

## Theoretical and experimental study of novel integrated magnetoplasmonic nanostructures

Lukas Halagacka

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par

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# Etude théorique et expérimentale de nanostructures magnétoplasmoniques intégrées

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I declare I elaborated this thesis by myself. All literary sources and publications I have used had been cited.

Dedicated to Soňa.

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## Abstracts

#### Abstract

This work studies the enhancement of the transverse magneto-optical Kerr effect by exploiting extraordinary resonances occurring in 1D periodic grating. The 1D periodic gold grating structure was designed, described, numerically simulated, and fabricated. A rigorous Coupled Wave Algorithm (RCWA) developed for parallel computing is used for the theoretical study of resonant modes in magnetoplasmonic gratings and for analysis of optical and magneto-optical data measured by Mueller matrix ellipsometry. The impact of coupling between Fabry-Perot modes inside grating air-gaps and surface plasmon mode at the interface between gold and MO garnet layer is studied via spectra of specular reflectivity and for the various angles of incidence. In a first step, the optical functions of the (CaMgZr)-doped gallium-gadolinium garnet (sGGG) substrate and the Bisubstituted gadolinium iron garnet (Bi:GIG) are obtained in the spectral range from 0.73 eV to 6.42 eV (wavelength range 193 nm – 1.7  $\mu$ m). Subsequently, the spectra of the magneto-optical tensor components are obtained by applying an external in-plane magnetic field in longitudinal and transverse geometry. The obtained functions are then used for numerical simulations demonstrating that by hybridization of surface and cavity resonances in this 1D plasmonic grating, the transverse Kerr effect can be further enhanced, extinguished or even switched in sign and that without inverting or modifying the film's magnetization. To confirm theoretical results a set of samples, gratings with a different width of an airgap, was fabricated using electron beam lithography and liftoff technique. To be able to reproduce Mueller matrix data from the samples, the models describing realistic structures were further developed and optimized. Experimental measurements of real structures confirm transverse MO effect enhancement using magnetoplasmonic effects and prove applicability of numerical models.

**Keywords:** magneto-optic, optical isolation, transverse Kerr effect, gratings, plasmonics, magnetoplasmonics, ellipsometry, RCWA

#### Abstrakt

Tato práce je zaměřena na studium zesílení transversáního magnetooptikého Kerrova jevu pomocí resonančních módů v jednodimenzionální (1D) periodické mřížce. Studovaná struktura sestává ze zlaté mřížky na dielektrickém substrátu tvořeném magnetooptickým granátem. Dva základní typy resonančních módů, resonance ve vzduchové kavitě mřížky a resonance povrchového plasmonu na rozhraní mezi zlatem a magnetooptickýcm granátem, jsou studovány samostatně a posléze je analyzován vliv jejich interakce na optickou a magnetooptickou odezvu. Optická a magnetooptická odezva je studována pomoci spekter spekulární reflektivity pro p-polarizovanou vlnu. Magnetoplasmonická struktura byla teoreticky studována prostřednictvím numerických simulací a posléze byl navrhnut a vyroben soubor vzorků pro experimentální optická a magnetooptická měření. Pro numerické simulace byl implementován algoritmus vázaných vln (Rigorous Coupled Wave Algorithm, RCWA) pro 1D periodické systémy, který byl paralelizován pro spektrální úlohy. Experimentální optická a magnetooptická data byla získána pomocí spektroskopické elipsometrie Muellerových matic ve spektrálním rozsahu 0.73-6.42 eV (193 nm-1.7  $\mu$ m). Elipsometrie Muellerových matic byla rovněž použita pro určení optických funkcí použitých materiálů. Pro substrát byl použit galium-gadoliniový granát dopovaný pomoci Ca, Mg a Zr. Na substrátu byla připravena vrstva magnetooptického, Bi-substituovaného gadolinium - železitého granátu (Bi:GIG). V dalším kroce bylo na vrstvu magnetooptického granátu (Bi:GIG) na sGGG substrátu aplikováno vnější magnetické pole v transvezální a longitudinální magnetooptické konfiguraci a byly určeny magnetooptické funkce. Takto získané materiálové parametry jsou použity v numerických simulacích. Podrobnou analýzou je předvedeno ovlivnění interakce mezi plasmonovým módem a módem v kavitě mřížky změnou geometrických parametrů mřížky. Následně je analyzován vliv interakce na transversální magnetooptickou odezvu a je demonstrován proces zesílení, ztlumení nebo dokonce změny znaménka Kerrova transversálního magnetooptikého jevu aniž by byla změněna magnetizace. Pro potvrzení teoretických výsledků byl navrhnut soubor vzorků s rozdílnou šířkou vzduchové mezery. Vzorky byly vyrobeny elektronovou litografií a procesem liftoff. Pro vyrobené vzorky byl vyvinut teoretický model, který byl následnou numerickou optimalizací fitován na experimentální optická data, čímž byl získám model věrně popisující optickou aktivitu vyrobených struktur. Shoda numerických dat, získaných pomocí optimalizovaného modelu, a změřených experimentálních dat potvrdila dřívěji získané teoretické poznatky o zesílení transversálního magnetooptického jevu pomocí magnetoplasmonické struktury a jeho ovlivnění vzájemnou interakcí resonančních módů.

**Klíčová slova:** magnetooptika, optická isolace, tranversání Kerrův jev, mřížka, povrchový plasmon, magnetoplasmon, elipsometrie, RCWA

#### Résumé

Ce travail porte sur l'exaltation de l'effet magnéto-optique (MO) Kerr transverse induite par des résonances « extraordinaires » dans un réseau d'or périodique 1D déposé sur un oxyde de grenat magnéto-optique. La structure complète incluant le réseau métallique 1D a été conçue, simulée numériquement, dimensionnée, fabriquée puis caractérisée. Un algorithme de type RCWA (Rigorous Coupled Wave Algorithm) adapté au calcul parallèle a été développé et utilisé d'une part pour l'étude théorique des modes résonants dans les réseaux magnétoplasmoniques et d'autre part pour l'analyse des données de mesures optiques et magnéto-optiques d'ellipsométrie à base de matrices de Mueller. L'impact sur la réflectivité angulospectrale du couplage entre les modes Fabry-Pérot des fentes du réseau et les plasmons de surface à l'interface entre l'or et la couche de grenat MO est ainsi étudié, en utilisant les paramètres optiques et magnéto-optiques réels des matériaux. Pour cela, les caractéristiques optiques du substrat en sGGG (grenat de gallium et gadolinium dopé CaMgZr) et du matériau Bi :GIG (grenat de fer et de gadolinium substitué bismuth) sont au préalable déterminés dans la gamme spectrale 0,73 - 6,42 eV (193 nm-1,7  $\mu$ m) par ellipsométrie à base de matrices de Mueller. Puis de même la dispersion des composantes magnéto-optiques du tenseur diélectrique est obtenue en appliquant un champ magnétique externe dans le plan, en configuration longitudinale ou transverse. Ces données mesurées sont alors utilisées dans les simulations. Il est ainsi démontré numériquement que grâce à l'interaction des résonances de surface et de cavité dans le réseau 1D l'effet Kerr transverse peut être exalté, éteint ou même de signe inversé, et cela sans renverser ou modifier l'aimantation de la couche magnéto-optique. Pour confirmer les résultats théoriques, une série d'échantillons comportant des réseaux de fentes différentes a été fabriquée par lithographie électronique et procédé de lift-off. Afin de reproduire les données des matrices de Mueller mesurées, les modèles ont été adaptés et optimisés pour tenir compte des imperfections des structures réelles. Les mesures expérimentales confirment l'exaltation de l'effet Kerr magnéto-optique transverse due aux effets magnéto-plasmoniques et prouvent la validité des modèles.

**Mots clés:** magnéto-optique, isolation optique, effect Kerr transverse, réseaux, plasmonique, magnéto-plasmonique, ellipsométrie, RCWA

## Contents

Acknow	ledgment i
Abstract	s iii
Contents	vii vii
<b>Résume</b> Introd Méthe Prépa Simu Résul Conc	S en françaisixductionixductionixode numérique employéexiiuration des échantillons et caractérisationxiiilations numériques et basesxviitats expérimentauxxxivclusion et perspectivesxxix
1 Intro 1.1 1.2 1.3 1.4	duction1Motivation: optical isolation3State of the art in nonreciprocal plasmonics9Objective of this work and used approaches11Organization of the thesis13
2 Theo 2.1 2.2 2.3 2.4 2.5 2.6 2.7 2.8	retical background15Light polarization15Maxwell equations in general media17Solution of Maxwell's equations in layered media21Boundary conditions - field matching at interfaces30Solution of the Maxwell equations in the 1D periodic media33Li-Factorization rules for 1D gratings41Experimental observables43Conclusion of the chapter47
<b>3 Samp</b> 3.1 3.2 3.3 3.4 3.5	<b>ble preparation and characterization 49</b> Fabrication of MO Bi:GIG layer by liquid phase epitaxy 49       49         Mueller matrix ellipsometry

4 Numerical simulations and fundamentals	71
4.1 Simulated structure - 1D grating	. 72
4.2 Analytical formulae of the grating's resonances	
4.3 Geometrical dispersion of resonant modes.	86
4.4 Anticrossing of resonant modes, field plots	95
4.5 Nonreciprocal optical response of grating's resonant modes .	96
4.6 Proposition of waveguiding structure with nonreciprocal di	S-
persion of TM modes	102
4.7 Conclusion of the chapter	108
5 Experiments	109
5.1 Optical characterization of samples	109
5.2 Global fit of fabricated samples	122
5.3 Transverse magneto-optical response of the sample	126
5.4 Impact of modes coupling to optical and MO response	130
5.5 Conclusion of the chapter	134
Achieved results and Perspectives	135
Achieved results	135
Perspectives	137
A Parallel implementation of the RCWA	139
A.1 Parallelization and scalability	139
Used abbreviations and symbols	143
List of figures	146
List of tables	151
List of publications	151
List of publications	152
References	155

## Résumé en français

#### Introduction

Dans ce travail intitulé Etude théorique et expérimentale de nanostructures magnétoplasmoniques intégrées innovantes, je me suis concentré sur l'étude optique et magnéto-optique de structures plasmoniques périodiques. La principale motivation de mes recherches était l'étude de structures avec une résonance optique non réciproque pour les télécoms optiques. Le domaine des fonctionnalités optiques non réciproques a été l'objet d'une étude approfondie dès l'essor des télécoms optiques

Les composants optiques non réciproques les plus connus sont les isolateurs optiques, qui sont utilisés dans les télécoms optiques pour la protection des diodes laser vis à vis de la rétroaction optique. Durant les dix dernières années ont été étudiés plusieurs concepts de non-réciprocité optique basés sur la non-linéarité optique [2–5], l'optomécanique [6] et l'optoacoustique [7]. Mais il est clair que la manière la plus directe et la plus naturelle pour parvenir à une isolation optique est l'utilisation d'un effet magnéto-optique.

Nous pourrions diviser les matériaux avec réponse magnéto-optique (MO) en deux groupes, à savoir les métaux et les matériaux diélectriques. Les métaux se distinguent par un effet MO plus grand, mais les pertes optiques y sont importantes. En revanche, les grenats substitués au bismuth sont transparents dans la lumière infrarouge et une partie de la zone du spectre visible. Bien que ces grenats se distinguent par une résonance MO moindre que les métaux, ils sont largement utilisés dans les composants et structures magnéto-optiques à faibles pertes.

#### Motivation : isolation optique

Avant de nous orienter sur les structures intégrées non réciproques, nous présentons une conception très simple, mais efficace de l'isolateur optique non intégré. L'isolateur MO typique, qui repose sur l'effet Faraday, consiste en la combinaison d'un rotateur Faraday à  $45^{\circ}$  et de deux polariseurs linéaires positionnés avec un angle relatif de  $45^{\circ}$ . Dans le sens transparent (vers l'avant), la lumière linéairement polarisée traverse le premier polariseur puis le matériau magnéto-optique. Cela entraîne du fait de l'effet Faraday une rotation de la polarisation d'un angle de  $45^{\circ}$ . Comme le deuxième polariseur est incliné par rapport au premier polariseur d'un angle de  $45^{\circ}$ , il peut y avoir transmission de la lumière. Dans le sens inverse, la non-réciprocité de l'effet Faraday entraîne une rotation de la polarisation d'un angle de  $-45^{\circ}$ , et donc la lumière ne peut pas être transmise à travers le polariseur de sortie. Depuis les années 80 [28–30] la conception

de l'isolateur optique Faraday non intégré pour les télécommunications optiques est bien connue. Elle est couramment utilisée dans un vaste domaine du spectre, des fréquences de la lumière infrarouge jusqu'au domaine de la lumière visible et de la lumière UV.

En 1995, Yokoi du groupe Mizumuto a montré l'intégration des grenats sur un substrat en InP [31] puis plus tard sur les alliages InGaAsP [32]. Le développement des techniques d'intégration des grenats avec des matériaux standards III-V est devenu un tournant dans le domaine de la conception de la photonique intégrée et a apporté de nouvelles possibilités de conception. Ont été démontrées et produites plusieurs versions d'isolateurs optiques se basant sur l'interféromètre de Mach-Zehnder (MZI) et utilisant le matériau InGaAsP, l'effet MO provenant de la couche de grenat [33–36].

Wang et Fan [40, 41] ont conçu une autre classe d'isolateur optique à base de grenat. Le composant est un cristal photonique 2D à symétrie triangulaire gravé dans un matériau magnéto-optique, tel que le grenat de bismuth fer (BIG). L'aimantation, normale au plan du composant, est orientée de manière opposée au centre et dans la partie périphérique de la structure. Cela entraine une levée de dégénérescence des modes contra-rotatifs de résonance de la cavité. W. Smigaj et al. ont perfectionné la conception de cette cavité non réciproque résonante. La cavité est alors constituée d'un réseau circulaire de Bragg, qui forme des cercles concentriques intérrompus par les guides d'approche. Cela permet un fonctionnement de la structure avec une aimantation uniforme [42,43].

L. Bi [39] a présenté en 2011 une structure différente d'isolateur optique monolithiquement intégré sur une plate-forme « Silicon-On-Insulator » (SOI). Il a conçu une structure de guide d'onde monomode en silicium et un résonateur en anneau où l'épaisseur de la couche de SiO<sub>2</sub> est de 1  $\mu$ m. Avec un certain intervalle de longueur d'onde (intervalle spectral libre), le couplage du guide d'onde et de l'anneau entraîne une excitation de la résonance de l'anneau. Il est important de souligner ici que la résonance de l'anneau se manifeste en tant que minima dans les spectres de transmission. En appliquant un champ magnétique, la fréquence de résonance de l'anneau se déplace du fait de l'effet magnéto-optique.

Dans le contexte de ces résultats déjà prometteurs, nous nous sommes intéressés au domaine des structures magnétoplasmoniques. Ces structures combinent la non-réciprocité de l'effet MO avec une augmentation du champ local dû à l'excitation des plasmons-polaritons de surface (SPP). L'augmentation locale du champ électromagnétique implique une augmentation de l'effet MO dans la structure.

