section, we introduce a concept of coherence matrices and use them to generalize the partial wave summation method to thick layers where the propagation is no longer a coherent process.

4.3.1 Coherence matrix formalism

The Jones matrix formalism used for coherent summation of partial waves is a useful tool for description of totally polarized light, however, it cannot be used for description of incoherent effects which cause depolarization. For more general description of light polarization, the coherence matrix [51–53] is defined as follows:

$$\mathbf{J}_c = \langle \mathbf{E} \otimes \mathbf{E}^* \rangle = \begin{bmatrix} \langle E_x E_x^* \rangle & \langle E_x E_y^* \rangle \\ \langle E_y E_x^* \rangle & \langle E_y E_y^* \rangle \end{bmatrix} = \begin{bmatrix} J_{xx} & J_{xy} \\ J_{yx} & J_{yy} \end{bmatrix}, \quad (4.15)$$

where $\otimes$ denotes the Kronecker product and the angle brackets denote the ensemble averaging. In contrast to the Jones formalism, which deals with field amplitudes, the coherence matrix is composed of second order moments and it enables us to describe partially polarized or depolarized light. Also, the information about the phase of light is lost. The total intensity of light I and the degree of polarization P can be expressed in terms of coherence matrix components as

$$I = \text{tr}(\mathbf{J}_c) = J_{xx} + J_{yy}, \quad (4.16a)$$

$$P = \left[1 - \frac{4 \det(\mathbf{J}_c)}{[\text{tr}(\mathbf{J}_c)]^2} \right]^{1/2}. \quad (4.16b)$$

For better manipulation, the coherence matrix elements can be rearranged to a column vector and the transformation of light upon interaction can be described as

$$\mathbf{J} = \begin{bmatrix} J'_{xx} \\ J'_{xy} \\ J'_{yx} \\ J'_{yy} \end{bmatrix} = \mathcal{T} \begin{bmatrix} J_{xx} \\ J_{xy} \\ J_{yx} \\ J_{yy} \end{bmatrix}, \quad (4.17)$$

where $\mathcal{T}$ is the 4×4 coherence-transforming matrix. The coherence-transforming matrix of a non-depolarizing system can be obtained from the corresponding Jones matrix as

$$\mathcal{T} = \mathbf{T} \otimes \mathbf{T}^* = \begin{bmatrix} T_{11}T_{11}^* & T_{11}T_{12}^* & T_{12}T_{11}^* & T_{12}T_{12}^* \\ T_{11}T_{21}^* & T_{11}T_{22}^* & T_{12}T_{21}^* & T_{12}T_{22}^* \\ T_{21}T_{11}^* & T_{21}T_{12}^* & T_{22}T_{11}^* & T_{22}T_{12}^* \\ T_{21}T_{21}^* & T_{21}T_{22}^* & T_{22}T_{21}^* & T_{22}T_{22}^* \end{bmatrix}. \quad (4.18)$$

In the rest of this thesis the script letters will denote the coherence-transforming matrices. The coherence vectors and coherence-transforming matrices are connected to the well-known Stokes vectors and Mueller matrices by simple transformation

$$\mathbf{S} = \mathbf{A}\mathbf{J}, \quad (4.19a)$$

$$\mathbf{M} = \mathbf{A}\mathcal{T}\mathbf{A}^{-1}, \quad (4.19b)$$

where

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & -i & i & 0 \end{bmatrix}. \quad (4.20)$$

However, in this thesis we will use the coherence-transforming matrices in our models for their more intuitive connection to the light reflection and transmission in layered structures. The same form of the recurrent formulae, as the one used for the coherence-transforming matrices, can be also used for the Mueller matrices.

4.3.2 Incoherent partial wave summation

The generalization of the parital wave summation method for incoherent propagation using coherence-transforming matrices is based on properties of the Kronecker product that introduces a symmetry between the product of Jones matrices and the product of the corresponding coherence-transforming matrices. It can be shown that the product $\mathbf{A} = \mathbf{B}\mathbf{C}$ corresponds to the product $\mathcal{A} = \mathcal{B}\mathcal{C}$. For example, in the case of the term A_{11} , which can be expressed as

$$A_{11} = B_{11}C_{11} + B_{12}C_{21}, \quad (4.21)$$

$$\mathcal{A}_{11} = (B_{11}C_{11} + B_{12}C_{21})(B_{11}C_{11} + B_{12}C_{21})^*, \quad (4.22)$$

or by multiplying corresponding coherency-transforming matrices

$$\mathcal{A}_{11} = \mathcal{B}_{11}\mathcal{C}_{11} + \mathcal{B}_{12}\mathcal{C}_{21} + \mathcal{B}_{13}\mathcal{C}_{31} + \mathcal{B}_{14}\mathcal{C}_{41} = (B_{11}C_{11} + B_{12}C_{21})(B_{11}C_{11} + B_{12}C_{21})^*. \quad (4.23)$$

We can see that both operations lead to the same result. The rest can be easily derived in the same way. Using these properties the same approach as in the Section 4.2 can be used to describe the incoherent propagation. There are infinite partial waves reflecting in the layer (as seen in Figure 4.1) that sum up and give the final wave leaving the structure. However, in this case the summation needs to be done incoherently in terms of coherence vectors based on intensities rather than amplitudes. The transformation during partial reflection/transmission is then described using the coherence-transforming matrices $\mathcal{R}^{(n)}, \mathcal{T}^{(n)}, \dot{\mathcal{R}}^{(n)}, \dot{\mathcal{R}}^{(n)}$ etc., which are obtained using relation (4.18) (this is true for continuous layers, the case of layers with lateral periodicity will be described in the later sections). It is good to note that coherency-transforming upward- and downward- propagation matrices are in this case the same

$$\mathcal{P}_{down}^{(k+1)} = \dot{\mathcal{P}}_{up}^{(k+1)} = \mathcal{P}^{(k+1)} = \begin{bmatrix} \exp[2 \Im(k_{z,s}^{(k+1)})d^{(k+1)}] & 0 & \vdots \\ 0 & \exp[ik_0(k_{z,s}^{(k+1)} - k_{z,p}^{(k+1)*})d^{(k+1)}] & \vdots \\ 0 & 0 & \vdots \\ 0 & 0 & \vdots \\ \vdots & 0 & 0 \\ \vdots & 0 & 0 \\ \vdots & \exp[ik_0(k_{z,p}^{(k+1)} - k_{z,s}^{(k+1)*})d^{(k+1)}] & 0 \\ \vdots & 0 & \exp[2 \Im(k_{z,p}^{(k+1)})d^{(k+1)}] \end{bmatrix} \quad (4.24)$$

and there is no information about the phase after propagating through the layer which prohibits the interference between partial waves. The only interference that can be present, is due to the cross-polarization coupling in anisotropic layers. According to the same logic as before, the partial waves form a geometric series and their summation leads to the same formulas as in (4.7), (4.8), (4.9) and (4.10):

$$\mathcal{T}^{(k \rightarrow k+2)} = \mathcal{T}^{(k+1)} \mathcal{P}^{(k+1)} (\mathcal{I} - \dot{\mathcal{R}}^{(k)} \mathcal{P}^{(k+1)} \mathcal{R}^{(k+1)} \mathcal{P}^{(k+1)})^{-1} \mathcal{T}^{(k)}, \quad (4.25a)$$

$$\mathcal{R}^{(k \rightarrow k+2)} = \mathcal{R}^{(k)} + \dot{\mathcal{T}}^{(k)} \mathcal{P}^{(k+1)} \mathcal{R}^{(k+1)} \mathcal{P}^{(k+1)} (\mathcal{I} - \dot{\mathcal{R}}^{(k)} \mathcal{P}^{(k+1)} \mathcal{R}^{(k+1)} \mathcal{P}^{(k+1)})^{-1} \mathcal{T}^{(k)}, \quad (4.25b)$$

$$\dot{\mathcal{T}}^{(k \rightarrow k+2)} = \dot{\mathcal{T}}^{(k)} \mathcal{P}^{(k+1)} (\mathcal{I} - \mathcal{R}^{(k+1)} \mathcal{P}^{(k+1)} \dot{\mathcal{R}}^{(k)} \mathcal{P}^{(k+1)})^{-1} \dot{\mathcal{T}}^{(k+1)}, \quad (4.25c)$$

$$\dot{\mathcal{R}}^{(k \rightarrow k+2)} = \dot{\mathcal{R}}^{(k+1)} + \mathcal{T}^{(k+1)} \mathcal{P}^{(k+1)} \dot{\mathcal{R}}^{(k)} \mathcal{P}^{(k+1)} (\mathcal{I} - \mathcal{R}^{(k+1)} \mathcal{P}^{(k+1)} \dot{\mathcal{R}}^{(k)} \mathcal{P}^{(k+1)})^{-1} \dot{\mathcal{T}}^{(k+1)} \quad (4.25d)$$

4.3.3 Partial wave summation for multilayers with gratings

The formula (4.18) can be used for obtaining the coherence-transforming matrices of continuous layers. However, in the case of layers with lateral periodicity, where many propagating

modes are present, it is no longer so easily applicable. The simple use of the Kronecker product would lead to emergence of cross-mode terms

$$\tilde{\mathcal{J}}^{(k)} = \begin{bmatrix} \vdots \\ A_n^{(k)} A_{n+1}^{(k)*} \\ \vdots \end{bmatrix}, \quad (4.26)$$

that would result in a correlation between amplitudes of different modes, which is not present in real structures. Two approaches to prevent this in our models are presented. The first one still uses the Kronecker product according to (4.18), but zeroes out the unwanted terms. This approach is easy to implement but more computationally demanding and algorithmic efficiency grows according to $\approx (2N+1)^2$ with the number of modes. The other approach is more formal. It treats the effects of individual propagating modes separately and after constructing the individual coherence-transforming matrices separately, the final total coherence-transforming matrices are constructed. As there are no redundant terms in the process, the final matrices describing the interactions have smaller dimensions and the algorithm is faster. However, because of non-trivial rearranging of the transmission and reflection matrices, this approach is more difficult to implement and deeper understading of the algorithm details is needed.