#### But de ce travail

Dans ce travail, nous nous sommes focalisés sur les structures et configurations indiquées ci-dessous :

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- Nous appliquons un Effet magnéto-optique transversal. L'avantage de cette configuration est que l'effet de non-réciprocité ne se manifeste qu'avec la polarisation p. Par conséquent aucune conversion de mode ou de polarisation n'apparait, ce qui est important pour le fonctionnement du composant.
- Pour une augmentation de l'effet magnéto-optique par l'influence de la concentration du champ local, nous avons utilisé des *plasmons de surface*. Générer des plasmons dans les structures réclame une interface entre le matériau diélectrique et le métal noble. Dans le cas de nos modèles, nous avons utilisé du grenat magnéto-optique (avec absorption négligeable dans la lumière infrarouge) et de l'or en tant que métal noble. Pour les modèles, nous utilisons la fonction optique des matériaux, déterminée à l'aide de l'ellipsométrie spectroscopique de la matrice de Mueller.
- La génération d'un plasmon de surface demande une constante de propagation élevée, qui est atteinte aux modes de diffraction d'ordre supérieur dans le réseau périodique. Nous avons utilisé un système périodique 1D (perpendiculaire au plan d'incidence) qui est efficace et optimal pour maximiser l'interaction avec le matériau magnéto-optique.

Notre étude a concerné la réponse optique et magnéto-optique d'un réseau périodique magnéto-plasmonique 1D (voir Figure 1). Le réseau en or est décrit par sa période  $\Lambda$ , son épaisseur  $h_1$  et son ouverture r. Le réseau a été créé sur une couche de grenat de gadolinium-fer bisubstitué (Bi :GIG). La couche de grenat MO a été épitaxiée sur un substrat de grenat de gadolinium-gallium (sGGG) dopé (CaMgZr).

Le principal objectif de ce travail est de présenter comment il est possible d'ajuster l'effet transversal Kerr magnéto-optique (TMOKE) par l'intermédiaire de la géométrie du réseau magnétoplasmonique. La démonstration théorique et la preuve expérimentale montrent que l'amplitude et le signe de l'effet TMOKE sont fortement influencés par l'interaction des modes de résonance dans la structure. En d'autres termes, le signe de l'effet TMOKE peut être modifié par optimisation de la géométrie du réseau (sans modification de l'orientation de l'aimantation), du fait d'une petite modification de l'interaction entre des résonances SPP (plasmons de surface) et FP (Fabry-Perot). Pour démontrer ce nouvel effet physique, nous avons dû résoudre les questions suivantes.

Dans la première partie, nous avons déterminé les fonctions optiques et magnétooptiques des matériaux utilisés. Elles ont été utilisées dans le cadre de l'étude théorique des résonances dans le réseau magnétoplasmonique 1D. Des modèles analytiques de modes de résonance (FP et SPP) ont été déduits. En outre, nous présentons un modèle décrivant le décalage du mode SPP par l'effet TMOKE. Les impacts sur l'effet TMOKE du changement de géométrie du réseau, à savoir son épaisseur, sa période et son ouverture r ont été étudiés et analysés.



Figure 1 – Illustration schématique de la structure étudiée : réseau en or avec période  $\Lambda$  et épaisseur  $h_1$  sur substrat de grenat magnéto-optique pour une configuration transversale avec onde au niveau de l'incidence au niveau y - z, avec angle d'incidence  $\varphi_0$  et polarisation *s*- ou *p*-.

Les conceptions de réseaux avec différentes ouvertures r ont été réalisées par lithographie électronique sur une surface de polyméthacrylate de méthyle (PMMA). Après évaporation de l'or, les motifs ont été créés par la technique de « lift-off ». Afin de retrouver numériquement la résonance optique mesurée, un modèle de structure de réseau a été développé et optimisé : les données de la matrice de Mueller ont ainsi été reproduites par le modèle. Pour finir, nous avons comparé le déplacement et la modification du signe des données calculées avec les données obtenues à partir d'un ensemble de 15 échantillons ; un très bon accord théorieexpérience a été obtenu.

#### Méthode numérique employée

Dans ce travail, nous avons utilisé pour toutes les simulations numériques et le fit des données optiques et magnéto-optiques notre code basé sur la méthode des modes couplés (RCWA, Rigorous Coupled Wave Algorithm). Ce code a été élargi selon les règles de factorisation Li pour le calcul des structures périodiques 1D anisotropes. De plus, introduit dans le programme Matlab, il a été conçu pour des simulations parallèles. Cela nous permet de procéder à des simulations de réseaux et de reproduire les données expérimentales avec les modèles dans des temps de calcul raisonnables. La RCWA découle des équations de Maxwell à l'aide de l'approche de Yeh et Berreman.

## Préparation des échantillons et caractérisation

Nous décrivons ici le processus technologique de fabrication des échantillons et la méthodologie de caractérisation optique et magnéto-optique. Pour le matériau MO des réseaux magnétoplasmoniques, nous avons choisi du grenat d'yttrium et de fer substitué au bismuth. Des films de cristal de grenats de fer bisubstitués ont été réalisés par épitaxie en phase liquide (LPE, Liquid Phase Epitaxial) sur des substrats orientés sGGG (111) dopés. La composition précise du substrat sGGG est la suivante :  $Gd_{2.7}Ca_{0.3}Ga_{4.1}Mg_{0.3}Zr_{0.6}O_{12}$ . Dans le cas d'un composant magnéto-optique la figure de mérite optique et les propriétés magnétiques, telles que l'aimantation et l'anisotropie, doivent être contrôlées simultanément. Afin d'incorporer une teneur en Bi élevée, et induire ainsi une grande rotation Faraday (ou une forte gyrotropie), les films réalisés sont constitués de combinaison de Gd, Pr, Lu sur des substrats CaMgZr-GGG, dont le paramètre de maille est élevé ( $a_S = 12.498$  Å). Pour la conception de la structure, les connaissances des fonctions optiques et magnéto-optiques des matériaux employés sont d'une très grande importance. L'ellipsométrie spectroscopique de la matrice de Mueller a été utilisée pour la caractérisation. Nous présentons ci-dessous le banc d'ellipsométrie de la matrice de Mueller et les grandeurs mesurées.

#### Ellipsométrie de la matrice de Mueller

L'ellipsomètre de la matrice de Mueller Woollam RC2-Di a été utilisé pour la caractérisation optique et magnéto-optique des matériaux. Cet ellipsomètre utilise comme source de lumière une combinaison d'ampoule halogène et de lampe au deutérium qui couvre une zone spectrale de 0.74 eV to 6.42 eV (193-1700 nm). Pour atteindre une matrice de Mueller pleine nous utilisons une configuration PCSCA (Polarisateur-Compensateur-Echantillon-Compensateur-Analyseur) à deux compensateurs rotatifs [99]. La matrice de Mueller décrit la transformation du vecteur de Stokes lors d'une réflexion (ou transmission) sur l'échantillon, la définition la plus souvent employée du vecteur de Stokes étant [90] :

$$\mathbf{S} = \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = \begin{bmatrix} I_p + I_s \\ I_p - I_s \\ I_{45^\circ} - I_{-45^\circ} \\ I_L - I_R \end{bmatrix}$$
(1)

Lors de l'interaction avec l'échantillon, le vecteur de Stokes est transformé par la matrice de Mueller  $S^{out} = MS^{in}$ . De manière générale, la matrice de Mueller possède seize composantes indépendantes. Dans le cas d'une structure isotrope sans effets dépolarisants, la matrice de Mueller lors d'une réflexion est diagonale

en bloc :

$$\mathbf{M} = \begin{bmatrix} 1 & -N & 0 & 0 \\ -N & 1 & 0 & 0 \\ 0 & 0 & C & -S \\ 0 & 0 & S & C \end{bmatrix}.$$
 (2)

La matrice de Mueller (2) est normalisée vis-à-vis de l'élément  $M_{11}$ , qui décrit l'intensité totale de réflexion.



Figure 2 – Illustration schématique de la configuration de l'ellipsomètre avec deux compensateurs rotatifs et orientation des composantes extérieures d'aimantation dans le plan.

La Figure 2 représente une illustration schématique de la configuration ellipsométrique. Pour une configuration en réflexion, l'angle d'incidence peut changer dans un intervalle de 19° jusqu'à 85°.La transmission peut être mesurée pour une configuration d'incidence normale, ou bien avec un échantillon incliné. Pour la caractérisation optique des petits échantillons, tels que nos réseaux, il est possible d'installer une optique focalisée. La distance du foyer des lentilles est de 27 mm et le diamètre du foyer est de 150  $\mu$ m.

Il est possible avec des sondes focalisées de changer l'angle d'incidence dans un intervalle allant de 19° à 70° et jusqu'à 60° en utilisant un aimant fixe, générant un champ magnétique au niveau de l'échantillon. Pour un alignement précis de l'échantillon vis-à-vis de la surface du spot incident et de la cartographie de la mesure une platine x - y motorisée a été utilisée.

#### Fonctions optiques des sGGG et Bi :GIG utilisés

Pour une analyse inverse (procédure de fit), la différence entre les données expérimentales et simulées est minimisée par l'optimisation du modèle. Pour l'ellipsométrie, nous avons utilisé la représentation de la sphère de Poincaré [100].La fonction optique a été ajustée à l'aide du modèle de Tauc-Lorentz avec queue d'Urbach (Urbach tail) [108]. La Figure 3 illustre les fonctions optiques obtenues du substrat sGGG et de la couche Bi :GIG. L'étape suivante nous a permis de déterminer les fonctions magnéto-optiques de la couche Bi :GIG. Pour



Figure 3 – Fonction optique du substrat sGGG (graphique à gauche) et de la couche Bi :GIG (graphique à droite). La composante réelle  $\Re{\epsilon_{11}}$  et la composante imaginaire  $\Im{\epsilon_{11}}$  de la fonction sont illustrées par une ligne pleine et pointillée.

la mesure magnéto-optique un aimant commandé par servomoteur générant un champ magnétique dans le plan de l'échantillon (in-plane) a été développé. L'aimant est actionné par un servomoteur, qui est commandé par ordinateur à l'aide de l'unité de commande T-Cube DC Servo Motor de la société Thorlabs. Cela nous a permis de commander l'orientation du champ magnétique avec une haute précision. L'aimant permanent fournit un volume suffisamment uniforme de champ magnétique d'une intensité de 300 Oe ,qui entoure le support de l'échantillon, l'écart des pôles de l'aimant étant de 20 mm. A l'aide de l'aimant, les configurations MO transverse ( $M_T^{sat.}$ ) et longitudinale ( $M_L^{sat.}$ )(voir ensemble de coordonnées sur la Figure 2) peuvent être obtenues. Après mesure de chaque spectre, l'orientation de l'aimantation est retournée. Dans le but de diminuer le bruit et d'accroître la sensibilité de la mesure, cinq mesures sont systématiquement moyennées, dans le cas de chaque configuration MO (longitudinale ou transverse, soit vers le, « haut » soit vers le « bas »). La Figure 4 illustre les fonctions magnetooptiques obtenues du substrat sGGG avec de la couche Bi :GIG.

#### Fabrication de structures de réseaux

Le réseau métallique est réalisé par évaporation d'Au sur un masque de résine positive (polyméthacrylate de méthyle (PMMA)), préalablement structurée par lithographie électronique. La résine PMMA appliquée à l'aide d'une tournette est recuite pendant une durée de 10 min. à une température de 180° C. Pour réaliser les différents rapports d'ouverture les réseaux ont été écrits par lithogra-



Figure 4 – Dépendance spectrale ajustée de la composante off-diagonale du tenseur obtenue par la mesure ellipsométrique Bi :GIG pour une configuration MO transverse et longitudinale.

phie électronique avec différentes doses d'exposition dans une étendue 890–1040  $\mu$ C/cm<sup>2</sup>, sous forme de carrés de 300 × 300 $\mu$ m. La période du réseau est maintenue constante avec une valeur  $\Lambda = 500$  nm. ne couche d'or d'une épaisseur d'approximativement 100nm est évaporée sur la résine développée, la structure du réseau ayant été réalisée par la technique de « lift-off ».

## Simulations numériques et bases des structures magnétoplasmoniques non réciproques

Dans cette partie nous présentons l'hybridation des plasmons polaritons de surface (SPP) du réseau magnétoplasmonique Au/grenat et des résonances des cavités (ou de Fabry-Perot, FP), nous procédons à son analyse et expliquons pourquoi elle a un impact considérable sur la réponse MO du réseau, notamment sur l'effet Kerr transverse. Nous illustrons numériquement l'impact des variations géométriques du réseau sur l'effet TMOKE via la réflexion des ondes p, son exaltation possible, son extinction, ou même, son inversion. Notre étude théorique qui a été publiée dans Optics Express [66] , a été améliorée par l'introduction de la dispersion des fonctions optiques et magnéto-optiques des matériaux employés, déterminée de manière expérimentale.

Dans le cadre de nos simulations, nous avons examiné le comportement de la structure à saturation de l'aimantation ( $M_T = M_T^{\text{sat}}$ ). Cette condition a été parfaitement remplie dans le cas des couches Bi :GIG, qui ont été soumises à l'action d'un champ magnétique externe de 300 Oe dans le plan. Dans notre cas, la résonance optique non réciproque se traduit par le glissement spectral des résonances et des anomalies de réflectivité. L'effet TMOKE est ensuite défini par la différence de réflectivité lors du renversement d'aimantation

$$\Delta R_p = R_p \left( + M_T^{\text{sat}} \right) - R_p \left( - M_T^{\text{sat}} \right).$$
(3)

La réflectivité spéculaire de la structure (ligne rouge au milieu) et le spectre TMOKE correspondant (courbe bleue en haut) de la lumière polarisée-p, tombant sous un angle  $\varphi_0 = 10^\circ$  sur le réseau avec configuration typique ( $\Lambda = 500 \text{ nm}, h_1 = 150 \text{ nm}, r = 20 \text{ nm}$ ) ont présentés sur la figure 5. En regardant la ligne verte en bas, nous pouvons voir les résonances de la transmission optique extraordinaire (EOT), qui correspondent aux minima de réflexion.

Sur la figure 6 sont illustrées les cartographies du champ magnétique  $H_x$  (concrètement  $|H_x|^2$ ), ayant été calculées pour les différentes résonances indiquées dans le spectre EOT (voir figure 5). Ces cartographies confirment que les résonances qui présentent un fort effet TMOKE (A) et (B) sont bien les SPP de l'interface Au/-grenat, couplés aux ordres de diffraction  $\pm 1$ .

#### Formules analytiques des résonances du réseau

Après avoir rappelé les résonances typiques du spectre magnétoplasmonique TMOKE, nous dirigeons notre attention sur leur dispersion, en fonction des paramètres géométriques du réseau. Le but est donc d'identifier si un (anti)croisement des modes des cavités et des modes des SPP se produit.



Figure 5 – Réflectivité spéculaire (ligne rouge au milieu), transmission spéculaire (ligne verte en bas) et spectre TMOKE correspondant (ligne bleue en haut) lors de l'incidence de la lumière polarisée-p sur la structure du réseau sur la Figure 1 où  $\Lambda = 500$  nm,  $h_1 = 150$  nm et r = 20 nm.

#### Dispersion des modes des SPP

Les minima locaux dans le spectre de réflectivité correspondent aux modes de résonance dans le réseau. Il ressort de l'illustration graphique des champs sur la figure 6 qu'il est possible d'exciter les SPP tant sur l'interface air/or que sur l'interface or/grenat. Les résonances résultent en bonne approximation de la combinaison de la courbe de dispersion des SPP sur une interface et de la diffraction induite par le réseau.