In the first approach, we use previously defined matrices of reflection and transmission coefficients (4.11a), (4.11b), (4.14a) and (4.14b) and transform them using the Kronecker product according to (4.18). This operation leads to an emergence of the unwanted cross-mode terms mentioned earlier. To set them zero, the modified coherence-propagation matrix $\mathcal{P}^{(n+1)'}$ is defined. The indexes of non-zero terms form a sequence

$$A_1 = 1, \quad A_n = A_{n-1} + (2N+1) + \frac{1}{2} - \left(-\frac{1}{2}\right)^n. \quad (4.27)$$

Using this sequence, we define a matrix $\mathbf{B}$ with dimensions $(4N+2)^2$:

$$b_{ij} = \begin{cases} 1, & i = j \in A_n, \\ 0, & \text{otherwise.} \end{cases} \quad (4.28)$$

$(2N+1)$ is the total number of modes present. The propagation matrix $\mathcal{P}^{(n+1)'}$ is then transformed using the matrix $\mathbf{B}$

$$\mathcal{P}^{(n+1)'} = \mathcal{P}^{(n+1)} \begin{bmatrix} \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{B} \end{bmatrix}. \quad (4.29)$$

Using the modified propagation matrix $\mathcal{P}^{(n+1)'}$, the partial wave summation algorithm can be used again in the same way as for non-periodic medium. However, as the matrices have a lot of redundant terms, the algorithm is slower then it needs to be.

The second approach treats the propagating modes separately. First, let's define the Jones matrices for the reflection and transmission of n -th to m -th mode.

$$\begin{bmatrix} A_{m,s,up}^{(k)} \\ A_{m,p,up}^{(k)} \end{bmatrix} = \begin{bmatrix} r_{mn,ss}^{(k)} & r_{mn,sp}^{(k)} \\ r_{mn,ps}^{(k)} & r_{mn,pp}^{(k)} \end{bmatrix} \begin{bmatrix} A_{n,s,down}^{(k)} \\ A_{n,p,down}^{(k)} \end{bmatrix} = \mathbf{R}_{mn}^{(k)} \begin{bmatrix} A_{n,s,down}^{(k)} \\ A_{n,p,down}^{(k)} \end{bmatrix}, \quad (4.30a)$$

$$\begin{bmatrix} A_{m,s,down}^{(l)} \\ A_{m,p,down}^{(l)} \end{bmatrix} = \begin{bmatrix} t_{mn,ss}^{(k)} & t_{mn,sp}^{(k)} \\ t_{mn,ps}^{(k)} & t_{mn,pp}^{(k)} \end{bmatrix} \begin{bmatrix} A_{n,s,down}^{(k)} \\ A_{n,p,down}^{(k)} \end{bmatrix} = \mathbf{T}_{mn}^{(k)} \begin{bmatrix} A_{n,s,down}^{(k)} \\ A_{n,p,down}^{(k)} \end{bmatrix}, \quad (4.30b)$$

and similarly the backward matrices

$$\dot{\mathbf{R}}_{mn}^{(k)} = \begin{bmatrix} \dot{r}_{mn,ss}^{(k)} & \dot{r}_{mn,sp}^{(k)} \\ \dot{r}_{mn,ps}^{(k)} & \dot{r}_{mn,pp}^{(k)} \end{bmatrix}, \quad (4.31a)$$

$$\dot{\mathbf{T}}_{mn}^{(k)} = \begin{bmatrix} \dot{t}_{mn,ss}^{(k)} & \dot{t}_{mn,sp}^{(k)} \\ \dot{t}_{mn,ps}^{(k)} & \dot{t}_{mn,pp}^{(k)} \end{bmatrix}. \quad (4.31b)$$

All of these coefficients can be extracted from the total S-matrix of thin film periodic system (3.42). Now let's define the propagation matrix of the n -th mode as

$$\mathbf{P}_n^{(l)} = \begin{bmatrix} \exp(\mp i k_0 k_{n,z,s} d^{(l)}) & 0 \\ 0 & \exp(\mp i k_0 k_{n,z,p} d^{(l)}) \end{bmatrix}. \quad (4.32a)$$

The corresponding coherence-transforming matrices $\mathcal{R}_{mn}^{(k)}, \mathcal{T}_{mn}^{(k)}, \dot{\mathcal{R}}_{mn}^{(k)}, \dot{\mathcal{T}}_{mn}^{(k)}, \mathcal{P}_n^{(l)}$, which now describe transformation of just one mode, can be obtained using the relation (4.18). The propagating waves at the k -th layer can be described in terms of the coherence vectors of N propagating waves as follows:

$$\mathcal{J}_n^{(k)} = \begin{bmatrix} A_{n,s}^{(k)} A_{n,s}^{(k)*}, & A_{n,s}^{(k)} A_{n,p}^{(k)*}, & A_{n,p}^{(k)} A_{n,s}^{(k)*}, & A_{n,p}^{(k)} A_{n,p}^{(k)*} \end{bmatrix}^T, \quad (4.33)$$

$$\tilde{\mathcal{J}}_{down}^{(k)} = \left[\mathcal{J}_{-N,down}^{(k)}, \mathcal{J}_{-N+1,down}^{(k)}, \dots, \mathcal{J}_{N,down}^{(k)} \right]^T, \quad (4.34)$$

$$\tilde{\mathcal{J}}_{up}^{(k)} = \left[\mathcal{J}_{-N,up}^{(k)}, \mathcal{J}_{-N+1,up}^{(k)}, \dots, \mathcal{J}_{N,up}^{(k)} \right]^T, \quad (4.35)$$

and upon interacting with an interface they are transformed according to

$$\begin{bmatrix} \mathcal{J}_{-N,up}^{(k)} \\ \mathcal{J}_{-N+1,up}^{(k)} \\ \vdots \\ \mathcal{J}_{N,up}^{(k)} \end{bmatrix} = \begin{bmatrix} \mathcal{R}_{-N,-N}^{(k)} & \mathcal{R}_{-N,-N+1}^{(k)} & \dots & \mathcal{R}_{-N,N}^{(k)} \\ \mathcal{R}_{-N+1,-N}^{(k)} & \mathcal{R}_{-N+1,-N+1}^{(k)} & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathcal{R}_{N,-N}^{(k)} & \dots & \dots & \mathcal{R}_{N,N}^{(k)} \end{bmatrix} \begin{bmatrix} \mathcal{J}_{-N,down}^{(k)} \\ \mathcal{J}_{-N+1,down}^{(k)} \\ \vdots \\ \mathcal{J}_{N,down}^{(k)} \end{bmatrix} = \tilde{\mathcal{R}}^{(k)} \tilde{\mathcal{J}}_{n,down}^{(k)}, \quad (4.36)$$

and for transmission

$$\tilde{\mathcal{T}}^{(k)} = \begin{bmatrix} \mathcal{T}_{-N,-N}^{(k)} & \mathcal{T}_{-N,-N+1}^{(k)} & \cdots & \mathcal{T}_{-N,N}^{(k)} \\ \mathcal{T}_{-N+1,-N}^{(k)} & \mathcal{T}_{-N+1,-N+1}^{(k)} & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathcal{T}_{N,-N}^{(k)} & \cdots & \cdots & \mathcal{T}_{N,N}^{(k)} \end{bmatrix}. \quad (4.37)$$

The same relations hold for the backward matrices $\dot{\mathcal{R}}_{mn}^{(k)}, \dot{\mathcal{T}}_{mn}^{(k)}$ too. To describe the incoherent propagation through a thick layer, the total propagation matrix is constructed out of the individual mode propagation matrices,

$$\tilde{\mathcal{P}}^{(l)} = \begin{bmatrix} \mathcal{P}_{-N}^{(l)} & 0 & \cdots & 0 \\ 0 & \mathcal{P}_{-N+1}^{(l)} & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \mathcal{P}_N^{(l)} \end{bmatrix}. \quad (4.38)$$

Matrices in this form can now be used in the partial wave summation formulas (4.25a), (4.25b), (4.25c) and (4.25d) as described earlier.

4.3.4 Dimension reduction

Most of the modes propagating through the structure are evanescent and decay exponentially from the interface. In the case of thick layers, evanescent modes become negligible and do not need to be included in the computations. Because of this fact, it is convenient to reduce the dimension of the problem only to modes that are not evanescent. The number of propagating modes is dependent on the period of the grating, wavelength of the light and the angle of incidence, so it needs to be determined on the case by case basis. First, the thin layer subsystems including the periodic layers are modelled using higher dimension of the problem. However, while constructing the total coherence matrices of the thin films system, the dimensions are reduced and only few modes are used. The convergence of the solution in relation to the number of modes used for partial wave summation can be seen in the Figure 4.2. Figure shows the convergence of the zero diffraction order reflectivity R_p of the sample structure with capping thick layer motivated by flexible diffractive components, which is more closely studied in Section 4.4. The reflectivity is modelled for wavelength 400 nm and several incidence angles. We can see different behaviour for every incidence angle due to the strong diffraction dependency on the incidence angle, however, the data stabilizes for five included modes. Higher modes are evanescent and do not propagate in the thick layer, therefore they do not need to be included in calculations.

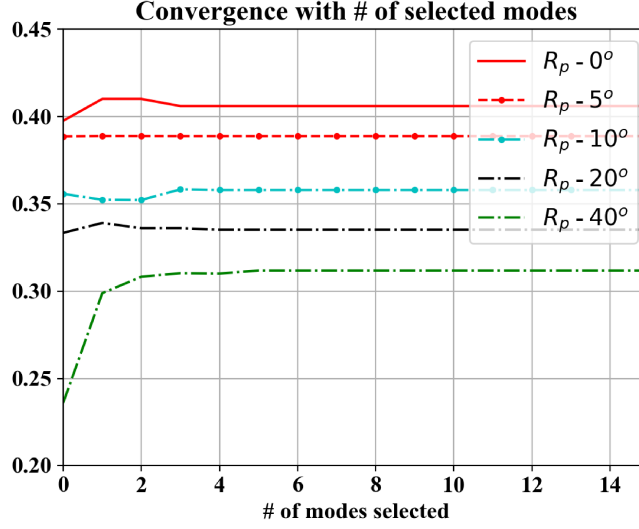


Figure 4.2: Convergence test for number of modes for the sample structure with capping thick layer motivated by flexible diffractive components studied more closely in Section 4.4. The convergence is done for the wavelength 400 nm and variable incidence angles. Dimension of the problem is twenty diffraction modes for RCWA algorithm and then reduced for incoherent partial wave summation. We can see that the reflectance R_p of the zero diffraction order converges differently for every incidence angle, but becomes stable for $N = 5$.

4.4 Multilayer system

So far in this chapter, the approach to describe a single thin/thick layer was presented. This section generalizes these methods for multilayer systems consisting of both thin and thick layers and the total reflection and transmission coherence-transforming matrices can be obtained by applying the following steps:

- The whole system of multilayers is reduced to the thin film sub-systems according to Figure 4.3.
- The reflection and transmission amplitude coefficients of these sub-systems can be obtained by applying RCWA and S-matrix algorithms.
- After calculating the reflection and transmission amplitude coefficients of the sub-systems, the Jones matrices of the subsystems are constructed. These matrices are then transformed to the corresponding coherence-transforming matrices of the interfaces and the coherence propagation matrices for the thick layers - by using the Kronecker product + B matrix, or

constructing the total coherence matrices from individual coherence-transforming matrices of the propagating modes.

- The dimension of problem is then reduced, so that only propagating waves are included.
- The incoherent partial wave summation formulae (4.25a), (4.25b), (4.25c) and (4.25d) are recurrently applied to obtain the total reflection and transmission coefficients of the whole system.

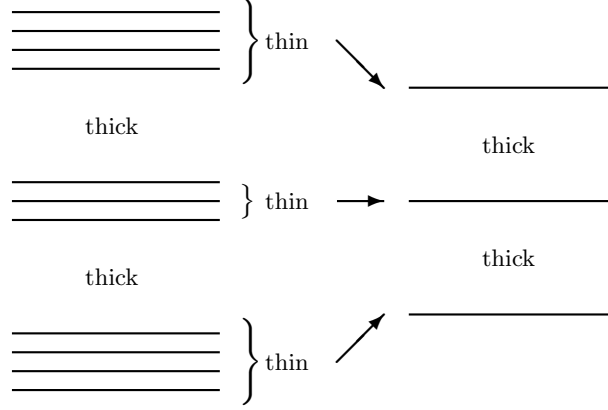


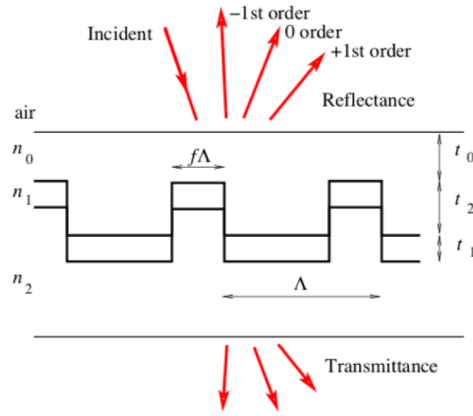
Figure 4.3: Recurrence for multilayer system consisting of thin and thick layers

4.5 Numerical models

In this section, we will study a real structure using presented methods and compare different approaches. The studied structure, seen in Figure 4.4, is motivated by flexible diffraction gratings. It consists of a relief grating in polycarbonate with applied reflective aluminium film immersed in thick UV-protection capping layer. The parameters of the model can be seen in Fig. 4.4. Due to the presence of the thick capping layer (which introduces incoherent effects), this structure is ideal for demonstration of our models for incoherent propagation in the systems with lateral periodicity.

4.5.1 Grating without the capping layer

In the first step, the grating without the capping layer was modelled. Figures 4.5 and 4.6 shows R_s and R_p reflectivities for zero and first two diffraction orders. We can see complex behaviour that is typical for gratings. The R_s for zero diffraction order vanishes around 600 nm and its energy is transferred into the first diffraction order that has its maximum around the same wavelength. Similar behaviour can be also observed for R_p reflectivity. We can see two



Thick capping UV-protected layer:
 $n_0 = 1.5$, $t_0 = 2 \mu\text{m}$
 Reflecting Aluminum film:
 $n_1 = 1 - 6i$, $t_1 = 20 \text{ nm}$
 Substrate (polycarbonate) with relief grating:
 $n_2 = 1.5$, $t_2 = 100 \text{ nm}$
 Grating period and filling factor:
 $\Lambda = 1000 \text{ nm}$, $f = 0.5$
 Angle of incidence: $\varphi_0 = 0^\circ$

Figure 4.4: Modelled grating structure motivated by flexible diffraction components.

oscillations in both figures around 525 and 750 nm. It is also interesting to note that for a wide range of wavelengths the reflectivity of the first diffraction orders is higher than that of zero diffraction orders. The second diffraction order appears only below 500 nm. Above this wavelength, the mode is evanescent and does not propagate outside the grating.

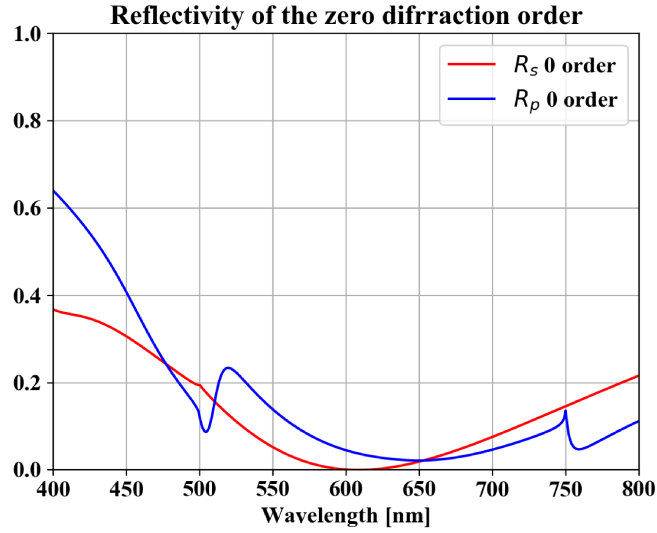


Figure 4.5: Reflectivity of the s- and p- polarization of zero diffraction order in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film motivated by flexible diffraction components. Model without the UV-protection capping layer.

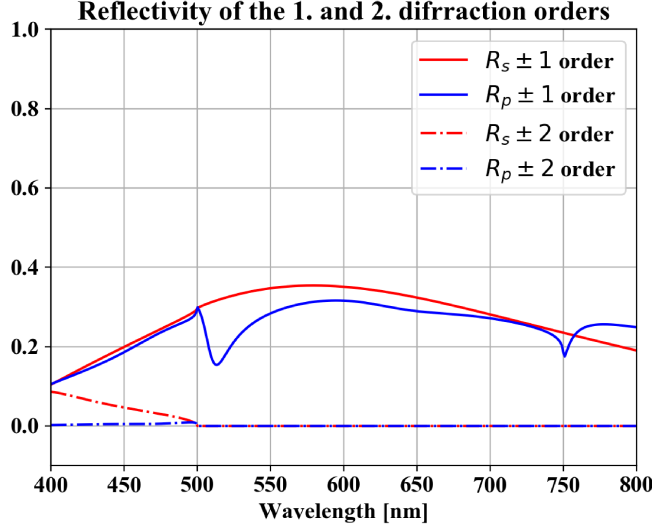


Figure 4.6: Reflectivity of the s- and p- polarization of first two diffraction orders in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film motivated by flexible diffraction components. The positive and negative diffraction orders are symmetric due to the normal incidence angle and the shape of the grating. The second orders vanish after specific wavelength.

4.5.2 Grating with the capping layer - coherent and partially coherent model

In the next step, the UV-protection capping layer was added into the model. The reflectivities R_s and R_p for zero diffraction order can be seen in Figure 4.7 and for higher diffraction orders in Figure 4.8. As the thickness of the capping layer is 2 μm , huge interference appears. However, due to the thickness non-uniformity of the capping, the propagation will not be in reality totally coherent and the observed interference will be attenuated.

Next model is assuming partially coherent propagation through the capping layer. The reflectivities are calculated for ten linearly spaced thicknesses of the capping layer in the interval from 1,8 to 2,2 μm . Then the weighted average of intensity-based quantities (reflectivity and transmittance) is calculated. The normal distribution is used as a weighting function with the mean 2 μm and 0,1 μ standard deviation (see Fig. 4.9). The averaging represents incoherent summation of waves and the interference effects are partially or completely suppressed. The results can be seen in Figures 4.10 and 4.11. We can observe the attenuation of interference, especially for shorter wavelengths, as their phase varies faster with distance. This approach is valid and correctly represents physical reality, however it is extremely computationally demanding and not practical for modelling of systems with lateral periodicity which need to work with

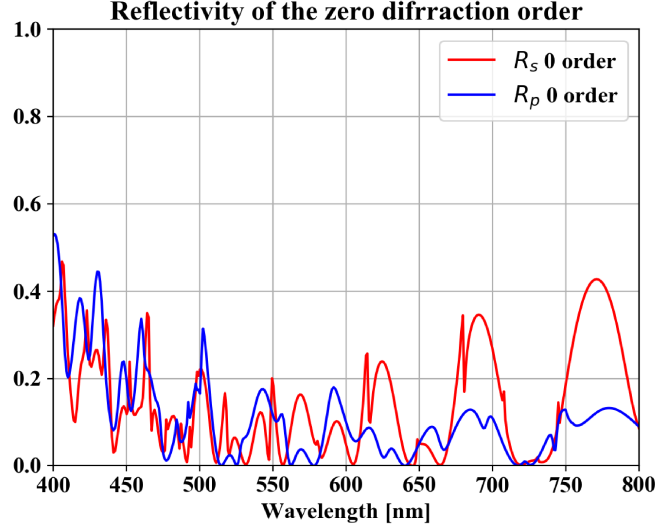


Figure 4.7: Reflectivity of the s- and p- polarization of zero diffraction order in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film immersed in UV-protection capping layer. Big interference in the capping layer appears due to the $2\text{ }\mu\text{m}$ thickness of the capping layer that would be not be observable in reality due to the effect of incoherent propagation.