En supposant que le matériau plasmonique est de l'or, et en notant  $\epsilon_2$  la permittivité de l'air (matériau diélectrique) et  $\epsilon_3$  celle du Bi :GIG, les modes SPP de notre système s'expriment à l'aide de la formule :

$$k_{\rm SP}(E) = k_y = k_0 \nu_y = k_0 n_{\rm eff} = \frac{2\pi}{hc} E \sqrt{\frac{\epsilon_2(E) \epsilon_i(E)}{\epsilon_2(E) + \epsilon_i(E)}}, \qquad i = 1, 3, \qquad (4)$$

où *E* est l'énergie des photons,  $\epsilon_2(E)$  la permittivité de l'or, i = 1 s'appliquant pour les SPP sur l'interface air/or, i = 3 s'appliquant pour les SPP sur l'interface





Figure 6 – Cartographie du module de la composante du champ magnétique  $H_x$  avec 0.973 eV (A), avec 1.097 eV (B), avec 1.403 eV (C), avec 1.683 eV (D), avec 2.053 eV (E), et avec 2.077 eV (F). La répartition du champ se rapporte à un réseau avec période  $\Lambda$  =500 nm, épaisseur  $h_1$  = 150 nm, largeur de l'ouverture r = 20 nm et angle d'incidence avec polarisation- $p \varphi_0 = 10^\circ$ .

or/grenat. Dans le cas d'une structure périodique 1D, les SPP sont excités par l'onde diffractée :

$$k_W(E) = \pm k_{\rm SP}(E) + m \frac{2\pi}{\Lambda}, \text{ with } m \in \mathbb{Z},$$
(5)

où  $k_W$  indique le vecteur d'onde SPP. Cette excitation des SPP est déjà connue comme le *Plasmon de Wood*, car elle a été observée à proximité des anomalies de Wood-Rayleigh [125]. Si nous posons  $k_W = \frac{2\pi}{hc} E \sin \varphi_0$  et résolvons l'équation (5) pour *E*, nous obtenons une approximation numérique du premier ordre pour les résonances SPP.

#### Dispersion des modes de cavités

Il est possible de prédire avec une bonne précision la position spectrale des résonances des fentes (modes de cavité) sur la base de la réponse d'un résonateur FP équivalent, constitué d'une couche d'indice de réfraction  $n_{\text{eff}}$ , de même épaisseur que celle du réseau en or, insérée entre l'air et le substrat de grenat. L'indice de réfraction effectif  $n_{\text{eff}}$  est celui du mode TM fondamental du guide d'onde



Figure 7 – Indice effectif du guide d'onde or/air/or,  $\lambda = 884$  nm.



Figure 8 – A gauche : illustration schématique du guide d'onde « or/air/or » et son insertion dans la cavité de résonance entre le grenat et l'air. A droite : Profil du champ du mode du guide d'onde.

Au/air/Au. Si nous considérons seulement des modes polarisés p-, la condition de guidage a la forme suivante [122] :

$$\tanh\left(\frac{r}{2}\sqrt{k_0^2 n_{\rm eff}^2 - k_0^2}\right) = -\frac{\sqrt{k_0^2 n_{\rm eff}^2 - k_0^2 \varepsilon_2}}{\varepsilon_2 \sqrt{k_0^2 n_{\rm eff}^2 - k_0^2}}.$$
(6)

La figure 7 illustre l'indice effectif ainsi obtenu en fonction de la largeur de la fente.

La position des résonances de cavité est ensuite déterminée par l'expression de la résonance bilatérale (round-trip) (voir schéma sur la figure 8) :

$$2k_0 n_{\text{eff}} h_1 + \phi_{r_1} + \phi_{r_3} = 2n\pi, \quad n \in \mathbb{Z},$$
(7)

où  $\phi_{r_i}$  est le déphasage induit par la réflexion à chaque extrémité de la cavité. Le

coefficient de réflexion peut être approximé par celui en incidence normale :

$$r_i = |r_i| \exp\left[\mathrm{i}\phi_{r_i}\right] = \frac{n_{\rm eff} - \sqrt{\varepsilon_i}}{n_{\rm eff} + \sqrt{\varepsilon_i}},\tag{8}$$

où i = 1 s'applique pour une permittivité de l'air et i = 3 pour la permittivité du grenat non aimanté. Cette approximation simple est suffisante pour le mode de cavité dans les zones où ne se produit pas d'interaction avec les modes plasmoniques.

A partir des équations (6) et (7), nous pouvons constater qu'il est possible d'ajuster la position spectrale du mode de cavité de deux façons. La première possibilité est la modification de la largeur de l'ouverture du réseau, qui entraine la modification de l'indice effectif lorsque la dispersion est suffisante (Figure 7). La deuxième possibilité est un ajustement de l'épaisseur de réseau, la longueur de résonance d'onde étant influencée par la condition d'accord de phase (7).

#### Impact du changement de l'ouverture du réseau sur TMOKE

Ici nous analysons l'impact de l'augmentation de la largeur des fentes du réseau sur la réponse TMOKE. Sur la figure 9, le graphe de gauche montre la réponse TMOKE en fonction de l'ouverture du réseau pour le  $-2^{nd}$  mode SPP. Il est possible d'observer un décalage important du mode couplé en fonction de la largeur de l'ouverture. A partir du graphique à gauche, il est visible que le TMOKE peut être maximisé (pour cette structure et le  $-2^{nd}$  mode SPP) lorsque l'ouverture du réseau varie dans un intervalle allant de 20 nm à 60 nm. Cette information est importante également pour le processus de fabrication. Le graphe à droite illustre l'effet TMOKE à 1,74 eV en fonction de la largeur des fentes. Lors du changement de la largeur de l'ouverture dans une gamme allant de 30 nm à 45 nm, il est possible d'observer un changement du signe TMOKE.

#### Proposition de structure du guide d'ondes avec dispersion non réciproque des modes TM

La figure 10 illustre la structure d'un guide d'onde silicium avec réseau plasmonique, où la couche MO, formée par le grenat BI :GIG, se trouve sur le réseau. Les matériaux employés dans le cas de la structure, c'est-à-dire silicium et SiO<sub>2</sub> ,ont été choisis pour leur contraste diélectrique élevé. Par conséquent, il est possible de parvenir à un guidage dans la couche de silicium. Dans cette étude, nous nous efforçons de déterminer le comportement non réciproque des modes du guide d'onde. Le principal objet est l'analyse du lien éventuel entre les modes du guide d'onde et les modes plasmoniques sur les interfaces du réseau. Le champ évanescent du mode du guide d'onde dans le silicium est utilisé pour l'excitation



Figure 9 – Le graphe de gauche illustre la dépendance spectrale TMOKE  $\Delta R_p$  en fonction de l'ouverture du réseau r dans un intervalle allant de 20 nm à 120 nm et une période  $\Lambda = 500$  nm. A droite : changement du signe TMOKE pour une énergie de photons fixée (1,74 eV) en fonction de la largeur de l'ouverture du réseau.

du mode des plasmons de surface sur le réseau. Pour parvenir à un comportement non réciproque, du grenat Bi :GIG est placé sur le réseau. L'excitation SPP et son contrôle à l'aide de l'aimantation entraînent alors un comportement non réciproque.



Figure 10 – Schéma de la structure du guide d'onde silicium avec réseau d'or et Bi :GIG.

La Figure 11 illustre les courbes de dispersion d'un indicateur de guidage noté  $1/\sigma_{max}$  calculé pour les modes TM, où les lignes droites sombres correspondent aux modes du guide d'onde. Le mode dominant avec  $\nu_y = 2.86$ apparait en tant que ligne verticale (le deuxième mode peut être observé avec  $\nu_y = 3.34$ ). Le graphe de droite représente un agrandissement de la zone où le mode vertical coupe divers modes de la structure et où se produit un intéressant comportement d'anticroisement. Nous pouvons observer une transformation progressive des modes. Les modes sont ensuite étudiés en utilisant des cartographies de



Figure 11 – A gauche : Courbe de dispersion de l'indicateur de guidage  $1/\sigma_{max}$ l'échelle logarithmique, calculé en fonction de l'indice effectif  $\nu_y$  et période de réseau  $\Lambda$ . A droite : Détail de la zone d'anticroisement du mode.

champ et sur la base d'une analyse de l'indice effectif des modes.

### Résultats expérimentaux

Nous présentons ici une analyse des données de la matrice de Mueller mesurée sur les échantillons que nous avons réalisés. Dans la première partie est décrit le développement du modèle de la structure. Ce modèle a été développé pas à pas, avec d'abord une description simple de la structure parfaite puis l'insertion dans le modèle de la rugosité de surface et de la présence de résine PMMA résiduelle à l'intérieur des fentes du réseau. A chaque étape, le fit des données expérimentales par le modèle est réalisé. La qualité du modèle développé est mise en évidence par la comparaison directe des grandeurs ellipsométriques mesurées et calculées N, C et S sur une large gamme d'angles d'incidence allant de 20° à 60°.

#### Développement du modèle de structure

Pour être capables de reproduire les résultats expérimentaux, il faut développer un modèle. Afin de parvenir aux meilleures données expérimentales a été appliquée pour le modèle une couche résiduelle de résine PMMA et une rugosité de surface sur la partie supérieure du réseau. La dispersion de la résine PMMA a été prise dans le lien [129]. La coupe du modèle est illustrée sur la Figure 12. Les paramètres les plus adaptés sont résumés dans le tableau 1 (désignés en gras). Nous avertissons du fait que l'épaisseur globale du réseau est indiquée en tant que  $t_1 + \frac{1}{2}t_3 + t_4 = 98.74$  nm. En tant qu'épaisseur de la couche représentant la dureté de la surface a été utilisée la valeur par rapport à la fraction volumique dure  $\frac{1}{2}t_3$  due to the fixed volume fraction f = 0.5. La Figure 13 illustre la très bonne conformité entre le modèle et les données. En outre a été atteinte une très bonne conformité entre la polarisation calculée et mesurée.



Figure 12 – Coupe de la structure du réseau avec rugosité de surface et PMMA résiduel.

Table 1 – Paramètres les plus appropriés

$\chi^2 = 0.0011$							
$arphi_0$	=	$44.33^{\circ}$	$\varphi_s$	=	$2.91^{\circ}$		
Λ	=	$502.6~{ m nm}$	r	=	<b>78.68</b> nm		
$t_1$	=	<b>68</b> . <b>16</b> nm	$t_2$	=	3988.4 nm		
$t_3$	=	$13.55~\mathrm{nm}$	$t_4$	=	23.8 nm		



Figure 13 – Comparaison entre le modèle avec rugosité de surface et PMMA résiduel et les données expérimentales.

#### Réponse transversale magnéto-optique de l'échantillon

Pour une autre analyse de la réponse optique de la structure (3), nous définissons la réflectivité relative  $R_p/R_s$  de la matrice de Mueller comme suit :

$$\frac{R_p}{R_s} = \frac{M_{11} + M_{12}}{M_{11} - M_{12}} = \frac{1 - \frac{M_{12}}{M_{11}}}{1 + \frac{M_{12}}{M_{11}}} = \frac{1 + N}{1 - N}.$$
(9)

Pour que nous puissions quantifier la résonance MO pour la configuration transversale, nous définissons la grandeur  $\delta R$  ainsi :

$$\delta R = \frac{R_p}{R_s} \left( + M_x^{\text{sat.}} \right) - \frac{R_p}{R_s} \left( - M_x^{\text{sat.}} \right), \tag{10}$$

La Figure 14 (gauche) compare la réflectivité relative  $R_/R_s$  des données mesurées et du modèle. Les données MO ont été obtenues pour la même configuration d'ellipsomètre, par conséquent nous pouvons utiliser les mêmes paramètres de fit. Le spectre de réflectivité-*s* calculé (ligne verte) montre que les effets caractéristiques n'apparaissent que pour la polarisation -p. Le graphique à droite illustre la grandeur MO calculée et mesurée  $\delta R$ . Cela illustre la façon dont le modèle décrit la résonance MO avec une très bonne conformité. Nous pouvons donc utiliser ce modèle pour déterminer l'origine de l'effet MO à l'aide de cartographies de champ, pour le calcul de la résonance MO pour divers angles d'incidence, etc.



Figure 14 – A gauche : Comparaison de la réflectivité relative calculée et mesurée  $R_p/R_s$ . A droite : Comparaison de l'effet MO mesuré et calculé.

#### Impact du couplage des modes sur la réponse optique et MO

Enfin est démontrée de manière expérimentale l'interaction du mode des plasmons de surface et des cavités. La figure 15 montre à gauche un zoom de la réponse MO, calculée pour différentes largeurs de fentes. Un décalage des pics vers le bleu avec l'augmentation de la largeur de la fente est clairement visible. Le graphique de droite représente la réponse MO mesurée pour divers échantillons (avec différentes largeurs de fente). Sur le graphique est clairement démontré le



Figure 15 – Décalage spectral de la réponse MO, extraite des mesures réalisées pour 15 échantillons avec différentes ouvertures r (droite), en comparaison avec les résultats de simulation (gauche).

décalage vers le bleu du pic MO en fonction d'un agrandissement de l'ouverture, prévu théoriquement.

Cette observation confirme la théorie de l'accordabilité géométrique de l'effet TMOKE dans le réseau magnétoplasmonique 1D, comme présenté précédemment.

## **Conclusion et perspectives**

#### **Résultats atteints**

Le but de ce travail était l'étude de la réponse TMOKE de réseaux magnétoplasmoniques périodiques 1D, l'analyse des différents modes résonants et l'impact de leur couplage sur l'augmentation de l'effet TMOKE. Le travail et les résultats peuvent être divisés en quatre groupes :

## 1. Couplage des modes de cavités et plasmoniques dans la structure magnétoplasmonique

- Le principal résultat de ce travail est l'explication et la confirmation expérimentale de l'augmentation de l'effet TMOKE, et l'inversion du signe de cet effet réalisable sans modification de l'aimantation. Cet effet a été expliqué numériquement par l'interaction entre les résonances du réseau (modes des cavités et modes des plasmons de surface). Il a également été montré qu'il est possible de le modifier par un léger changement de la géométrie du réseau – publié dans [65,66].
- Afin de confirmer les résultats théoriques un ensemble de quinze réseaux magnétoplasmoniques ont été fabriqués par lithographie électronique et structuration du réseau par lift-off. La réponse magnéto-optique des échantillons a été mesurée à l'aide de l'ellipsomètre de la matrice de Mueller et les données expérimentales ont démontré l'effet prédit avec une très bonne conformité.

#### 2. Détermination du spectre optique et magnéto-optique des matériaux utilisés :

- Les fonctions optiques du matériau employé pour la production des échantillons ont été déduites de la réflexion et de l'intensité des spectres de transmission de la matrice de Mueller – publié dans [130].
- UUne analyse des effets de dépolarisation provoqués par le réglage ellipsométrique, de la définition spectrale finale et de la focalisation du faisceau a été réalisée.
- L'ellipsomètre de la matrice de Mueller a été complété par un aimant permanent générant un champ magnétique dans le plan (in-plane) et commandé par ordinateur. L'aimant a été utilisé pour la caractérisation des propriétés MO Bi :GIG et pour les expérimentations MO sur les réseaux magnétoplasmoniques – publié dans [131].
- 3. Développement de modèles réalistes de structures magnétoplasmoniques :
- Un modèle de réseau plasmonique 1D, qui prend en compte les imperfections de fabrication, comme la rugosité de surface sur le réseau, la résine PMMA résiduelle à l'intérieur des fentes du réseau et une divergence du
rayon focalisé, a été développé. Le modèle développé conduit à un très bon accord théorie-expérience des données MO mesurées et calculées – publié dans [130].