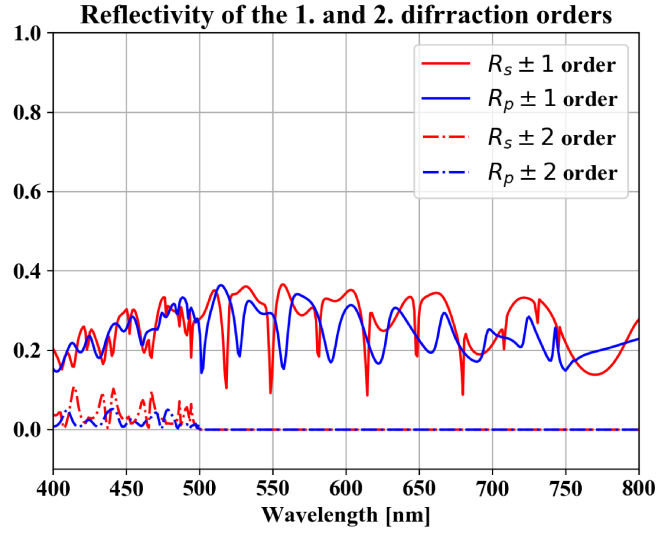


Figure 4.8: Reflectivity of the s- and p- polarization of the first two diffraction orders in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film immersed in UV-protection capping layer. Big interference in the capping layer can be also observed.

high number of modes.

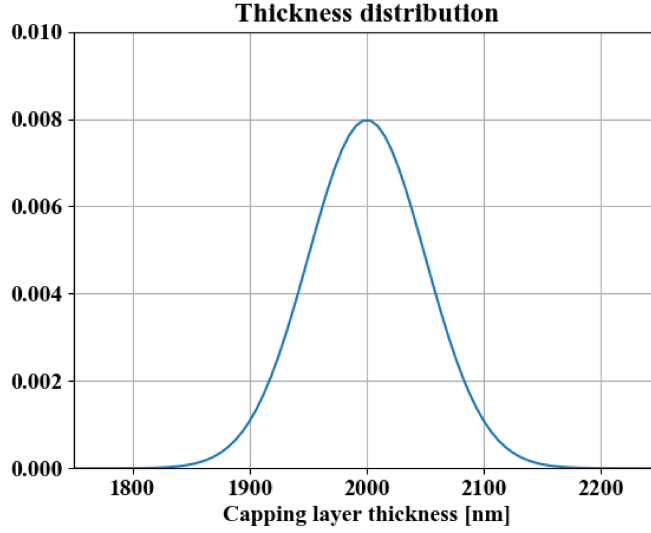


Figure 4.9: Distribution of capping layer thickness used for weighted averaging to model thickness non-uniformity, which causes incoherent propagation in the thick capping layer.

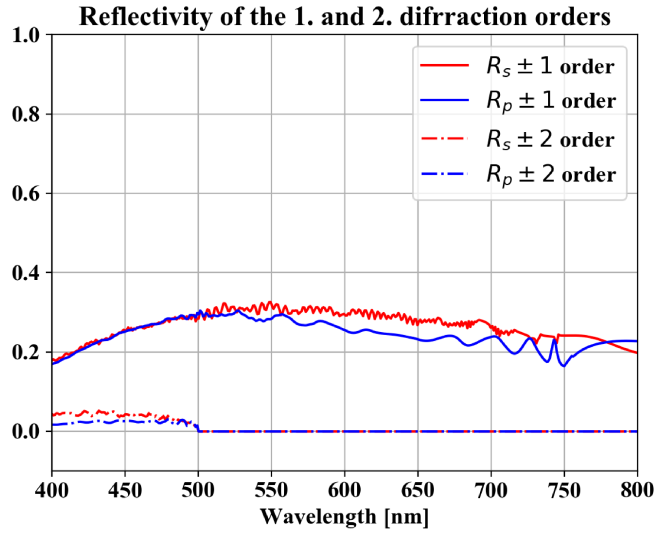


Figure 4.11: Reflectivity of the s- and p- polarization of the first two diffraction orders in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film immersed in UV-protection capping layer. The reflectance is averaged over variable thickness of capping layer to model partially coherent propagation.

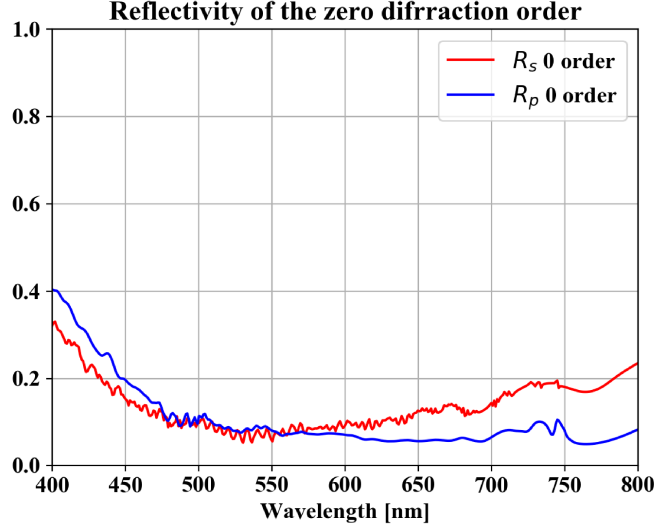


Figure 4.10: Reflectivity of the s- and p- polarization of the first two diffraction orders in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film immersed in UV-protection capping layer. The reflectance is averaged over variable thickness of capping layer to model partially coherent propagation. We can see partial attenuation of the interference, especially for shorter wavelengths, however, this model is extremely computationally demanding.

4.5.3 Grating with the capping layer - incoherent model

The last model uses incoherent partial wave summation approach developed in Section 4.3.3. The system is divided into the thin layer subsystems, consisting of the relief grating with aluminium reflective film and the interface between capping layer and air. The response of this subsystems is calculated using S-matrix and RCWA algorithms. From the reflection and transmission coefficients of these subsystems the total coherence-transforming matrices are constructed, their dimension is reduced to five propagating modes, and then they are used in partial wave summation formulae.

The results can be seen in Figures 4.12 and 4.13. We can observe that interference disappeared. If we compare this model with the grating without the capping layer, we can see that the effects of the grating are slightly less prominent. There is still a visible transfer of energy to higher modes around 500 and 750 nm, however, the reflectivity R_s of the zero diffraction order does not approach zero as for the grating without the capping layer. The trend also oscillates. The oscillations are denser in the region below 500 nm and get weaker above. This shows correlation with the appearance of higher orders below 500 nm. Both of these effects, less

prominent transfer of energy to higher modes and oscillating behaviour of reflectivity, are caused by reflections in the capping layer. The light inside the capping layer is reflected a number of times back and forth before it leaves the structure and a complex interaction with the grating takes place.

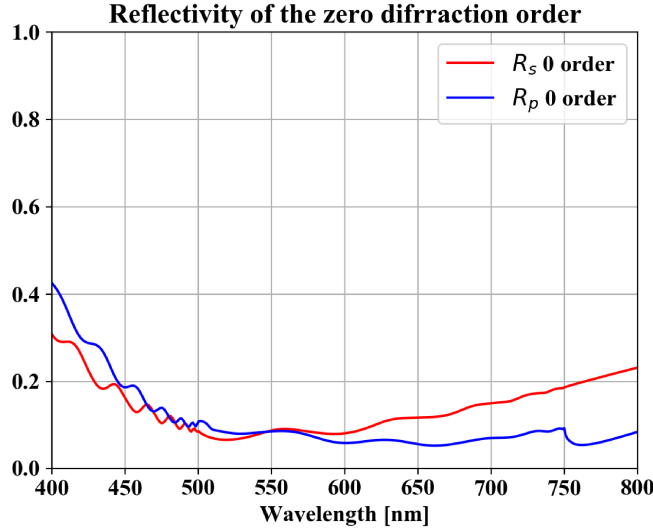


Figure 4.12: Reflectivity of the s- and p- polarization of the first two diffraction orders in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film immersed in UV-protection capping layer. The data is modelled using incoherent partial wave summation method for gratings. The interference effects in thick layer disappeared. The presence of the thick capping layer decreased the effect of the grating.