 Le fit des résultats expérimentaux des 15 échantillons a été réalisé de manière globale, avec des largeurs de fentes qui font apparaître la même tendance que les fentes qui ont été observées avec un microscope électronique à balayage (SEM).

#### 4. Développement du logiciel pour la modélisation du réseau

- Pour la modélisation de la réponse optique du réseau périodique 1D un nouveau logiciel a été développé dans MATLAB. Ce programme se base sur la méthode RCWA (méthode de l'onde couplée) et est optimisé pour le calcul parallèle des problèmes spectraux.
- Une optimisation de l'implémentation parallèle du code a été réalisée et des simulations spectrales avec divergence intégrée du rayon focalisé ont été effectuées (avec utilisation d'un centre de superinformatique IT4I), jusqu'à 256 cpus.

#### Perspectives

Dans le cadre de ce travail nous avons réalisé la démonstration expérimentale de plusieurs résultats prédits théoriquement. Une grande quantité d'études pourraient être menées dans le futur à partir de ces premiers résultats. Nous indiquons ici quelques unes de ces idées. Nous avons par exemple prédit au chapitre 4 un lien entre les modes SPP et les modes des cavités par l'intermédiaire d'un changement de l'épaisseur du réseau et de la largeur de l'ouverture. Mais les échantillons expérimentaux produits par cette méthode, qui est décrite dans le chapitre 3, ne confirment que les prédictions dans le cas d'un changement de l'ouverture du réseau. Il serait pertinent de procéder à une analyse du couplage et de comparer la réponse magnéto-optique atteinte en fonction de l'épaisseur du réseau. Les échantillons pour ces expérimentations sont déjà disponibles. En outre, les structures qui ont fait l'objet de ce travail sont unidimensionnelles, à angles droits et ont été étudiées pour une configuration avec diffraction plane et aimantation transversale. Des travaux futurs pourront s'orienter vers des configurations avec diffraction conique, sur les structures périodiques 2D et dans le cas d'une aimantation longitudinale ou polaire. La configuration avec diffraction conique devrait permettre une caractérisation optique précise et l'étude de la conversion non réciproque des modes. Ces structures 2D pourront faire apparaître d'intéressantes propriétés optiques tant en réflexion qu'en transmission. Leur étude pourra apporter de nouvelles possibilités d'ajustement des modes des cavités, ainsi que des informations importantes sur le processus de fabrication. La proposition théorique de la structure du guide d'onde ouvre un nouvel axe possible de recherche. Une autre étude et optimisation de la structure seront alors nécessaires. La structure devra être conçue avec des matériaux compatibles (du point de vue de la fabrication) et pour le mode fondamental du guide d'onde. Le composant intégré peut fonctionner en tant qu'isolateur optique ou modulateur, selon que l'aimantation est constante ou modulée. Et enfin, les résultats théoriques et expérimentaux présentés concernant la structure magnétoplasmonique pourront être transposés dans le domaine de l'IR lointain et du THz, pour les utiliser lors de la conception de nouveaux composants optiques.

# English Text

### 1 Introduction

In this thesis entitled *Theoretical and experimental study of novel integrated magnetoplasmonics nanostructures* I am focused on optical and magneto-optical study of periodic plasmonic structures for applications in non-reciprocal optics.

Before giving a detailed presentation of the theoretical and experimental work, the phenomena of optical non-reciprocity are introduced. Usual passive linear optical systems obeys so called *time reversal symmetry*. Figure 1.1 shows an example of such symmetrical system schematically - two silica prisms which couple and decouple light from the single mode waveguide<sup>1</sup>. A single mode waveguide is used in order to avoid transmission into higher-orders modes, which caused a lof of confusion during last years [1]. In such kind of linear passive systems forward and backward modes inside the waveguide are equivalent. The only difference is the sign of the wavevector k. A change of the sign of the wavevector k  $\rightarrow -k$  is equivalent to time reversal  $t \rightarrow -t$ , this is consistent with time-invariance of the Maxwell's equations. System which allows propagation of modes with the wavevector  $\pm k$  are called *reciprocal*. Optoelectronic



Figure 1.1: Prism coupling and decoupling of guided forward and backward modes is shown schematically.

structures with preferred propagation direction of guided modes (+k or -k) are required. Optical isolators are typical non-reciprocal optical devices used in optical telecommunication technology to protect laser diodes (with positive feedback) against spurious back reflections. During last decades several concepts for optical non-reciprocity based on the optical nonlinearity [2–5], opto-mechanic [6] and opto-acoustic [7] have been explored. Finally a lot of work was done on optical isolation using magneto-optic effects. But obviously the most straightforward and natural way to obtain optical isolation is using magneto-optic effect.

The first observation of magneto-optic (MO) effect was done by Michael Faraday in 1845. For the propagation in parallel to magnetic field (H||k) through flint glass rod, Faraday observed rotation of the plane of linearly polarized light. The

<sup>1.</sup> Considered refractive index of prisms is n' and n < n' for surrounding medium.

azimuth of the rotation is linearly proportional to the applied magnetic field and to the propagation length. The phenomenon is known as *Faraday rotation* [8]. In 1898 Woldemar Voigt discovered a magneto-optical effect in transmission with magnetic field perpendicular to the propagation ( $\mathbf{H} \perp \mathbf{k}$ ) [9]. The *Voigt* or *Cotton–Mouton* effect is similar to the Faraday effect, but while the Faraday effect is linear in the applied field, the Voigt effect is quadratic, i.e. effect is proportional to the square of magnetization.

In reflection three magneto-optical configurations are distinguished according to the orientation of the magnetization vector with respect to the interface plane and the incident wave [10,11]. Magneto-optical effect upon the reflection of polarized light from a perpendicularly (i.e. in the polar direction) magnetized air-iron interface was proposed in 1877 by Reverend John Kerr [12]. The longitudinal MO Kerr effect for magnetization parallel to both the plane of incidence and the interface was described in 1878 [13]. Upon reflection in both cases, polar and longitudinal configuration, the linearly polarized incident light is transformed into an elliptical one. The third magneto-optical effect when magnetization is perpendicular to the plane of incidence and lies in plane of interface, i.e. transverse Kerr effect, was observed by Peter Zeeman in 1898. The transverse Kerr effect change both phase and amplitude only for TM (or *p*-) polarized mode.

The presence of magnetic field or magnetization inside the crystal breaks timesymmetry of the crystal. As a consequence, material properties exhibit reduced symmetry as well. In case of optical properties, the reduced crystal symmetry due to magnetization gives rise to so-called magneto-optical (MO) effects. In general, those effects can be linear, quadratic [14], etc. in magnetization. From the macroscopic point of view, the MO effects linear in magnetization provides non-zero antisymmetric off-diagonal elements in the permittivity tensor. From microscopic point of view the MO effect occurs due to different light absorption for different magnetization directions. For example, when light propagates along magnetization direction, than there is different absorption for circular left and circular right polarizations [15]. The light absorption itself originates from probability of photon be absorbed by the matter, while exciting electron from the ground state to the excited state. Note, that in the optical spectral range, the absorption is dominated by electric dipole absorption (i.e. absorption is caused by electric part of the electromagnetic wave). Therefore, magnetic part of the electromagnetic-wave does not interacts with spin of the electron at optical frequencies. Hence dependence of absorption on magnetization direction (i.e. on spin of electrons) is provided only indirectly, due to spin-orbit coupling. To avoid canceling of the effect due to symmetry of the spin-orbit interaction, the electronics structure must be split by magnetic field, either external or internal, in later case usually called as exchange splitting. In following work, the linear transverse magneto-optical Kerr effect (TMOKE) is used for its unique property: the polarization state does not change

2

upon reflection. The linear TMOKE reflection coefficient for *p*-polarization can be defined as:

$$r_{pp}^{(\mathbf{M})} = r_{pp}^{(0)} + \delta r_{pp} \left(\mathbf{M}\right), \qquad (1.1)$$

where  $r_{pp}^{(0)}$  is the Fresnel reflection coefficients from non-magnetized media and  $\delta r_{pp}$  (**M**) is the linear perturbation introduced by the transverse MO effect. Total phase and amplitude changes upon reflection is given by both reflection without magnetization and the MO contribution. The nonreciprocal phase shift and absorption are then related to the perturbation  $\delta r_{pp}$  (**M**).

Despite the fact that the family of MO active materials is very wide and almost each feromagnetic material which can sustain spontaneous magnetization will have some magneto-optical response, two basic groups of MO materials can be established. These are the ferromagnetic metals (and their alloys and compounds) and the ferromagnetic garnets and oxides. Ferromagnetic metals (especially Co, Fe, and Ni), their alloys and compounds were studied for decades. Their popularity comes from their large MO effect, well known properties (optical, magnetic) and relatively easy manipulation and fabrication (thin film deposition). Moreover they can be mixed in binary or ternary compound with other chemical elements {for example like a Heusler compounds [16]}, which makes their MO response widely tunable. In the past, ferromagnetic metals were deeply studied for magnetic recording [17–19]. Metals provide relatively strong MO response, but they have also large optical losses, therefore they are hard to use for waveguide configuration<sup>2</sup>.

Second group of promising materials for magneto-optical applications are ferrimagnetic garnets. Those very complex cubic crystals with spinel-like structure were discovered in 1959. First films of magnetic garnet were prepared in 70s by liquid phase epitaxy (LPE) on gadolinium gallium garnet substrate. At that time, magnetic garnets were studied for application in magnetic bubble memories [22–25]. Because of their unique combination of sufficiently strong magnetooptical properties<sup>3</sup> and transparency in near-infrared region, MO garnets found use in optical switching and modulation in waveguiding structures [26,27].

# 1.1 Motivation: optical isolation

Before going into integrated non-reciprocal structures a very simple, but efficient, concept of non-integrated optical isolator should be introduced. Figure

<sup>2.</sup> But in a special configuration with active loss-compensation it is possible as was demonstrated in work of M. Vanwolleghem [20,21].

<sup>3.</sup> Of course, MO properties of transparent garnets are weaker than MO properties of metals (Co, Fe, Ni)

1.2 shows a typical MO isolator based on the Faraday effect. A free space optical isolator based on Faraday rotator is achieved by combination of  $45^{\circ}$  Faraday rotator and two linear polarisers tilted by  $45^{\circ}$ . In the transparent direction (for-



Figure 1.2: Basic principle of free space polarization-dependent optical isolator.

ward) a linearly polarized light passes through the first polarizer. Then the plane of polarization is rotated by  $45^{\circ}$  by the Faraday effect. Because the second polarizer is tilted by  $45^{\circ}$  with respect to the first polarizer, the light can propagate. In the opposite direction, the non-reciprocity of Faraday effect leads to a rotation of the polarization plane by  $-45^{\circ}$ , therefore, in the ideal case, the backward propagation mode is perfectly blocked. Free-standing (non-integrated) optical isolator for optical telecomunication based on Faraday effect is well-known concept from the 80s [28–30]. Till now, concept of optical isolator based on Faraday rotator is commonly used in a wide spectral domain from infrared frequencies to visible and UV light domain.

On the other hand, functionality of Faraday effect-based optical isolators is directly related to the propagation length through MO material. Therefore, simple miniaturization of a device is not possible for design of on-chip integrable nonreciprocal optical structures and advanced design of novel structures and new approaches are required. During last two decades several concept of waveguiding structures based on garnets were proposed and experimentally demonstrated. Moreover, bonding techniques for combination of garnets with standard silicon or III-V semiconductor were developed. But due to fabrication difficulties, sensitivity to precise dimension of fabricated structures, temperature of surrounding, etc., it is hard to transfer laboratory devices into large-scale commercial production.

In 1995 Yokoi, from group of Mizumuto, reported first successful results on

boning of garnets onto InP substrate [31] and later on InGaAsP alloys [32]. Development of bonding techniques of garnets with standard III-V materials was milestone in design of integrated photonic and it brings new design possibilities. Several designs of optical isolators based on Mach-Zender interferometer (MZI) developed in a InGaAsP material where the MO effect is introduced by MO garnet cladding were demonstrated and fabricated [33–36]. Figure 1.3 shows layout of structure with Ce-substituted yttrium iron garnet (Ce:YIG) cladding proposed by Sobu et. al. [37]. The optical isolator is composed of multi-mode interference (MMI) couplers, a reciprocal phase shifter on one (upper) interferometer arm, and nonreciprocal phase shifters on two arms. The reciprocal phase shift is accomplished by the difference in optical path lengths between the two arms. The nonreciprocal phase shifters are composed of a Ce:YIG upper cladding layer magnetized transverse to the light propagation direction on film plane [38]. In order to obtain non-reciprocal TMOKE phase shift, external magnetic fields are applied to the two interferometer arms in anti-parallel directions. As a consequence, the phase shift generated by the first-order MO effect becomes different in the two arms. In the forward propagation, the phase difference, measured in the upper arm with respect to the lower arm, is set to be  $-\pi/2$  by proper adjustment of the length of the nonreciprocal phase shifters. When the reciprocal phase shifter gives a phase shift of  $\pi/2$ , the phase difference is canceled. The light waves propagating in the two waveguide arms become in-phase and interfere constructively in the output of  $1 \times 2$  MMI coupler. The forward light wave is output from the central port of the MMI coupler. In the backward propagation, the phase difference given by the nonreciprocal phase shifters changes its sign. Namely, the phase difference of  $\pi/2$  is given by the TMOKE, whereas the reciprocal phase shift remains giving a  $\pi/2$  phase difference. As a result, the total phase difference between the two arms becomes  $\pi$ . The light waves propagating in the two waveguide arms emerge in anti-phase, and destructive interference occurs in the  $2 \times 3$  MMI coupler. The light wave does not come out from the initial input port, but is radiated from the side waveguides. In order to suppress the reflection at the front edges of the side waveguides, a lateral taper is introduced at the ends of side waveguides. The light wave is radiated to the substrate effectively. Thus, the device exhibits direction-dependent and nonreciprocal transmission behavior and works as an optical isolator.

Different design of monolithically integrated optical isolator on Silicon-On-Insulator (SOI) platform was presented in 2011 by L. Bi [39]. Figure 1.4 shows on the right subplot proposed structure of a single-mode silicon waveguide and racetrack resonator fabricated on an SOI wafer with a top cladding of 1  $\mu$ m thick SiO<sub>2</sub>. Middle subplot shows SEM image of the part of the ring where cladding was etched and Ce:YIG was deposited. At a certain wavelength the coupling between waveguide and the ring leads to the excitation of ring resonance. Here it is



Figure 1.3: Schematic illustration of an integrated GaInAsP MZI optical isolator developed by Sobu et. al. [37].

important to point out, that resonance of the ring appears as a dip in transmission spectra. By application of transversal magnetic field, the resonant frequency of the ring is shifted. The shift originates from the TMOKE non-reciprocal phase-shift. Therefore under the fixed magnetization resonant frequency of the ring modes propagating in a clockwise (CW) and counter clockwise (CCW) direction are different. Right subplot of Fig. 1.4 shows operation principle for optical isolation schematically. Maximum achieved isolation ratio was 19.2 dB.



Figure 1.4: Structure of the monolithic nonreciprocal optical-resonator-based isolator introduced by L. Bi [39] (left subplot), transverse cross-sectional SEM image of the resonator ring covered with MO garnet layer (middle subplot), and operation principle for optical isolation. Maximum isolation ratio (19.2 dB), corresponding insertion loss and operation wavelength range are shown.

Another class of garnet-based optical isolator was proposed by Wang and Fan [40,41]. The proposed device, shown in the left subplot of Fig. 1.5, consists

of three branches of waveguides (ports  $S_{1,2,3}$ ) evanescently coupled to a resonant cavity at the center. The device (inset in right subplot of Fig. 1.5) was considered as 2D photonic crystal with triangular symmetry of air holes in gyrotropic material, such a bismuth iron garnet (BIG). The right subplot shows transport properties of the structure. The magnetization was applied in normal direction with a special profile. The magnetization in the center of the structure (dark grey) had opposite orientation than magnetization in surrounding structure (light grey). This leads to the splitting of resonant rotating modes inside the cavity. If the input port  $(S_1)$  and direction of magnetization are fixed, than the injected mode is coupled to exactly one of the output  $(S_3)$  waveguide and second port  $(S_2)$  is isolated. For the opposite orientation of magnetizations, the mode is coupled to previously isolated port (which becomes to be output), and the previous output port becomes isolated. The concept of the nonreciprocal resonant cavity was further improved by W. Śmigaj, et. al. They surround the resonant cavity by the circular Bragg grating formed by the concentric full and split rings. This lead to functionality of the structure under uniform magnetization [42,43].



Figure 1.5: Left: Schematic of a three-port Y-junction circulator. The straight arrows indicate the incoming and outgoing waves. The curved arrows represent the two counter-rotating modes in the resonator. Right: Transmission spectra at the output and isolated ports of a three-port junction circulator.

In the text above we have summarized milestones in the designs of optical structures with nonreciprocal optical behavior. Common factor of all mention structures is that non-reciprocity has been achieved by the phase shift originating from the linear MO transverse Kerr effect. Despite the fact, that the presented functionality of different designs achieves very high efficiency, their operation bandwidth is always limited by the resonant character of all discussed designs or by MO effect of transparent MO dielectrics (i.e. MO garnets) itself. For that reason it is very important to study structures, which can provide enhancement of the MO effect and/or wider operational broadband, because it can lead to

further increase of the efficiency of optical isolators. In this work we are focused on enhancement of the transverse MO Kerr effect by the effect of surface plasmon polaritons (SPP) excitation at the interface between noble metal (gold) and MO garnet. Structures which combine plasmonic behavior with MO effect are call *magnetoplasmonic*.

8

# **1.2** State of the art in nonreciprocal plasmonics

Since about half a decade the rich variety of research activities in the field of plasmonics has seen the addition of yet another interesting application, namely *magnetoplasmonics*. In search of active functionality in plasmonic circuitry, the use of an external magnetic control field and magneto-optic (MO) effects has been proposed both in surface plasmon waveguide layouts as well as in grating configurations [44, 45] and has been successfully verified experimentally [46, 47]. Moreover the inherent nonreciprocity of magneto-optical ferromagnetic metals has been exploited to obtain ultracompact and integratable optical magnetoplasmonic isolators [48–50]. The main focus of magnetoplasmonic research has been on the enhancement of the magneto-optic response of a MO material via the excitation of surface plasmon polaritons (SPP) [51]. Even though some interesting results have been reported on Kerr effect enhancement in nanoparticles of pure ferromagnetic metals [52, 53], by far the strongest MO Kerr effect enhancements have been seen by combining the SPP resonance of a noble metal with the gyrotropy of a ferromagnetic metal [54].

The most spectacular effect however has been reported by Belotelov et al. [55, 56] where it was predicted and demonstrated that a very strong transverse MO Kerr effect (TMOKE) of the order of 30% is induced by incorporating a nanostructured Au grating on top of a dielectric transparent magnetic iron garnet that is magnetized in plane and parallel to the gold stripes. TMOKE manifests itself as the relative change of the reflected intensity of p-polarized light incident along a plane perpendicular to the magnetization upon reversal of the latter. Magnetooptics textbooks [57] show that TMOKE is only appreciable on lossy magnetic materials, and that for smooth homogeneous ferromagnetic metal films it is only of the order 0.1%. A TMOKE of 30% predicted and measured in a system where the only magnetically active layer is transparent, is therefore a clear demonstration of the enhancement via plasmonic resonances. It was explained how the nonreciprocal splitting of the dispersion of the SPP's guided by the garnet/Au grating interface causes a nonreciprocal shift of the Wood-plasmon resonances in the extraordinary optical transmission (EOT) and reflection spectrum of this structure, and hence is at the origin of the Kerr effect enhancement.

On the other hand, it has been known for some time now, that EOT effects in 1D gratings are governed both by SPP resonances at the grating's interfaces and Fabry-Perot (FP) cavity resonances in its slits, and possibly even by their mutual coupling [58,59]. The latter hybridization of these resonances is strongly dependent on the precise geometrical parameters of the grating and can greatly influence the efficiency of the EOT effects at play [60, 61]. In EOT gratings on MO substrates [62–64], the role of the FP cavity modes has commonly been neglected in view of the limited interaction with the MO material until 2012, when we demonstrated how the FP cavity modes can play an important role in the control of the TMOKE [65,66].

# 1.3 Objective of this work and used approaches

Objective of this thesis is study of structures for enhancement of the magnetooptical effect. We combine a local field enhancement by surface plasmon resonance with magneto-optical properties of the garnet. We use the transverse magneto-optical Kerr effect, because it does not provide mode conversion. For the plasmon generation we used 1D periodic grating made of gold. The gold was used as a well known and stable plasmonic metal. The 1D structure was chosen for its tunability and effective surface plasmon generation.

Our study is focused on the optical and magneto-optical response of a magnetoplasmonic 1D periodic grating, shown on Fig. 1.6. The considered gold grating is parametrized by a period  $\Lambda$ , a thickness  $h_1$ , and a width r for the air gap . The grating was fabricated on a layer of Bi-substituted gadolinium iron garnet (Bi:GIG). The MO garnet layer was prepared on a (CaMgZr)-doped galliumgadolinium garnet (sGGG) substrate.



Figure 1.6: Schematic representation of the studied structure: gold grating with a period  $\Lambda$  and a thickness  $h_1$  on a magneto-optic garnet substrate in transversal configuration with incident plane wave in y - z plane at the incident angle  $\varphi_0$  and with *s*- or *p*-polarization.

It is the main issue of this work to present how the TMOKE in the magnetoplasmonic grating can be tuned via the grating geometry. It is demonstrated theoretically and proved experimentally, that the amplitude and sign of the TMOKE is strongly affected by the interaction of resonant modes in the structure. In other words, it is shown that the sign of the TMOKE can be even switched by optimization of grating geometry (without change of an orientation of magnetization), i.e. by slight change of interaction between SPP and FP resonances. In order to demonstrate a new physical phenomena, we had to pass through following issues.

In the first part we have determined optical and magneto-optical functions of the used materials. The experimental data were measured by a Mueller matrix Ellipsometer Woollam RC2 with dual-rotating compensators. For the MO characterization the ellipsometer was extended with a PC controlled in-plane magnet. Our parallel implementation of the fully vectorial anisotropic Rigorous Coupled Wave Algorithm (RCWA) was used for simulations and analysis of data measured on the gratings.

Determined optical functions were used in the theoretical study of resonances in 1D magnetoplasmonic gratings. The analytical models of resonant modes (FP and SPP) were derived. Moreover, a model describing shift of the SPP mode by TMOKE is presented. The impacts of a variation of the grating geometry, namely its thickness, period, and width of the air-gap r to the TMOKE was studied and analyzed.

Proposed designs of gratings with various width of the air gap r were fabricated by electron beam writing into polymethyl-metacrylate photoresist. After gold evaporation motives were fabricated by liftoff technique. To be able to reproduce measured optical response, the model of the grating structure was developed and optimized: Mueller matrix data were fitted to the model. Finally we have compared calculated shift and the sign change of calculated data and data obtained from a set of 15 samples and a very good agreement was achieved.

# 1.4 Organization of the thesis

This thesis is organized in four chapters.

*Chapter 2* introduces the polarization properties of light and the formulation of the Maxwell equations used in rest of text. The solution of the Maxwell's equations in layered medium is introduced in two steps. First, the eigenmodes in each medium are found, after that the boundary conditions are applied for the interfaces. Then the Rigorous Coupled Wave Algorithm (RCWA) is introduced as a solution of the Maxwell equations in 1D periodic media by its expansion into Fourier series. The chapter is finished by the introduction of the Li-factorization rules for 1D gratings and definition of the experimental observables.

*Chapter 3* is devoted to the description of the methods used for the fabrication and optical and magneto-optical characterization. We introduce the technique of magneto-optical Bi:GIG garnet layer fabrication on the sGGG substrate. In the next step, optical functions of the Bi:GIG, sGGG and the reference gold are determined using Mueller matrix ellipsometry. The characterization work is finished by the determination of the magneto-optical functions of Bi:GIG. The chapter is finished by the description of the fabrication of the magnetoplasmonic gratings.

*Chapter 4* is focused on numerical simulations of the optical and magneto-optical properties of the 1D periodic magnetoplasmonic grating. A detailed analysis of resonant modes in the structure and analytical formulae describing these resonances are introduced. The main part of the chapter is devoted to the analysis of the geometrical dispersion of the resonant modes for various grating's thickness, fill-factor and period and to the analysis of impact of modes interaction to the TMOKE response. The chapter is finished with proposition of waveguiding structures based on magnetoplasmonics.

*Chapter 5* is devoted to the experiments on fabricated magnetoplasmonic structures. In this chapter we will show experimental confirmation of the previous theoretical results on the interaction of resonant modes. The chapter consist of three main parts. In the first we are focused on the optical characterization of the fabricated structure in order to develop a realistic model of the structure, which can describe the measured data (optical and magneto-optical) with a good agreement. In the second part the developed model is used to fit experimental data measured on the set of 15 samples. Finally, the analysis of the TMOKE response is presented and the experimental confirmation of previous theoretical results is shown.

### 2 Theoretical background

This chapter introduces numerical method, the Rigorous Coupled Wave Algorithm (RCWA), used in the thesis for modeling and data analysis. The Berreman and Yeh formalism is used for solution of the Maxwell's equations for plane waves. By application of the boundary conditions of the Maxwell's equations the T-matrix algorithm is derived. For the 1D periodic gratings the Maxwell's equations are solved in Fourier domain, the S-matrix algorithm, and the factorization of the finite Fourier series are presented. Chapter is finished by definition of the experimental observables.

# 2.1 Light polarization

Light in a general medium can be described as a solution of Maxwell equations [67]. In our approach we use the solution for monochromatic plane waves which can describe far field physical processes, for instance the reflection, transmission, and the polarization changes of the light after interactions with matter.

For the plane monochromatic waves we use the complex representation [67, 68]:

$$\mathbf{E}(\mathbf{r},t) = E_0 \mathbf{e} \exp\left[i\left(\mathbf{k} \cdot \mathbf{r} - \omega t\right)\right],$$
(2.1a)

$$\mathbf{H}(\mathbf{r},t) = H_0 \mathbf{h} \exp\left[i\left(\mathbf{k} \cdot \mathbf{r} - \omega t\right)\right], \qquad (2.1b)$$

where  $E_0$  and  $H_0$  are the complex field amplitudes and the vectors e and h represent the polarization states of the field and they are independent on *z*-coordinate.  $\omega = \frac{2\pi}{\lambda}$  where  $\lambda$  is the wavelength, and k is the wavevector. Real (physical) electric and magnetic fields are the real parts of the field vectors (2.1a) and (2.1b).

Considering propagation of the plane wave in *z*-direction, the endpoint of the electric field vector traces in general an ellipse (Fig 2.1). The polarization ellipse can be described by two parameters, the azimuth  $\theta$  and the ellipticity  $\varepsilon$ . The azimuth  $\theta$  is the angle describing rotation of the major axis of the ellipse (in the range from  $-\pi/2$  to  $\pi/2$ ) and tan  $\varepsilon$  is the ratio between major and minor axis of the ellipse (in the range from  $-\pi/4$  to  $\pi/4$ ). With the rotation and ellipticity the expression of the electric field component in Fig 2.1 leads to the relation:

$$\begin{bmatrix} e_x \\ e_y \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\varepsilon \\ i\sin\varepsilon \end{bmatrix} = \begin{bmatrix} \cos\theta\cos\varepsilon - i\sin\theta\sin\varepsilon \\ \sin\theta\cos\varepsilon + i\cos\theta\sin\varepsilon \end{bmatrix}, \quad (2.2)$$

where  $e_x$ ,  $e_y$  are the components of the polarization vector e. According to parameters  $\theta$  and  $\varepsilon$  we can define two basic states of light polarization. If the transverse



Figure 2.1: Real part of elliptically polarized vector e for propagation in *z*-axis direction.

field components  $E_0e_x$ ,  $E_0e_y$  have the same magnitude and the phase between them is  $\pi/2$  and  $-\pi/2$ , polarization states are referred as left and right circular polarization respectively. Normalized electric field components of the left and right circular polarization are in the following form:

$$\mathbf{e}_{\text{left}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\ i \end{bmatrix}, \qquad (2.3a)$$

$$\mathbf{e}_{\text{right}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\ -i \end{bmatrix}.$$
(2.3b)

If the polarization components are in phase ( $\varepsilon = 0$ ) the polarization is linear. In experiments and simulations we define the polarization with respect to the plane of incidence. When the electric field vector is perpendicular to the plane of incidence the polarization state is called transverse electric (TE) or *s*-polarized. If the electric field vector is in the plane of incidence the polarization state is transverse magnetic (TM) or *p*-polarized. Normalized field vectors for the linear polarizations can be expressed in the form:

$$\mathbf{e}_{\mathrm{TE}} = \begin{bmatrix} 1\\0 \end{bmatrix}, \qquad (2.4a)$$

$$\mathbf{e}_{\mathrm{TM}} = \begin{bmatrix} 0\\1 \end{bmatrix}. \tag{2.4b}$$

# 2.2 Maxwell equations in general media

An electromagnetic field and its interactions with a medium is described by the Maxwell equations defining relations between the electric field  $\mathbf{E}(\mathbf{r}, t)$ , the magnetic field  $\mathbf{H}(\mathbf{r}, t)$ , the electric displacement  $\mathbf{D}(\mathbf{r}, t)$ , the magnetic flux density  $\mathbf{B}(\mathbf{r}, t)$ , the volume density of the free charges  $\rho(\mathbf{r}, t)$ , and the current density  $\mathbf{j}(\mathbf{r}, t)$  in the form:

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \mathbf{j}(\mathbf{r},t) + \frac{\partial \mathbf{D}(\mathbf{r},t)}{\partial t},$$
 (2.5a)

$$abla imes \mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t},$$
(2.5b)