Figures 4.14 and 4.15 show the comparison of all three approaches. We can see that interferences in both coherent and partially coherent models follow the trend of incoherent model, as expected. The main advantage of the presented model of incoherent propagation in the structures with lateral periodicity is its reduced computational complexity. The computational complexity depends on many factors, such as number of propagating modes that need to be included in calculation, the efficiency of algorithms used for different matrix operations etc. In the case of our simulations, this model proved to be around 20-times faster than the model based on weighted averaging. The speed of the calculations can be further improved by reducing the dimension to the minimum amount. In Figure 4.16, we can observe the convergence of R_s zero diffraction order reflectivity for different number of modes included in incoherent summation. Above 750 nm the model converges even for single mode included in incoherent summation. In the range of 500 - 750 nm only two modes are needed and below 500 nm another higher mode appears

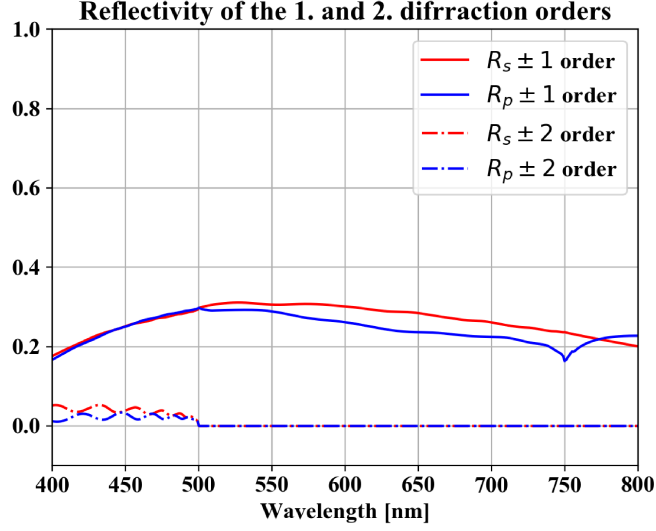


Figure 4.13: Reflectivity of the s- and p- polarization of the first two diffraction orders in the case of one dimensional relief grating in polycarbonate with applied reflective aluminium film immersed in UV-protection capping layer. The incoherent partial wave summation is used to model incoherent propagation in the thick capping layer.

and the model converges for three included modes. This is however only true for the normal incidence angle. With a change of the incidence angle new modes can appear, as we have seen in Figure 4.2, and they need to be included in the summation.

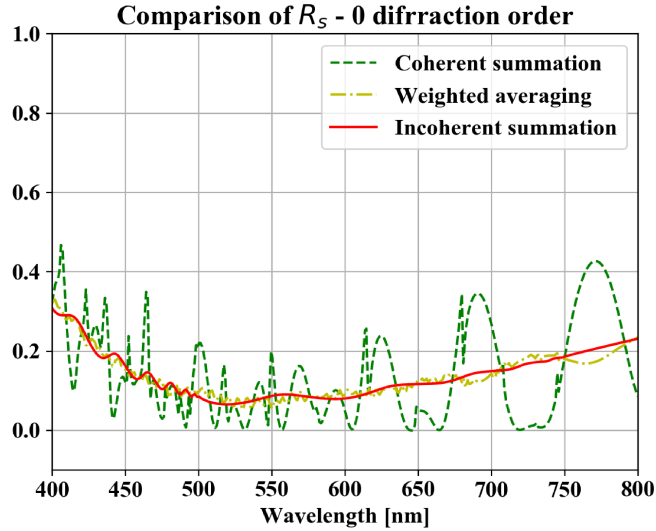


Figure 4.14: The comparison of zero diffraction order reflectivity R_s modelled by three different approaches. The data obtained using coherent and partially coherent models oscillates around the trend of the data obtained using incoherent model of propagation.

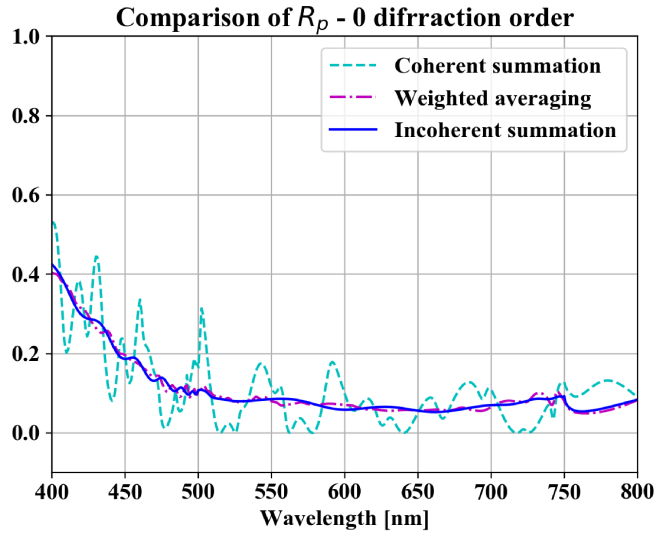


Figure 4.15: The comparison of zero diffraction order reflectivity R_p modelled by three different approaches. There is a the same trend as we have seen for the case of R_s . The same holds true for all other diffraction orders.

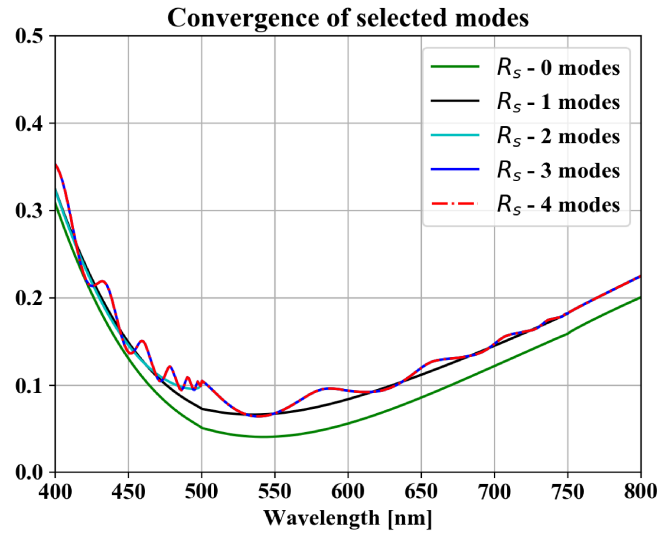


Figure 4.16: Reflectivity of the zero diffraction order R_s for two, three and four modes that were included in incoherent summation. The model converges for three included modes below 500 nm and for two modes above. Higher modes vanish above 500 nm and do not propagate out of the structure.

5. Light emission from multilayers

This chapter is devoted to modelling of light emission from multilayers containing active dipole layers, such as LEDs and VCSELs. The matrix method presented is based on the work of Fördös et. al. [17, 18, 38] and it has been used for modelling of light emission profile and polarization properties of spin-VCSELs in dependence on the spin-polarization of the injected current. However, this method relies on the averaging over random phase to account for incoherent emission processes. With the goal of combining this method with RCWA to model VCSELs containing periodic structures, this method is expressed using coherence-matrices in order to model these incoherent effects. This will bring the method into the same formalism developed in the previous chapter and it will enable the combination of the two.

5.1 Multilayers with active dipole sources

Figure 5.1 shows structure with an active layer surrounded by multilayers. $\mathbf{A}^{(0)}$ denotes the amplitudes in the superstrate, $\mathbf{A}'$ denotes the amplitudes right above the active layers and they are together related by transfer matrix $\mathbf{M}^{(1)}$ as follows:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}^{(0)} \end{bmatrix} = \begin{bmatrix} \mathbf{M}_{uu}^{(1)} & \mathbf{M}_{ud}^{(1)} \\ \mathbf{M}_{du}^{(1)} & \mathbf{M}_{dd}^{(1)} \end{bmatrix} \begin{bmatrix} \mathbf{A}'_{up} \\ \mathbf{A}'_{down} \end{bmatrix}, \quad \begin{bmatrix} \mathbf{A}'_{up} \\ \mathbf{A}'_{down} \end{bmatrix} = \begin{bmatrix} \dot{\mathbf{M}}_{uu}^{(1)} & \dot{\mathbf{M}}_{ud}^{(1)} \\ \dot{\mathbf{M}}_{du}^{(1)} & \dot{\mathbf{M}}_{dd}^{(1)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}^{(0)} \end{bmatrix}, \quad (5.1)$$

where

$$\dot{\mathbf{M}}^{(1)} = [\mathbf{M}^{(1)}]^{-1}. \quad (5.2)$$

Similarly, the amplitudes right below the active layer $\mathbf{A}''$ and the amplitudes in the substate $\mathbf{A}^{(N+1)}$ are related by transfer matrix $\mathbf{M}^{(2)}$

$$\begin{bmatrix} \mathbf{A}''_{up} \\ \mathbf{A}''_{down} \end{bmatrix} = \begin{bmatrix} \mathbf{M}_{uu}^{(2)} & \mathbf{M}_{ud}^{(2)} \\ \mathbf{M}_{du}^{(2)} & \mathbf{M}_{dd}^{(2)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(N+1)} \\ \mathbf{A}_{down}^{(N+1)} \end{bmatrix}. \quad (5.3)$$

There are four propagating modes in the multilayer structures, the waves 1 and 3 are propagating down and the waves 2 and 4 are propagating up,

$$\mathbf{A}_{down}^{(0)} = \begin{bmatrix} A_1^{(0)} \\ A_3^{(0)} \end{bmatrix}, \mathbf{A}_{up}^{(0)} = \begin{bmatrix} A_2^{(0)} \\ A_4^{(0)} \end{bmatrix}, \quad (5.4)$$

and we are also assuming that no light is entering the structure:

$$\mathbf{A}_{down}^{(0)} = \mathbf{A}_{up}^{(N+1)} = \mathbf{0}. \quad (5.5)$$

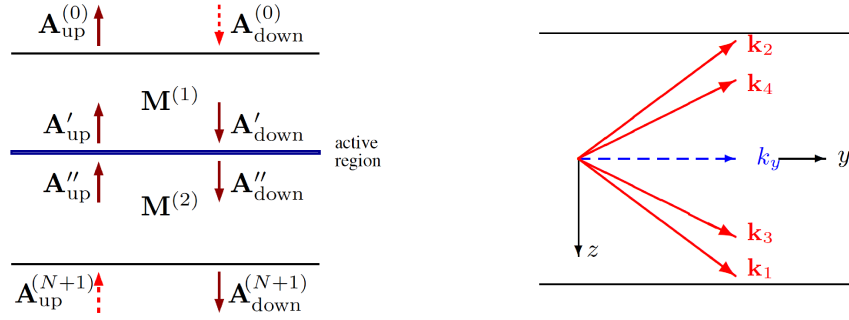


Figure 5.1: Description of the structure with a single active layer using transfer matrix approach and waves propagating in anisotropic medium. [38]