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = \rho(\mathbf{r}, t), \tag{2.5c}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0. \tag{2.5d}$$

An additional constitution relations between the polarization  $\mathbf{P}(\mathbf{r}, t)$  and the magnetization  $\mathbf{M}(\mathbf{r}, t)$  are expressed:

$$\mathbf{D}(\mathbf{r},t) = \epsilon_0 \mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t), \qquad (2.6a)$$

$$\mathbf{B}(\mathbf{r},t) = \mu_0 \mathbf{H}(\mathbf{r},t) + \mu_0 \mathbf{M}(\mathbf{r},t), \qquad (2.6b)$$

where  $\mu_0$  is the free space permeability and  $\epsilon_0$  is the free space permittivity. In the following calculations, let's consider the magnetization for optical frequencies M = 0 and linear material properties without free charges at the interfaces:

$$\rho\left(\mathbf{r},t\right) = 0. \tag{2.7}$$

The charge volume density **j** can be expressed using the conductivity tensor  $\hat{\sigma}$  by the relation:

$$\mathbf{j}(\mathbf{r},t) = \widehat{\sigma} \mathbf{E}(\mathbf{r},t). \tag{2.8}$$

Using the electric susceptibility tensor  $\hat{\chi}_{e}$ , defining the relation between the polarization density and the electric intensity:

$$\mathbf{P}(\mathbf{r},t) = \epsilon_0 \widehat{\chi_e} \mathbf{E}(\mathbf{r},t), \qquad (2.9)$$

the permittivity tensor  $\hat{\epsilon}$  is defined as:

$$\widehat{\epsilon} = \epsilon_0 \left( \widehat{\mathbb{I}} + \widehat{\chi}_e \right) \tag{2.10}$$

Those premises let us write Maxwell equations (2.5) in the new form:

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \hat{\epsilon} \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} + \hat{\sigma} \mathbf{E}(\mathbf{r}, t), \qquad (2.11a)$$

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t},$$
(2.11b)

$$\nabla \cdot [\hat{\epsilon} \mathbf{E}(\mathbf{r}, t)] = 0, \qquad (2.11c)$$

 $\nabla \cdot \mathbf{H}(\mathbf{r}, t) = 0. \tag{2.11d}$ 

During following calculations let us consider only monochromatic plane waves and restrict to harmonic solution  $\exp(-i\omega t)$ . Then the electric and magnetic field vector can be expressed in the form:

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})\exp\left(-\mathrm{i}\omega t\right), \qquad (2.12a)$$

$$\mathbf{H}(\mathbf{r},t) = \mathbf{H}(\mathbf{r})\exp\left(-\mathrm{i}\omega t\right),\tag{2.12b}$$

where the complex amplitudes  $E(\mathbf{r})$ ,  $H(\mathbf{r})$  are time independent. Relations (2.11) together with (2.12) lead to the final expression of Maxwell's equations with eliminated time-dependency :

$$\nabla \times \mathbf{H}(\mathbf{r}) = -\mathrm{i}\omega\widehat{\epsilon}\,\mathbf{E}(\mathbf{r}) + \widehat{\sigma}\,\mathbf{E}(\mathbf{r}) = -\mathrm{i}\omega\widehat{\epsilon}'\mathbf{E}(\mathbf{r}),\tag{2.13a}$$

$$\nabla \times \mathbf{E}(\mathbf{r}) = i\omega\mu_0 \mathbf{H}(\mathbf{r}), \tag{2.13b}$$

$$\nabla \cdot [\hat{\epsilon}' \mathbf{E}(\mathbf{r})] = 0, \qquad (2.13c)$$

$$\nabla \cdot \mathbf{H} \left( \mathbf{r} \right) = 0, \tag{2.13d}$$

where  $\hat{\epsilon}'$  is the complex permittivity tensor:

$$\widehat{\epsilon}' = \epsilon_0 \widehat{\epsilon_R} = \widehat{\epsilon} + \frac{\mathrm{i}}{\omega} \widehat{\sigma}.$$
(2.14)

This tensor describes optical properties of both anisotropic and absorbing materials.

#### 2.2.1 Material properties

The optical response of a material is affected by material parameters, which are the permittivity  $\hat{\epsilon}'$  and permeability  $\mu$ . For optical frequencies the permeability is assumed to be equal to the permeability of free space,  $\mu = \mu_0$ . General permittivity tensor in (2.13a) has the following form:

$$\widehat{\epsilon_R} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix}.$$
(2.15)

The material tensor can be simplified, for special anisotropies and for special orientations as follows:

#### - Isotropic material

An isotropic material has rotation symmetry around all exes:

$$\widehat{\epsilon_R} = \begin{bmatrix} \epsilon_{xx} & 0 & 0\\ 0 & \epsilon_{xx} & 0\\ 0 & 0 & \epsilon_{xx} \end{bmatrix}.$$
(2.16)

#### – Uniaxial anisotropy

An uniaxial anisotropic material has rotation symmetry around one symmetry axis (here the *y*-axis):

$$\widehat{\epsilon_R} = \begin{bmatrix} \epsilon_{xx} & 0 & 0\\ 0 & \epsilon_{yy} & 0\\ 0 & 0 & \epsilon_{xx} \end{bmatrix}.$$
(2.17)

#### Biaxial anisotropy

The tensor of a biaxial anisotropic material with axes parallel to the coordinate system axis has all diagonal elements different:

$$\widehat{\epsilon_R} = \begin{bmatrix} \epsilon_{xx} & 0 & 0\\ 0 & \epsilon_{yy} & 0\\ 0 & 0 & \epsilon_{zz} \end{bmatrix}.$$
(2.18)

#### 2.2.2 Magneto-Optic anisotropy

Linear dependence of the components of the permittivity tensor on the magnetization vector M defines the linear magneto-optic effects. Using the Einstein summation convention the dependence of the permittivity tensor components on magnetization components can be expressed [69]:

$$\epsilon_{ij} = \varepsilon_{ij}^{(0)} + K_{ijk}M_k, \tag{2.19}$$

where  $K_{ijk}$  represent the components of the linear magneto-optic tensor and  $\varepsilon_{ij}^{(0)}$  denotes the permittivity tensor components without the effect of the magnetization M. The permittivity has to fulfill Onsager symmetry [70,71]:

$$\epsilon_{ij}\left(\mathbf{M}\right) = \epsilon_{ji}\left(-\mathbf{M}\right). \tag{2.20}$$

Considering M = 0 in (2.19) and (2.20) the following relations of symmetry are obtained:

Full linear magneto-optic permittivity tensor can be written in the form:

$$\hat{\epsilon}_{R} = \begin{bmatrix} \varepsilon_{xx}^{(0)} & \varepsilon_{xy}^{(0)} - K_{xyk}M_{k} & \varepsilon_{xz}^{(0)} + K_{xzk}M_{k} \\ \varepsilon_{xy}^{(0)} + K_{xyk}M_{k} & \varepsilon_{yy}^{(0)} & \varepsilon_{yz}^{(0)} - K_{yzk}M_{k} \\ \varepsilon_{xz}^{(0)} - K_{xzk}M_{k} & \varepsilon_{yz}^{(0)} + K_{yzk}M_{k} & \varepsilon_{zz}^{(0)} \end{bmatrix}.$$
 (2.22)

Figure 2.2 shows system of coordinates and basic directions of the magnetization vector. Plane y - z is chosen to be the plane of incidence. According to orientation of the magnetization vector M with respect to the plane of incidence three basic MO configurations are defined: polar, longitudinal, and transversal.



Figure 2.2: Directions of magnetization for basic magneto-optic configurations: polar, longitudinal, and transversal.

#### Polar magneto-optical configuration

In the polar magneto-optical configuration the magnetization is perpendicular to the surface (first subplot of Fig. 2.2):

$$\mathbf{M}_P = [0, 0, M_z]^T \,. \tag{2.23}$$

Considering isotropic material the permittivity tensor for polar magnetization is obtained using relations (2.22):

$$\widehat{\epsilon_{RP}} = \begin{bmatrix} \epsilon_{xx} & -K_{xyz}M_z & 0\\ K_{xyz}M_z & \epsilon_{xx} & 0\\ 0 & 0 & \epsilon_{xx} \end{bmatrix},$$
(2.24)

#### Longitudinal magneto-optical configuration

In the longitudinal magneto-optical configuration the magnetization is parallel to the surface and to the plane of the incidence (second subplot on Fig. 2.2):

$$\mathbf{M}_{L} = [0, M_{y}, 0]^{T} \,. \tag{2.25}$$

Permittivity tensor of isotropic media for longitudinal magnetization has following form:

$$\hat{\epsilon_{RL}} = \begin{bmatrix} \epsilon_{xx} & 0 & K_{xzy}M_y \\ 0 & \epsilon_{xx} & 0 \\ -K_{xzy}M_y & 0 & \epsilon_{xx} \end{bmatrix}, \qquad (2.26)$$

#### Transversal magneto-optical configuration

In the transversal magneto-optical configuration the magnetization is parallel to the surface and perpendicular to the plane of the incidence (third subplot on Fig. 2.2):

$$\mathbf{M}_T = [M_x, 0, 0]^T \,. \tag{2.27}$$

Permittivity tensor of isotropic media for transverse magnetization has following form:

$$\widehat{\epsilon}_{RT} = \begin{bmatrix} \epsilon_{xx} & 0 & 0\\ 0 & \epsilon_{xx} & -K_{yzx}M_x\\ 0 & K_{yzx}M_x & \epsilon_{xx} \end{bmatrix}, \qquad (2.28)$$

# 2.3 Solution of Maxwell's equations in layered media

This section is focused on a description of the electromagnetic field in a layered structure. Plane wave solution simplifies the description of the field inside the structure. Figure 2.3 shows the layered structure schematically. In the layered structure we are interested mostly in the tangential field components (here xand y components) which are continuous at interfaces - the boundary conditions can be directly applied [72–74]. There are two common approaches to solve the Maxwell's equations in layered media. Berreman's approach uses plane wave solution and transforms Maxwell equations into a set of four equations for tangential field components [72]. In Yeh's approach Maxwell's equations are transformed into a wave equation [73].



Figure 2.3: System of coordinates for planar structure

#### 2.3.1 Berreman approach for solving Maxwell's equations

Berreman calculations starts from (2.13a,2.13b) and expand them into a system of linear differential equations with constant coefficients. By this the Maxwell's equations can be easily solved in each layer of the system. To derive this Maxwell's

equations are first transformed as follows. The first step is applying the normalization:

$$\mathbf{E}'(\mathbf{r}) = \sqrt[4]{\mu_0^{-1}\epsilon_0} \mathbf{E}(\mathbf{r}), \qquad (2.29a)$$

$$\mathbf{H}'(\mathbf{r}) = \sqrt[4]{\epsilon_0^{-1} \mu_0 \mathbf{H}(\mathbf{r})},$$
(2.29b)

into (2.13a,2.13b):

$$\nabla \times \mathbf{H}'(\mathbf{r}) = -\mathrm{i}k_0 \hat{\epsilon_R} \, \mathbf{E}'(\mathbf{r}), \qquad (2.30a)$$

$$\nabla \times \mathbf{E}'(\mathbf{r}) = \mathrm{i}k_0 \mathbf{H}'(\mathbf{r}), \qquad (2.30b)$$

where  $k_0 = \frac{\omega}{c}$  is the amplitude of the wave vector in free space. For the general permittivity tensor (2.15), these equations can be written in matrix notation as follows:

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

$$= ik_0 \begin{bmatrix} -\epsilon_{xx} & -\epsilon_{xy} & -\epsilon_{xz} & 0 & 0 & 0 \\ -\epsilon_{yx} & -\epsilon_{yy} & -\epsilon_{yz} & 0 & 0 & 0 \\ -\epsilon_{zx} & -\epsilon_{zy} & -\epsilon_{zz} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} E'_x(\mathbf{r}) \\ E'_y(\mathbf{r}) \\ E'_z(\mathbf{r}) \\ H'_x(\mathbf{r}) \\ H'_y(\mathbf{r}) \\ H'_y(\mathbf{r}) \\ H'_z(\mathbf{r}) \end{bmatrix}.$$
(2.31)

Assuming plane wave solution:

$$\mathbf{E}'(\mathbf{r}) = \mathbf{E}'(x, y, z) = E_0' \mathbf{e}(z) \exp\left[\mathrm{i}k_0 \left(\nu_x x + \nu_y y\right)\right], \qquad (2.32a)$$

$$\mathbf{H}'(\mathbf{r}) = \mathbf{H}'(x, y, z) = H_0' \mathbf{h}(z) \exp\left[\mathrm{i}k_0 \left(\nu_x x + \nu_y y\right)\right].$$
(2.32b)

tangential derivatives can be factored out and only the *z*-derivatives remain:

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\partial}{\partial z} & \mathrm{i}k_0\nu_y \\ 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & -\mathrm{i}k_0\nu_x \\ 0 & 0 & 0 & -\mathrm{i}k_0\nu_y & \mathrm{i}k_0\nu_x & 0 \\ 0 & -\frac{\partial}{\partial z} & \mathrm{i}k_0\nu_y & 0 & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & -\mathrm{i}k_0\nu_x & 0 & 0 & 0 \\ -\mathrm{i}k_0\nu_y & \mathrm{i}k_0\nu_x & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \\ e'_z(z) \\ h'_x(z) \\ h'_y(z) \\ h'_z(z) \end{bmatrix} =$$

$$= ik_0 \begin{bmatrix} -\epsilon_{xx} & -\epsilon_{xy} & -\epsilon_{xz} & 0 & 0 & 0 \\ -\epsilon_{yx} & -\epsilon_{yy} & -\epsilon_{yz} & 0 & 0 & 0 \\ -\epsilon_{zx} & -\epsilon_{zy} & -\epsilon_{zz} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \\ e'_z(z) \\ h'_x(z) \\ h'_y(z) \\ h'_z(z) \end{bmatrix},$$
(2.33)

where  $\nu_x$ ,  $\nu_y$  are the components of the normalized wave vector  $\mathbf{N} = \mathbf{k}/k_0$ . The wavevector  $\mathbf{k}$  is defined as:

$$\mathbf{k} = k_0 \left( \mathbf{i}_{\mathbf{x}} \nu_x + \mathbf{i}_{\mathbf{y}} \nu_y + \mathbf{i}_{\mathbf{z}} \nu_z \right).$$
(2.34)

Let's first introduce the vector of tangential components  $\mathbf{F}(z)$  depending on *z*-coordinate:

$$\mathbf{F}(z) = \left[e'_{x}(z), h'_{y}(z), e'_{y}(z), h'_{x}(z)\right]^{T},$$
(2.35)

Using the F-vector it is possible to obtain explicit formulas for the normal components  $e_z^{'}, h_z^{'}$ :

$$\begin{bmatrix} -\epsilon_{zz}^{-1}\epsilon_{zx} & -\epsilon_{zz}^{-1}\nu_x & -\epsilon_{zz}^{-1}\epsilon_{zy} & \epsilon_{zz}^{-1}\nu_y \\ -\nu_y & 0 & \nu_x & 0 \end{bmatrix} \underbrace{\begin{bmatrix} e'_x(z) \\ h'_y(z) \\ e'_y(z) \\ h'_x(z) \end{bmatrix}}_{\mathbf{F}(z)} = \begin{bmatrix} e'_z(z) \\ h'_z(z) \end{bmatrix}.$$
 (2.36)

Separating the normal components one can write (2.33) as:

$$\begin{bmatrix} 0 & 0 & 0 & -\frac{\partial}{\partial z} \\ 0 & 0 & \frac{\partial}{\partial z} & 0 \\ 0 & -\frac{\partial}{\partial z} & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \\ h'_x(z) \\ h'_y(z) \end{bmatrix} + ik_0 \begin{bmatrix} \nu_y e'_z(z) \\ -\nu_x e'_z(z) \\ \nu_y h'_z(z) \\ -\nu_x h'_z(z) \end{bmatrix} =$$
$$= ik_0 \begin{bmatrix} -\epsilon_{xx} & -\epsilon_{xy} & 0 & 0 \\ -\epsilon_{yx} & -\epsilon_{yy} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} e'_x(z) \\ e'_y(z) \\ h'_x(z) \\ h'_y(z) \end{bmatrix} + \begin{bmatrix} -\epsilon_{xz} e'_z(z) \\ \epsilon_{yz} e'_z(z) \end{bmatrix}.$$
(2.37)

The system is reorganized with respect to the vector  $\mathbf{F}(z)$  (2.35) and  $e'_z(z)$ ,  $h'_z(z)$  are substituted according to (2.36):

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial z} \\ 0 & 0 & -\frac{\partial}{\partial z} & 0 \\ \frac{\partial}{\partial z} & 0 & 0 & 0 \end{bmatrix} + \mathbf{i}k_0 \begin{bmatrix} -\nu_y^2 & 0 & \nu_y\nu_x & 0 \\ \nu_y\nu_x & 0 & -\nu_x^2 & 0 \\ -\nu_y\epsilon_{zz}^{-1}\epsilon_{zx} & -\nu_y\epsilon_{zz}^{-1}\nu_x & -\nu_y\epsilon_{zz}^{-1}\epsilon_{zy} & \nu_y\epsilon_{zz}^{-1}\nu_y \\ \nu_x\epsilon_{zz}^{-1}\epsilon_{zx} & \nu_x\epsilon_{zz}^{-1}\nu_x & \nu_x\epsilon_{zz}^{-1}\epsilon_{zy} & \nu_x\epsilon_{zz}^{-1}\nu_y \end{bmatrix} \end{bmatrix} \mathbf{F}(z) =$$

$$= \left[ \begin{bmatrix} -\epsilon_{xx} & 0 & -\epsilon_{xy} & 0 \\ -\epsilon_{yx} & 0 & -\epsilon_{yy} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} \epsilon_{xz}\epsilon_{zz}^{-1}\epsilon_{zx} & \epsilon_{xz}\epsilon_{zz}^{-1}\nu_{x} & \epsilon_{xz}\epsilon_{zz}^{-1}\epsilon_{zy} & -\epsilon_{xz}\epsilon_{zz}^{-1}\nu_{y} \\ \epsilon_{yx}\epsilon_{zz}^{-1}\epsilon_{zx} & \epsilon_{yz}\epsilon_{zz}^{-1}\nu_{x} & \epsilon_{yz}\epsilon_{zz}^{-1}\epsilon_{zx} & -\epsilon_{yz}\epsilon_{zz}^{-1}\nu_{y} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \right] ik_{0}\mathbf{F}(z)$$

$$(2.38)$$

From Eq. (2.33) we can derive a system of 4 equations for only the tangential components of the fields. A system of four coupled differential equations is obtained and it can be solved by different techniques. By proper reorganization it is possible to transform this problem into an eigenvalue problem that can be solved with high efficiency (in numerical simulations). The final form of the eigenvalue problem is:

$$\frac{\partial}{\partial z} \mathbf{F}(z) = \mathrm{i}k_0 \mathrm{C}\mathbf{F}(z), \qquad (2.39)$$

where the matrix C follows from (2.38):

$$C = \begin{bmatrix} -\nu_{x}\epsilon_{zz}^{-1}\epsilon_{zx} & 1 - \nu_{x}\epsilon_{zz}^{-1}\nu_{x} & -\nu_{x}\epsilon_{zz}^{-1}\epsilon_{zy} & \nu_{x}\epsilon_{zz}^{-1}\nu_{y} \\ -\nu_{y}^{2} + \epsilon_{xx} - \epsilon_{xz}\epsilon_{zz}^{-1}\epsilon_{zx} & -\epsilon_{xz}\epsilon_{zz}^{-1}\nu_{x} & \nu_{y}\nu_{x} + \epsilon_{xy} - \epsilon_{xz}\epsilon_{zz}^{-1}\epsilon_{zy} & \epsilon_{xz}\epsilon_{zz}^{-1}\nu_{y} \\ -\nu_{y}\epsilon_{zz}^{-1}\epsilon_{zx} & -\nu_{y}\epsilon_{zz}^{-1}\nu_{x} & -\nu_{y}\epsilon_{zz}^{-1}\epsilon_{zy} & \nu_{y}\epsilon_{zz}^{-1}\nu_{y} - 1 \\ -\nu_{x}\nu_{y} - \epsilon_{yx} + \epsilon_{yz}\epsilon_{zz}^{-1}\epsilon_{zx} & \epsilon_{yz}\epsilon_{zz}^{-1}\nu_{x} & \nu_{x}^{2} - \epsilon_{yy} + \epsilon_{yz}\epsilon_{zz}^{-1}\epsilon_{zy} & -\epsilon_{yz}\epsilon_{zz}^{-1}\nu_{y} \end{bmatrix}$$

$$(2.40)$$

Equation (2.39) is soluble as the eigenvalue problem of the C matrix.

#### Eigenvalue decomposition

The eigenvalue decomposition of the matrix C is defined as follows:

$$CT = TV, \qquad (2.41)$$

where T is a column matrix of eigenvectors and V is a diagonal matrix of eigenvalues, i.e. normal components of normalized wave vectors. Because of linear independence of eigenvectors, any vector which is in conformity with Maxwell equations (2.13) can be expressed as a linear combination of eigenvectors with amplitudes g(z):

$$\mathbf{F}(z) = \mathrm{Tg}(z). \tag{2.42}$$

The final system of differential equations for the amplitudes is obtained by substituting (2.42) into (2.39):

$$\frac{\partial}{\partial z}\mathbf{g}(z) = \mathrm{i}k_0 \mathrm{V}\mathbf{g}(z), \qquad (2.43)$$

and the solution g(z) can be written:

$$\mathbf{g}(z) = \exp\left(\mathrm{i}k_0 z \mathbf{V}\right) \mathbf{A},\tag{2.44}$$

where A is vector of the amplitudes of each mode.

#### T and V matrices of isotropic homogeneous material

Let the plane of incident wave be identical with the *y*-*z* plane (according to Fig. 2.3) and the medium be isotropic and homogeneous. Then the component of normalized wave vector  $\nu_x = 0$ , the permittivity tensor  $\hat{\epsilon}$  is in the form of a diagonal matrix,  $\hat{\epsilon} = diag(\epsilon, \epsilon, \epsilon)$  and the C matrix describing this medium can be written in the form:

$$C_{iso} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \epsilon - \nu_y^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \nu_y \epsilon^{-1} \nu_y - 1 \\ 0 & 0 & -\epsilon & 0 \end{bmatrix}.$$
 (2.45)

The next step is the calculation of the eigenvalues  $V_{iso}$  of the  $C_{iso}$  matrix

$$\mathbf{V}_{iso} = \begin{bmatrix} \sqrt{\epsilon - \nu_y^2} & 0 & 0 & 0\\ 0 & -\sqrt{\epsilon - \nu_y^2} & 0 & 0\\ 0 & 0 & \sqrt{\epsilon - \nu_y^2} & 0\\ 0 & 0 & 0 & -\sqrt{\epsilon - \nu_y^2} \end{bmatrix},$$
(2.46)

and its eigenvectors  $T_{iso}$ 

$$T_{iso} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ \sqrt{\epsilon - \nu_y^2} & -\sqrt{\epsilon - \nu_y^2} & 0 & 0 \\ 0 & 0 & (\sqrt{\epsilon})^{-1} \sqrt{\epsilon - \nu_y^2} & (\sqrt{\epsilon})^{-1} \sqrt{\epsilon - \nu_y^2} \\ 0 & 0 & -\sqrt{\epsilon} & \sqrt{\epsilon} \end{bmatrix}.$$
 (2.47)

At this point it is necessary to discuss ordering of columns and rows of the V and T matrices (2.46), (2.47). The analytical expression of modes in the isotropic homogeneous material (2.47) represents tangential components of the the *s*-polarized (first and second columns) and *p*-polarized modes (third and fourth columns). The *s*- and *p*-polarized modes are further distinguished as up and/or down propagating according to the related propagation constant. For straightforward calculation the flowing ordering of modes (columns) in the T is commonly used :

$$\mathbf{T}_{iso} = [S_{down}, S_{up}, P_{down}, P_{up}].$$

$$(2.48)$$

The ordering was already used in construction of the  $V_{iso}$ -matrix, where the signs of the  $[V_{iso}]_{11}$  and  $[V_{iso}]_{22}$  are opposite (and  $[V_{iso}]_{33}$ ,  $[V_{iso}]_{44}$  as well). Columns of the  $T_{iso}$  were ordered according to the propagation constants. The situations becomes complicated when the T-matrix is calculated by the eigenvalue decomposition of the C-matrix. Depending on algorithm, the arrangement of the eigenvalues and eigenvectors may be different. Therefore ordering criteria has to be established. For the chosen sign convention downward propagating waves have positive real part of the propagation constant and positive imaginary part if the wave is attenuated. Naturally, *up* and *down* modes can be distinguished according their real or/and imaginary part. In our implementation we have used combined criteria for ordering of modes. According to the numerical tests we have set threshold for the absolute value of the propagation constant imaginary part as 0.05. If the value is above the threshold, the mode is recognized as *up* or *down* according to the sign of the imaginary part. If the value is under the threshold, the sign of the real part is used for *up* and *down* ordering. This combined criteria is not necessary for a layered structures, but it improves computing stability if the same code is used for a grating calculation, which will be discussed further.

#### 2.3.2 Yeh approach for solving Maxwell equations

Another way to solve the electromagnetic wave propagating in an anisotropic layered medium has been introduced by Yeh [73, 75]. Instead of solving system of linear first-order differential equations, the system is transformed into one second-order equation. The equation has to be solved for each medium in a single system separately. With the aid of Yeh's approach it is easy to get analytical formulas for some special media. For example isotropic homogeneous media or media with a special anisotropy caused by an external magnetic field. Firstly the Helmholtz wave equation is derived from Maxwell's equations (2.11) and assuming plane wave solution (2.1):

$$\mathbf{k} \times [\mathbf{k} \times \mathbf{E}] + \frac{\omega^2}{c^2} \hat{\epsilon}_R \mathbf{E} = 0, \qquad (2.49)$$

and equation for H:

$$\mathbf{H} = \sqrt{\frac{\epsilon_0}{\mu_0}} \mathbf{N} \times \mathbf{E},\tag{2.50}$$

where  $\mathbf{N} = \mathbf{k}/k_0$  is normalized wavevector defined by (2.34).

#### Matrix of tangential component with Yeh approach applied to isotropic homogeneous material

Equation (2.49) is expanded and simplified as follows for an isotropic medium:

$$\underbrace{\begin{bmatrix} \epsilon - \nu_y^2 - \nu_z^2 & \nu_y \nu_x & \nu_z \nu_x \\ \nu_x \nu_y & \epsilon - \nu_x^2 - \nu_z^2 & \nu_z \nu_y \\ \nu_x \nu_z & \nu_y \nu_z & \epsilon - \nu_x^2 - \nu_y^2 \end{bmatrix}}_{\mathrm{B}} \times \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = 0$$
(2.51)

The problem (2.51) is solved for nontrivial solutions  $\nu_z$  assuming the tangential  $\nu_x$  and  $\nu_y$  are given by the incident wave. The solutions  $\nu_z$  are the solutions of the det(B) = 0:

$$\nu_{z,1} = +\sqrt{\epsilon - \nu_x^2 - \nu_y^2} \\ \nu_{z,2} = -\nu_{z,1} = -\sqrt{\epsilon - \nu_x^2 - \nu_y^2} \\ \nu_{z,3} = +\sqrt{\epsilon - \nu_x^2 - \nu_y^2} \\ \nu_{z,4} = -\nu_{z,3} = -\sqrt{\epsilon - \nu_x^2 - \nu_y^2}$$
(2.52)

The propagation constants with positive real parts ( $\nu_{z,1}$ ,  $\nu_{z,3}$ ) represent *down*-propagating modes, those with negative real part *up*-propagating modes ( $\nu_{z,2}$ ,  $\nu_{z,4}$ ). This propagation constants are connected to two *up*- and two *down*-propagating plane waves. Propagating modes are chosen as a *s*- and *p*-polarized waves, however each wave satisfying wave equation (2.51) can be used.

$$\mathbf{e}_{1} = \begin{bmatrix} \nu_{y} \\ -\nu_{x} \\ 0 \end{bmatrix}, \quad \mathbf{h}_{1} = \begin{bmatrix} \nu_{x}\nu_{z,1} \\ \nu_{y}\nu_{z,1} \\ -(\nu_{x}^{2} + \nu_{y}^{2}) \end{bmatrix}, \\
\mathbf{e}_{2} = \begin{bmatrix} \nu_{y} \\ -\nu_{x} \\ 0 \end{bmatrix}, \quad \mathbf{h}_{2} = \begin{bmatrix} -\nu_{x}\nu_{z,1} \\ \nu_{y}\nu_{z,1} \\ -(\nu_{x}^{2} + \nu_{y}^{2}) \end{bmatrix}, \\
\mathbf{e}_{3} = \begin{bmatrix} \nu_{x}\nu_{z,3} \\ \nu_{y}\nu_{z,3} \\ (\nu_{x}^{2} + \nu_{y}^{2}) \end{bmatrix}, \quad \mathbf{h}_{3} = \begin{bmatrix} \nu_{y}\nu_{z,3}^{-1} \left(\nu_{x}^{2} + \nu_{y}^{2} - \nu_{z,3}^{2}\right) \\ \nu_{x}\nu_{z,3}^{-1} \left(\nu_{x}^{2} + \nu_{y}^{2} - \nu_{z,3}^{2}\right) \\ 0 \end{bmatrix}, \\
\mathbf{e}_{4} = \begin{bmatrix} -\nu_{x}\nu_{z,3} \\ -\nu_{y}\nu_{z,3} \\ (\nu_{x}^{2} + \nu_{y}^{2}) \end{bmatrix}, \quad \mathbf{h}_{4} = \begin{bmatrix} -\nu_{y}\nu_{z,3}^{-1} \left(\nu_{x}^{2} + \nu_{y}^{2} - \nu_{z,3}^{2}\right) \\ \nu_{x}\nu_{z,3}^{-1} \left(\nu_{x}^{2} + \nu_{y}^{2} - \nu_{z,3}^{2}\right) \\ 0 \end{bmatrix}.$$
(2.53)

Relation (2.50) has been used for calculation of magnetic fields. The atrix of the tangential components T is assembled from the components of the field vectors (2.53) according to the column vector F (2.35) and propagation direction (constant  $\nu_z$ ).