In the active medium, the propagating waves are amplified by interaction with active dipoles. The amplification of propagating waves is described using the Jones vectors of the source,

$$\mathbf{A}_{down}^d = \begin{bmatrix} A_1^d \\ A_3^d \end{bmatrix}, \mathbf{A}_{up}^d = \begin{bmatrix} A_2^d \\ A_4^d \end{bmatrix}. \quad (5.6)$$

The polarization of the source vectors is related to the emission process and is discussed in Section 5.3. The propagating wave is partially amplified by stimulated emission and it is added with light emitted by spontaneous emission (for more detailed discussion see [17]) as follows:

$$\begin{bmatrix} \mathbf{A}'_{up} \\ \mathbf{A}''_{down} \end{bmatrix} = \begin{bmatrix} \mathbf{T}_{uu} & \mathbf{0} \\ \mathbf{0} & \mathbf{T}_{dd} \end{bmatrix} \begin{bmatrix} \mathbf{A}''_{up} \\ \mathbf{A}'_{down} \end{bmatrix} + \gamma \begin{bmatrix} \mathbf{A}_{up}^d \\ \mathbf{A}_{down}^d \end{bmatrix}, \quad (5.7)$$

where γ denotes the coefficient of spontaneous emission and matrices $\mathbf{T}_{uu}$ and $\mathbf{T}_{dd}$ are in the form

$$\mathbf{T}_{uu} = \begin{bmatrix} 1 + \delta \frac{A_2^d A_2^{d*}}{|\mathbf{A}_{up}^d|} & \delta \frac{A_2^d A_4^{d*}}{|\mathbf{A}_{up}^d|} \\ \delta \frac{A_4^d A_2^{d*}}{|\mathbf{A}_{up}^d|} & 1 + \delta \frac{A_4^d A_4^{d*}}{|\mathbf{A}_{up}^d|} \end{bmatrix}, \quad (5.8a)$$

$$\mathbf{T}_{dd} = \begin{bmatrix} 1 + \delta \frac{A_1^d A_1^{d*}}{|\mathbf{A}_{down}^d|} & \delta \frac{A_1^d A_3^{d*}}{|\mathbf{A}_{down}^d|} \\ \delta \frac{A_3^d A_1^{d*}}{|\mathbf{A}_{down}^d|} & 1 + \delta \frac{A_3^d A_3^{d*}}{|\mathbf{A}_{down}^d|} \end{bmatrix}, \quad (5.8b)$$

where δ is the coefficient of stimulated emission (gain) and the norms $|\mathbf{A}_{up}^d|$ and $|\mathbf{A}_{down}^d|$ are defined as

$$|\mathbf{A}_{up}^d| = \sqrt{A_2^d A_2^{d*} + A_4^d A_4^{d*}}, \quad (5.9a)$$

$$|\mathbf{A}_{down}^d| = \sqrt{A_1^d A_1^{d*} + A_3^d A_3^{d*}}. \quad (5.9b)$$

By combining equations (5.1), (5.3) and (5.7), we get a compact matrix form [38] of the problem,

$$\begin{bmatrix} -\mathbf{M}_{uu}^{(2)} & \mathbf{T}_{uu}\mathbf{M}_{ud}^{(2)} \\ \mathbf{T}_{dd}\mathbf{M}_{du}^{(1)} & -\mathbf{M}_{dd}^{(1)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}^{(N+1)} \end{bmatrix} = -\gamma \begin{bmatrix} \mathbf{A}_{up}^d \\ \mathbf{A}_{down}^d \end{bmatrix}. \quad (5.10)$$

As spontaneous emission is not a coherent process, the terms $\mathbf{A}_{up}^d$ and $\mathbf{A}_{down}^d$ need to be added incoherently to the propagating wave. One way of achieving this is to introduce random phase factors to the source terms

$$\begin{bmatrix} A_2^d \\ A_4^d \\ A_1^d \\ A_3^d \end{bmatrix} \longrightarrow \begin{bmatrix} e^{i\varphi_2} A_2^d \\ e^{i\varphi_4} A_4^d \\ e^{i\varphi_1} A_1^d \\ e^{i\varphi_3} A_3^d \end{bmatrix} = e^{i\varphi_1} \begin{bmatrix} e^{i(\varphi_2-\varphi_1)} A_2^d \\ e^{i(\varphi_4-\varphi_1)} A_4^d \\ A_1^d \\ e^{i(\varphi_3-\varphi_1)} A_3^d \end{bmatrix} = e^{i\varphi_1} \begin{bmatrix} e^{i\Delta\varphi_2} A_2^d \\ e^{i\Delta\varphi_4} A_4^d \\ A_1^d \\ e^{i\Delta\varphi_3} A_3^d \end{bmatrix}, \quad (5.11)$$

and average intensity based quantites over random phase as follows

$$S_{out} = \langle S_{out}(\Delta\varphi_2, \Delta\varphi_3, \Delta\varphi_4) \rangle_{\varphi_2, \varphi_3, \varphi_4}, \quad (5.12)$$

where S_{out} is the Stokes vector in the form (in the case that the A_2 described s- polarization and A_2 described p-polarization)

$$\begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix} = \begin{bmatrix} A_2^{(0)} A_2^{(0)*} + A_4^{(0)} A_4^{(0)*} \\ A_2^{(0)} A_2^{(0)*} - A_4^{(0)} A_4^{(0)*} \\ A_2^{(0)} A_4^{(0)*} + A_4^{(0)} A_2^{(0)*} \\ i(A_4^{(0)} A_2^{(0)*} - A_2^{(0)} A_4^{(0)*}) \end{bmatrix}. \quad (5.13)$$

Furthermore, in case of spin-polarized light emission, certain polarizations are preferred [17] according to the quantum selection rules. Thus,

$$\varphi_2 = \varphi_4, \quad (5.14)$$

$$\varphi_1 = \varphi_3 = 0, \quad (5.15)$$

and the problem simplifies to

$$S_{out} = \langle S_{out}(\Delta\varphi_2) \rangle_{\varphi_2}. \quad (5.16)$$

5.2 Description by S-matrix algorithm

The same model as in the last section can be expressed using the S-matrix algorithm instead of the M-matrix algorithm. It is important step for integration with RCWA, as it uses the S-matrices for better stability of the algorithm, instead of the M-matrices, as boundary condition realization. Figure 5.2 shows the same multilayer structure, however, now using S-matrices to describe the propagation through multilayer above and below the active region. Similarly to (5.1) and (5.3), the amplitudes in superstrate $\mathbf{A}^{(0)}$ and right above the active region $\mathbf{A}'$ are related by the S-matrix $\mathbf{S}^{(1)}$ and the amplitudes in substrate $\mathbf{A}^{(N+1)}$ and right below the active region $\mathbf{A}''$ are related by the S-matrix $\mathbf{S}^{(2)}$ as follows:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}' \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{uu}^{(1)} & \mathbf{S}_{ud}^{(1)} \\ \mathbf{S}_{du}^{(1)} & \mathbf{S}_{dd}^{(1)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}' \\ \mathbf{A}_{down}^{(0)} \end{bmatrix} = \mathbf{S}^{(1)} \begin{bmatrix} \mathbf{A}_{up}' \\ \mathbf{A}_{down}^{(0)} \end{bmatrix}, \quad (5.17a)$$

$$\begin{bmatrix} \mathbf{A}_{up}'' \\ \mathbf{A}_{down}^{(N+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{uu}^{(2)} & \mathbf{S}_{ud}^{(2)} \\ \mathbf{S}_{du}^{(2)} & \mathbf{S}_{dd}^{(2)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(N+1)} \\ \mathbf{A}_{down}'' \end{bmatrix} = \mathbf{S}^{(2)} \begin{bmatrix} \mathbf{A}_{up}^{(N+1)} \\ \mathbf{A}_{down}'' \end{bmatrix}. \quad (5.17b)$$

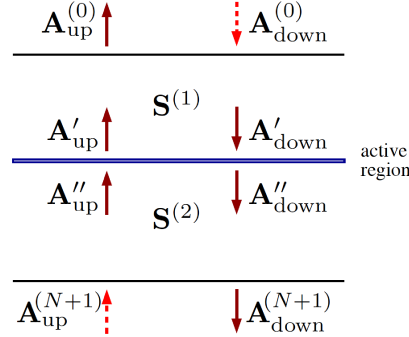


Figure 5.2: Scattering matrix description of the multilayer system with a single active layer. [38]

Again, by assuming there is no light entering the structure

$$\mathbf{A}_{down}^{(0)} = \mathbf{A}_{up}^{(N+1)} = \mathbf{0}, \quad (5.18)$$

and using the same description of amplification process as before, according to (5.7), the equations (5.17a), (5.17b) and 5.7) can be expressed in a compact matrix form [38]:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}^{(N+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{uu}^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_{dd}^{(2)} \end{bmatrix} \begin{bmatrix} \mathbf{I} & -\mathbf{T}_{uu}\mathbf{S}_{ud}^{(2)} \\ -\mathbf{T}_{dd}\mathbf{S}_{du}^{(1)} & \mathbf{I} \end{bmatrix}^{-1} \gamma \begin{bmatrix} \mathbf{A}_{up}^d \\ \mathbf{A}_{down}^d \end{bmatrix}. \quad (5.19)$$

This equation is an alternative formulation of the same problem (5.10). The treatment of the spontaneous emission is the same as before, described by (5.11) and (5.12). If the structure

consists of more active layers, it can be treated by using a recurrent approach described in Ref. [38].

5.3 Modelling of the source amplitude

This section is devoted to the discussion about finding source terms $\mathbf{A}_{up}^d$ and $\mathbf{A}_{down}^d$ that are used in the previous models. As our models aim at use for modelling of spin-polarized lasers, we will focus on recombination processes in semiconductors. Two different cases are mentioned and described. First corresponds to the light sources without spin polarized current, for which there is no preferred polarization of the emitted light. The second is the case of spin-polarized light emission, for which particular optical polarizations are preferred. However, as this topic is not the main focus of this thesis, the models are not exhaustively described and more details can be found in Ref. [17,18]. The emission process is closely related to the actual mechanisms of emission concerned and in most cases it depends on the emission angle φ . It is established that emission in a semiconductor can be represented by the electric dipole emission in the weak coupling regime (emitters are basically incoherent). The electric dipoles are vectorial point sources with any possible orientation, however, in the case of quantum well structures, typical for VCSELs, there is a preference for emission by horizontally aligned dipoles.

5.3.1 Sources without preferred polarization

In the semiconductors without spin-polarized current, there is no preference for the emitted polarization. This model was presented by Benisty et. al. [21] (see Reference for detailed explanation of the problem). The emitted intensity depends on the mutual orientation of the wave vector $\mathbf{k}$ and the dipole moment and can be decomposed into p- and s- componets as follows

$$A_s^h = A \sin \varphi, \quad (5.20)$$

$$A_p^h = A \cos \theta^{(n)} \cos \varphi = A \frac{k_z^{(n)}}{n^{(n)} k_0} \cos \varphi, \quad (5.21)$$

where φ is the azimuth and θ is elevation of $\mathbf{k}$. Furthermore, the dipole moment can have any orientation in the plane of the quantum well, so the emitted amplitudes can be averaged over φ and normalized for emitted power. The result is in the following form:

$$A_s^h = \pm \frac{3}{16\pi}, \quad (5.22)$$

$$A_p^h = \pm \frac{3}{16\pi} \frac{k_z^{(n)}}{n^{(n)} k_0}. \quad (5.23)$$

We can see, that the polarization of the emitted light changes with the emission angle. This approach was used in Reference [21] to study resonant cavity LED structures.

5.3.2 Sources with preferred circular polarization

In the case of spin-polarized lasers, circularly polarized photons are emitted due to the conservation of angular momentum during recombination process. Such sources can be viewed as two-crossed linear sources with the phase shift of $\pi/2$ and can in general be modelled by parametrized function [17] as

$$\mathbf{A}_{down,L}^d = \mathbf{A}_{up,R}^d = \begin{bmatrix} \mathcal{A}_s + \mathcal{B}_s \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0}) \\ -i(\mathcal{A}_p + \mathcal{B}_p \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0})) \end{bmatrix}, \quad (5.24)$$

$$\mathbf{A}_{down,R}^d = \mathbf{A}_{up,L}^d = \begin{bmatrix} \mathcal{A}_s + \mathcal{B}_s \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0}) \\ i(\mathcal{A}_p + \mathcal{B}_p \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0})) \end{bmatrix}, \quad (5.25)$$

where $\mathcal{A}$, $\mathcal{B}$ and l are positive constants determined by theory or experiment and the indexes R and L denote the right- and the left- circular polarizations. The total source vector is then combination of these two circularly polarized independent sources

$$\mathbf{A}_{up,down}^d = \alpha \begin{bmatrix} \mathcal{A}_s + \mathcal{B}_s \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0}) \\ -i(\mathcal{A}_p + \mathcal{B}_p \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0})) \end{bmatrix} + \beta e^{i\tilde{\varphi}} \begin{bmatrix} \mathcal{A}_s + \mathcal{B}_s \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0}) \\ i(\mathcal{A}_p + \mathcal{B}_p \cos^l(\frac{k_z^{(n)}}{n^{(n)}k_0})) \end{bmatrix}, \quad (5.26)$$

where the coefficients α and β depend on the transition probabilities and spin-current polarization. As the two sources are incoherent, random phase factor $\tilde{\varphi}$ for isotropic case is introduced. This approach is used in Ref. [17] to calculate the emission profiles and the polarization of the emitted light from spin-VCSEL structures containing magneto-optically active layers as a function of spin-polarization and it leads to the combination of the dipole sources

$$\mathbf{A}_{up,down}^d = \frac{n_+}{n_+ + n_-} \left[\sqrt{\xi_{HH}} \begin{pmatrix} 1 \\ -i \cos \theta^{(n)} \end{pmatrix} + e^{i\tilde{\varphi}} \sqrt{\xi_{LH}} \begin{pmatrix} 1 \\ i \cos \theta^{(n)} \end{pmatrix} \right] + \frac{n_-}{n_+ + n_-} \left[\sqrt{\xi_{LH}} \begin{pmatrix} 1 \\ -i \cos \theta^{(n)} \end{pmatrix} + e^{i\tilde{\varphi}} \sqrt{\xi_{HH}} \begin{pmatrix} 1 \\ i \cos \theta^{(n)} \end{pmatrix} \right], \quad (5.27)$$

where n_+ , n_- are spin-polarized carriers densities and ξ_{HH} , ξ_{LH} are normalized transition probabilities for light and heavy hole transitions. This model assumes independence of stochastic HH and LH transitions.

5.3.3 Transformation of emitted field upon refraction

For the process of calculating outside power emitted by the structure, it is important to also account for the change of the solid angle upon refraction. This section briefly introduces the approach described by Benisty et. al. and for more detailed discussion see [21]. The power per unit solid angle and surface area $\Pi = dP/d\Omega dS$ is related to the same quantity in the source layers as

$$\frac{\Pi}{\Pi_i} = \frac{dP}{dP_i} \frac{d\Omega_i}{d\Omega}, \quad (5.28)$$

where the index i denotes the source layer. The first factor denotes the power transmission coefficient, which is related to the Poynting vector flux $\mathbf{S}_p$ as

$$\frac{dP}{dS} = \frac{\mathbf{S}_p \cdot d\mathbf{S}}{dS} = |E|^2 \frac{k_z}{k}, \quad (5.29)$$

therefore [see also (2.66b)],

$$\frac{dP}{dP_i} = \frac{|E|^2 \frac{k_z}{k}}{|E_i|^2 \frac{k_{z,i}}{k}}. \quad (5.30)$$

The second term describing the change of the solid angle can be expressed as (see Ref. [55] for examples and more detailed description)

$$\frac{d\Omega_i}{d\Omega} = \frac{nk_z}{n_i k_{z,i}} \quad (5.31)$$

The total outside power is then

$$\Pi = |E|^2 \frac{nk_z^2}{n_i k_{z,i}^2} \Pi_i = |E_{out}|^2 \frac{nk_z^2}{n_i k_{z,i}^2}, \quad (5.32)$$

where E_{out} denotes the calculated outside field, according to (5.10) or (5.19), modulated by the refraction factor.

5.4 Coherence-matrix based approach

The approach to modelling of multilayers with active dipole layers is so far dependent on averaging over random phase factor to take into account incoherent effects. As we mentioned before, this processes is not efficient and becomes extremely computationally demanding in the case of multilayers containing layers with lateral periodicity. Here we propose an alternative approach for modelling of incoherent propagation based on coherence-transforming matrices can be used. This would enable incorporating layers with lateral periodicity into multilayers above

or below the active region and it would enable us modelling of VCSELs with periodic gratings or photonic crystals.

The main issue with expressing models of active layers using coherence-transforming matrices is to correctly separate the coherent and incoherent processes in the equation. The terms with the same random phase factor need to be added coherently, so it needs to be done by adding the amplitude-based Jones matrices. After adding all the coherent terms, we are left with the terms with different random phase factors that need to be added incoherently. In this step, the Jones matrices are transformed into coherence-transforming matrices and the final expression is obtained. Let's demonstrate this process on the following example. We have a system containing the source with preferred polarization described by the equation

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}^{(N+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{uu}^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_{dd}^{(2)} \end{bmatrix} \begin{bmatrix} \mathbf{I} & -\mathbf{T}_{uu}\mathbf{S}_{ud}^{(2)} \\ -\mathbf{T}_{dd}\mathbf{S}_{du}^{(1)} & \mathbf{I} \end{bmatrix}^{-1} \gamma \begin{bmatrix} e^{i\Delta\varphi_2} \mathbf{A}_{up}^d \\ \mathbf{A}_{down}^d \end{bmatrix}. \quad (5.33)$$

There are two different phase factors, terms with vector $\mathbf{A}_{up}^d$ and with vector $\mathbf{A}_{down}^d$. All the terms containing the same phase factor are coherent processes. They can be summed up and expressed using single compact matrix as follows:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}_{down}^{(N+1)} \end{bmatrix} = \mathbf{G} \begin{bmatrix} e^{i\Delta\varphi_2} \mathbf{A}_{up}^d \\ \mathbf{A}_{down}^d \end{bmatrix} = \begin{bmatrix} \mathbf{G}_{uu} & \mathbf{G}_{ud} \\ \mathbf{G}_{du} & \mathbf{G}_{dd} \end{bmatrix} \begin{bmatrix} e^{i\Delta\varphi_2} \mathbf{A}_{up}^d \\ \mathbf{A}_{down}^d \end{bmatrix}. \quad (5.34)$$

Now, there are only two terms with different phase factors that need to be added incoherently. The submatrices can be transformed into the coherence-transforming matrices using the Kronecker product

$$\mathcal{G}_{uu} = \mathbf{G}_{uu} \otimes \mathbf{G}_{uu}^*, \quad (5.35)$$

$$\mathcal{G}_{ud} = \mathbf{G}_{ud} \otimes \mathbf{G}_{ud}^*, \quad (5.36)$$

$$\mathcal{G}_{du} = \mathbf{G}_{du} \otimes \mathbf{G}_{du}^*, \quad (5.37)$$

$$\mathcal{G}_{dd} = \mathbf{G}_{dd} \otimes \mathbf{G}_{dd}^*, \quad (5.38)$$

and the final equation takes the form

$$\begin{bmatrix} \mathcal{A}_{up}^{(0)} \\ \mathcal{A}_{down}^{(N+1)} \end{bmatrix} = \begin{bmatrix} \mathcal{G}_{uu} & \mathcal{G}_{ud} \\ \mathcal{G}_{du} & \mathcal{G}_{dd} \end{bmatrix} \begin{bmatrix} \mathcal{A}_{up}^d \\ \mathcal{A}_{down}^d \end{bmatrix}, \quad (5.39)$$

where the transformation is no longer expressed using the Jones vector but by using the Coherence vectors. Coherence vectors can then be transformed into the Stokes vectors according to (4.19a) and the same result as from averaging over the random phase factors in (5.16) is obtained. As this approach doesn't depend on averaging over the phase factor $\delta\varphi_2$, it is a more efficient and it allows adding of layers with lateral periodicity into the model.

	air superstrate	$n^{(0)} = 1$
	incident wavelength	$\lambda = 680 \text{ nm}$
$\lambda \backslash n^{(1)}$ thick	layer 1	$n^{(1)} = 2$
$\lambda \backslash n^{(2)}$ thick	layer 2	$n^{(2)} = 3.6$
	active layer	
	coefficient of spontaneous emission	$\gamma = 1$
	coefficient of stimulated emission	$\delta = 0$
$\lambda \backslash n^{(2)}$ thick	layer 2	$n^{(2)} = 3.6$
$\lambda \backslash n^{(1)}$ thick	layer 1	$n^{(1)} = 2$
	air substrate	$n^{(0)} = 1$

Table 5.1: Parameters of the modelled LED structure.

5.5 Numerical models

In this section, we demonstrate validity of the approach based on coherence-matrices in comparison to result obtained by averaging over random phase on a simple LED structure. The modelled structure can be seen in Figure 5.3. It consists of one active layer surrounded by symmetrical multilayer and the emission is modelled for the parameters seen in Tab. 5.1. As our goal is just to compare both algorithms, very simple isotropic model without stimulated emission was chosen. Also for simplicity, the simple source vectors emitting only s- polarization

$$\mathbf{A}_{down}^d = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \mathbf{A}_{up}^d = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad (5.40)$$

that are not dependent on the emission angle, were chosen.

The comparison of the normalized S_0 component of the emitted Stokes vector modelled by both approaches can be seen in Figure 5.4. The emission profile without averaging is also shown. We can see typical emission profile with the maximum for the normal emission angle. Both algorithms give us the same result with a small difference for the normal emission due to the statistical nature of averaging over a finite set of values. The model without averaging is completely different. All components of the emitted Stokes vector can be seen in Figure 5.5. The data shows that the s- polarized light was emitted ($S_0 = S_1$ and other components are zero) for every emission angle, as expected for the isotropic system and the source term chosen. For better view of the emission profile, the polar plot of emitted intensity is also shown in Figure

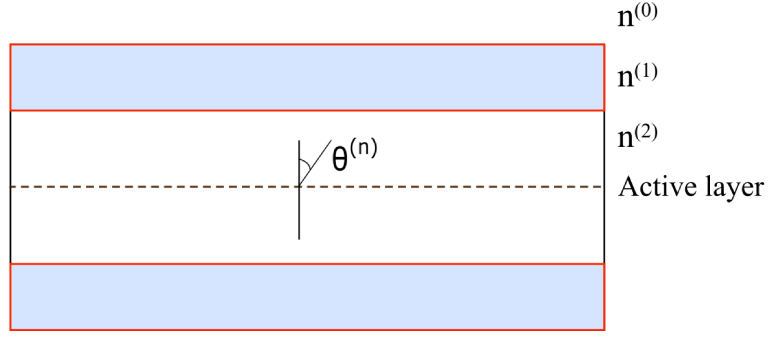


Figure 5.3: Simple LED structure that is modelled for comparison of coherence-matrix based approach with averaging over random phase factor.

5.6.

As the coherence-matrix based model shows a good agreement with previously developed models, it proves to be a useful approach of modelling of the incoherent processes in the structures with active layers. It is also more efficient approach and can help us incorporate layers with lateral periodicity into multilayer models with active regions, where we now avoid averaging over many phase factors.

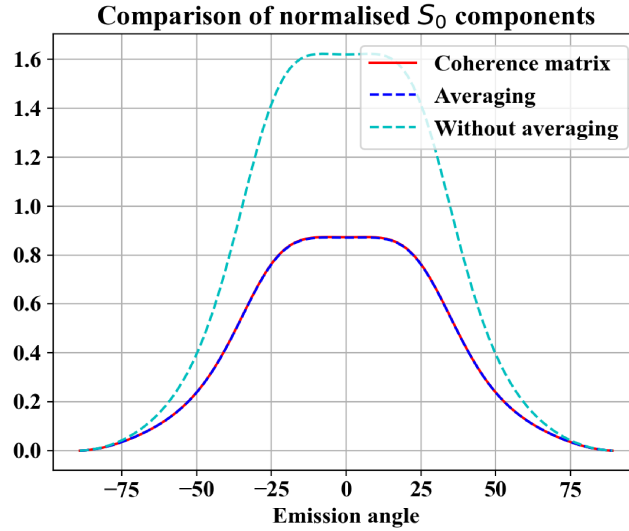


Figure 5.4: Comparison of S_0 component of emitted light obtained using coherence-matrix based model, model of averaging over random phase factor and without averaging. Both coherence-matrix and statistical approach gave us the same result with small differences for normal emission due to the averaging over finite set of values.

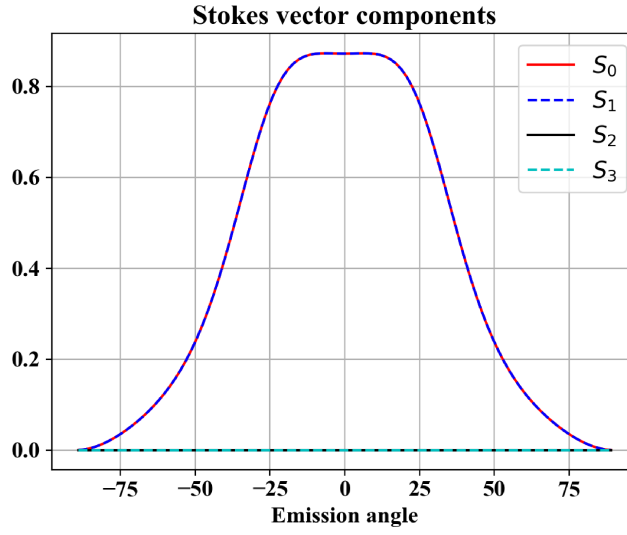


Figure 5.5: Dependence of Stokes components of emitted light on emission angle. The s-polarization is emitted for every emission angle, as expected for isotropic multilayer and the source choosen.

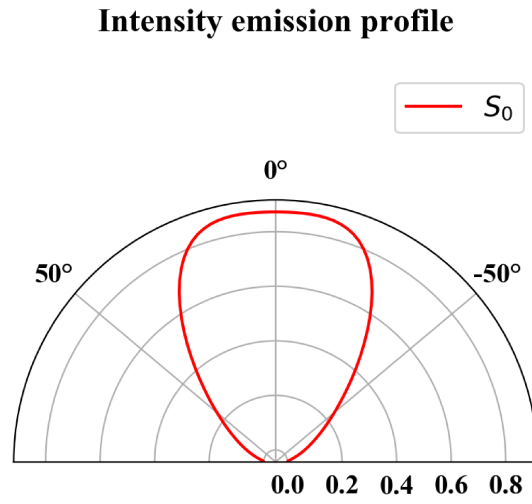


Figure 5.6: Emission profile of the emitted intensity. The light is emitted in a cone with maximum at normal emission.

6. Conclusions

The goal of this thesis was understanding of RCWA, its application to anisotropic 1D grating structures and modelling of light emission from structures containing active layers with the aim of combining these approaches to model active structures containing layers with lateral periodicity. In order to do so, a new formalism for modelling of incoherent propagation in grating structures was developed.

The original results of the thesis are:

- Developing a new formalism for modelling of incoherent propagation in grating structures (Sections 4.3 and 4.4) that solves the problem of combining models of active structures with RCWA due to the treatment of incoherent processes by averaging over random phase factor.
 - Application of the developed formalism to models of flexible diffractive components including incoherent propagation in the thick capping layer and the comparison with the coherent and partially coherent models (Section 4.5).
- Expressing the models of active structures in terms of coherence matrix based formalism making them compatible with RCWA (Section 5.4).
 - Demonstrating the validity of the coherence matrix based approach on a simple LED structure and comparing it with the method of averaging over random phase factor (Section 5.5).

The results of this thesis leave us with a lot of future prospects. The goals of the future research are following:

- To check models validity by comparing results of our models with the actual experimental data measured on the flexible diffractive gratings by Mueller matrix ellipsometry.

- To combine RCWA with the models of active structures by the use of the formalism developed in this thesis.
- Use of the models of incoherent propagation in grating structures for modelling of flexible diffractive optics components, such as security holograms.
- To generalize the developed formalism of incoherent propagation for 2D periodic structures, such as arrays of quantum dots [56, 57] or photonic crystals.
- To model actual spin-VCSEL structures in order to understand the underlying processes and to design spin-lasers for future applications.

I will continue in my research during my PhD studies that I will do in co-tutelle program at Ècole Polytechnique in Paris and VŠB-Technical University of Ostrava on the topic of Modeling of spin-lasers with lateral periodicity, for which I was granted the French Government scholarship.

Contributions:

P. Ciompa, K. Postava, T. Fördös, H. Jaffrès, J. Peřina, J. Piřtora, "Modelling of incoherent propagation in periodic structures", *Optics Express*, to be submitted

K. Postava, P. Ciompa, J. Piřtora, "Modelling of ellipsometric response from periodic structures including incoherent propagation", *10th Ellipsometry Workshop*, 19th - 21st March, 2018 in Chemnitz, Germany

P. Ciompa, K. Postava, T. Fördös, H. Jaffrès, J. Piřtora, "Modelling of incoherent propagation in periodic structures", *21st Czech-Polish-Slovak Optical conference on Wave and Quantum aspects of contemporary optics*, 3. 7. September, 2018, Lednice, Czech Republic

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