Let the plane of incidence wave be in y - z plane ( $\nu_x = 0$  according to Figure. 2.3) and assume a isotropic homogeneous medium ( $\hat{\epsilon} = diag(\epsilon, \epsilon, \epsilon)$ ). Then the solution of the (2.53) is identical with (2.46) and (2.47).

#### 2.3.3 Analytical formulae for magneto-optical media

Considering media with anisotropy induced only by linear magneto-optical effect in an isotropic medium (i.e.  $\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz}$ ), the permittivity tensor (2.22) is

defined as follows:

$$\widehat{\epsilon_R} = \epsilon_1 \begin{bmatrix} 1 & -iQ_P & iQ_L \\ iQ_P & 1 & -iQ_T \\ iQ_L & iQ_T & 1 \end{bmatrix},$$
(2.54)

where parameters  $Q_P$ ,  $Q_L$ , and  $Q_T$  are the linear magneto-optical parameters of polar, longitudinal and transverse magneto-optical effect, respectively.

#### Polar magneto-optical effect

Here we consider the polar magneto-optical configuration ( $Q_L = Q_T = 0$ ) and the incident plane wave in y - z plane ( $\nu_x = 0$ ). The Helmholtz equation for the plane waves 2.49 is expanded as follows:

$$\underbrace{\begin{bmatrix} \epsilon_1 - \nu_y^2 - \nu_z^2 & -i\epsilon_1 Q_P & 0\\ i\epsilon_1 Q_P & \epsilon_1 - \nu_z^2 & \nu_z \nu_y\\ 0 & \nu_y \nu_z & \epsilon_1 - \nu_y^2 \end{bmatrix}}_{\mathbf{B}} \times \begin{bmatrix} e_x\\ e_y\\ e_z \end{bmatrix} = 0.$$
(2.55)

The problem (2.55) is solved for nontrivial solutions  $\nu_z$  assuming the tangential  $\nu_y$  is given by the incident wave. The solutions  $\nu_z$  are the solutions of the det(B)=0:

$$\nu_{z,1,3} = -\nu_{z,2,4} = \sqrt{\epsilon_1 - \nu_y^2 \pm Q_P \sqrt{\epsilon_1 \left(\epsilon_1 - \nu_y^2\right)}}.$$
(2.56)

Solution of the problem are the elliptically polarized plane waves and the matrix of tangential fields is defined as:

$$T_{polar} = \begin{bmatrix} T_{11} & T_{11} & T_{11} & T_{11} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & T_{33} & T_{34} \\ T_{41} & T_{42} & T_{43} & T_{44} \end{bmatrix},$$
(2.57)

where

$$T_{11} = \epsilon_1 Q_P \left( \epsilon_1 - \nu_y^2 \right),$$
  

$$T_{2,j} = \epsilon_1 Q_P \nu_{z,j} \left( \epsilon_1 - \nu_y^2 \right),$$
  

$$T_{3,j} = i \nu_y \nu_{z,j} \left( \epsilon_1 - \nu_y^2 - \nu_{z,j}^2 \right),$$
  

$$T_{4,j} = i \nu_y \nu_{z,j}^4 - i \nu_y \epsilon_1^2 + 2i \epsilon_1 \nu_y^3 - i \nu_y^5.$$
  
(2.58)

#### Longitudinal magneto-optical effect

Here we consider the longitudinal magneto-optical configuration ( $Q_P = Q_T = 0$ ) and the incident plane wave in y - z plane ( $\nu_x = 0$ ). The Helmholtz equation for the plane waves 2.49 is expanded as follows:

$$\underbrace{\begin{bmatrix} \epsilon_1 - \nu_y^2 - \nu_z^2 & 0 & i\epsilon_1 Q_L \\ 0 & \epsilon_1 - \nu_z^2 & \nu_z \nu_y \\ -i\epsilon_1 Q_L & \nu_y \nu_z & \epsilon_1 - \nu_y^2 \end{bmatrix}}_{\mathrm{B}} \times \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = 0.$$
(2.59)

The problem (2.59) is solved for nontrivial solutions  $\nu_z$  assuming the tangential  $\nu_y$  is given by the incident wave. The solutions  $\nu_z$  are the solutions of the det(B) = 0:

$$\nu_{z,1,3} = -\nu_{z,2,4} = \sqrt{\epsilon_1 - \nu_y^2 - \frac{1}{2}\epsilon_1 Q_L^2 \pm \frac{1}{2}Q_L \sqrt{\epsilon_1^2 Q_L^2 + 4\epsilon_1 \nu_y^2}}.$$
 (2.60)

Solution of the problem are the elliptically polarized plane waves and the matrix of tangential fields is defined as:

$$T_{long} = \begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & T_{33} & T_{34} \\ T_{41} & T_{42} & T_{43} & T_{44} \end{bmatrix},$$
(2.61)

where

$$T_{1,j} = i\epsilon_1 \nu_y Q_L \nu_{z,j},$$

$$T_{2,j} = i\epsilon_1 \nu_y Q_L \nu_{z,j}^2,$$

$$T_{3,j} = -\nu_y \nu_{z,j} \left(\epsilon_1 - \nu_y^2 - \nu_{z,j}^2\right),$$

$$T_{4,j} = \nu_y \epsilon_1^2 - 2\epsilon_1 \nu_y^3 + \nu_y^5 - \nu_y \epsilon_1^2 Q_L^2 - \nu_y \nu_{z,j}^4.$$
(2.62)

#### Transverse magneto-optical effect

Considering the transverse magneto-optical configuration ( $Q_P = Q_T = 0$ ) and the incident plane wave in y - z plane ( $\nu_x = 0$ ). The Helmholtz equation for plane waves (2.49) is expanded as follows:

$$\underbrace{\begin{bmatrix} \epsilon_1 - \nu_y^2 - \nu_z^2 & 0 & 0\\ 0 & \epsilon_1 - \nu_z^2 & -i\epsilon_1 Q_T + \nu_y \nu_z\\ 0 & i\epsilon_1 Q_T + \nu_y \nu_z & \epsilon_1 - \nu_y^2 \end{bmatrix}}_{\mathbf{B}} \times \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = 0.$$
(2.63)

The problem (2.63)) is solved for nontrivial solutions  $\nu_z$  assuming the tangential  $\nu_y$  is given by the incident wave. The solutions  $\nu_z$  are the solutions of the det(B)=0:

$$\nu_{z,1,2} = \pm \sqrt{\epsilon_1 - \nu_y^2}, \qquad \nu_{z,3,4} = \pm \sqrt{\epsilon_1 - \nu_y^2 - \epsilon_1 Q_T^2}.$$
 (2.64)

Solution of the problem are the linear polarized plane waves and the matrix of tangential fields is defined as:

$$\mathbf{T}_{long} = \begin{bmatrix} T_{11} & T_{11} & 0 & 0 \\ T_{21} & -T_{21} & 0 & 0 \\ 0 & 0 & T_{33} & T_{33} \\ 0 & 0 & T_{43} & T_{44} \end{bmatrix},$$
 (2.65)

where

$$T_{1,1} = 1,$$

$$T_{2,1} = \sqrt{\epsilon_1 - \nu_y^2},$$

$$T_{3,3} = \epsilon_1 - \nu_y^2,$$

$$T_{4,3} = -i\epsilon_1\nu_yQ_T - \epsilon_1\sqrt{\epsilon_1 - \nu_y^2 - \epsilon_1Q_T^2},$$

$$T_{4,4} = -i\epsilon_1\nu_yQ_T + \epsilon_1\sqrt{\epsilon_1 - \nu_y^2 - \epsilon_1Q_T^2},$$
(2.66)

Note that from the (2.65) it is directly seen, that transverse MO Kerr effect affects only *p*-polarization.

# 2.4 Boundary conditions - field matching at interfaces

In this section the theoretical results about solving of the Maxwell equations in the medium based on the tangential components continuity (Sec. 2.3.) are applied to the system of planar layers. Figure 2.4 shows the discussed case with the layer [with index (*i*)] surrounded by a system of layers and the superstrate (0) and a substrate (n + 1). Assuming homogeneous, isotropic substrate and superstrate the eigenmodes in this semi-infinite media are given by analytical form of the T-matrix (2.47). The eigenmodes in a homogeneous layer (i + 1) with a general anisotropy are calculated as an eigenvector problem (2.43) of a general C<sup>(1)</sup> matrix (2.40).



Figure 2.4: Wave transformation in propagation through a system of planar layers.

The vector  $\mathbf{A}^{(i)}(z_i)$  represents the vector of amplitudes of field components at the interface  $z_i$ . From the C-matrix of a general material (anisotropic, homogeneous), the eigenvector matrix T is obtained as follows:

$$\mathbf{T}^{(i)} = \begin{bmatrix} e_{1,x}^{(i)} & e_{2,x}^{(i)} & e_{3,x}^{(i)} & e_{4,x}^{(i)} \\ h_{1,y}^{(i)} & h_{2,y}^{(i)} & h_{3,y}^{(i)} & h_{4,y}^{(i)} \\ e_{1,y}^{(i)} & e_{2,y}^{(i)} & e_{4,y}^{(i)} \\ h_{1,x}^{(i)} & h_{2,x}^{(i)} & h_{3,x}^{(i)} & h_{4,x}^{(i)} \end{bmatrix}.$$
(2.67)

The vector of amplitudes  $\mathbf{A}^{(i)} = \left[A_{1_{down}}^{(i)}, A_{2_{up}}^{(i)}, A_{3_{down}}^{(i)}, A_{4_{up}}^{(i)}\right]^T$  is defined for each mode in the structure. Therefore the product of  $T^{(i)}\mathbf{A}^{(i)}$  represents total tangential field components:

$$\begin{bmatrix}
e_{1,x}^{(i)} & e_{2,x}^{(i)} & e_{3,x}^{(i)} & e_{4,x}^{(i)} \\
h_{1,y}^{(i)} & h_{2,y}^{(i)} & h_{3,y}^{(i)} & h_{4,y}^{(i)} \\
e_{1,y}^{(i)} & e_{2,y}^{(i)} & e_{3,y}^{(i)} & e_{4,y}^{(i)} \\
h_{1,x}^{(i)} & h_{2,x}^{(i)} & h_{3,x}^{(i)} & h_{4,x}^{(i)}
\end{bmatrix}
\begin{bmatrix}
A_{1_{down}}^{(i)} \\
A_{2_{up}}^{(i)} \\
A_{3_{down}}^{(i)} \\
A_{4_{up}}^{(i)}
\end{bmatrix} =
\begin{bmatrix}
e_{x}^{(i)} \\
h_{y}^{(i)} \\
e_{y}^{(i)} \\
h_{x}^{(i)}
\end{bmatrix}.$$
(2.68)

Continuity of the tangential components at the interface leads to the following relation for the top interface:

$$T^{(i)}\mathbf{A}^{(i)}(z_i) = T^{(i+1)}\mathbf{A}^{(i+1)}(z_i), \qquad (2.69a)$$

(2.69b)

To be able to describe total optical response of the structure or to calculate field distribution it is necessary to propagate fields through a media. This is described with the following T-matrix algorithm.
#### 2.4.1 T-matrix algorithm

For description of the optical response of a multilayered structure it is necessary to include field propagation through the system. The propagation from interface  $(z_i)$  to  $(z_{i+1})$  is described with propagation matrix  $P^{(i+1)}$ :

$$\mathbf{P}^{(i+1)} = \begin{bmatrix} \exp\left[ik_0\left[\mathbf{V}^{(i+1)}\right]_{1,1}d^{(i+1)}\right] & 0 & 0 & 0 \\ 0 & \exp\left[ik_0\left[\mathbf{V}^{(i+1)}\right]_{2,2}d^{(i+1)}\right] & 0 & 0 \\ 0 & 0 & \exp\left[ik_0\left[\mathbf{V}^{(i+1)}\right]_{3,3}d^{(i+1)}\right] & 0 \\ 0 & 0 & 0 & \exp\left[ik_0\left[\mathbf{V}^{(i+1)}\right]_{4,4}d^{(i+1)}\right] \end{bmatrix} \end{bmatrix}$$

where  $[V]_{ii}$  are the propagation constants from matrix V, i.e. propagation constants  $\nu_{z,i}$ , and  $d_i$  is the thickness of i + 1-th layer. The vector of amplitudes is transformed according to the relation:

$$\mathbf{A}^{(i+1)}(z_{i+1}) = \mathbf{P}^{(i+1)}\mathbf{A}^{(i+1)}(z_i).$$
(2.71)

The relation between the wave  $\mathbf{A}^{(i)}(z_i)$  and  $\mathbf{A}^{(i+2)}(z_{i+1})$  is given combining (2.69-2.71):

$$\mathbf{A}^{(i)}(z_i) = \left(\mathbf{T}^{(i)}\right)^{-1} \mathbf{T}^{(i+1)} \left(\mathbf{P}^{(i+1)}\right)^{-1} \left(\mathbf{T}^{(i+1)}\right)^{-1} \mathbf{T}^{(i+2)} \mathbf{A}^{(i+2)}(z_{i+1}).$$
(2.72)

For a system with N planar layers the relation between the vector of the amplitudes in the superstrate and the substrate has the following form <sup>1</sup>:

$$\mathbf{A}^{(0)} = \left(\mathbf{T}^{(0)}\right)^{-1} \left(\prod_{i=1}^{N} \mathbf{T}^{(i)} \left(\mathbf{P}^{(i)}\right)^{-1} \left(\mathbf{T}^{(i)}\right)^{-1}\right) \mathbf{T}^{(N+1)} \mathbf{A}^{(N+1)} = \mathbf{T} \mathbf{A}^{(N+1)}.$$
 (2.73)

The presented T-matrix algorithm is straightforward and effective approach how to propagate field in a layered media. At this point it is time to point out, that the algorithm propagates fields from the top to the bottom side. In means, that back reflected waves from the bottom are propagated in opposite directions. In other worlds, amplitude of the propagating mode is being exponentially increased, because it is calculated in the opposite direction that it really propagates. Despite this fact, the T-matrix algorithm is stable for calculation of layered structures. But it can becomes unstable when highly evanescent modes exists in a structure.

<sup>1.</sup> It is not necessary to calculate inversion to matrix  $P^{(i)}$  in numerical implementation, changing the sign in exponential factor reduces calculation time.

# 2.5 Solution of the Maxwell equations in the 1D periodic media

This section deals with solution of Maxwell's equations in a 1D periodic media, using rigorous coupled wave analysis (RCWA). Figure 2.5 schematically illustrates 1D periodic structure. In the following calculations let's assume the



Figure 2.5: System of coordinates for 1D grating.

plane of incidence is parallel to the y-z plane, and it is perpendicular to the lamellas of the grating. Because the permittivity tensor of the periodic layer is a discontinuous function (in y-direction) it is necessary to use more advanced method than the T-matrix algorithm (2.73). The algorithm discussed in this section is the Rigorous Coupled Wave Analysis (RCWA) based on approximation of permittivity function and field components by their truncated Fourier series [76,77].

## 2.5.1 Maxwell equation in Fourier domain

Starting from the normalized Maxwell equations defined in (2.30):

$$\nabla \times \mathbf{H}'(\mathbf{r}) = -\mathrm{i}k_0 \hat{\epsilon_R} \mathbf{E}'(\mathbf{r}), \qquad (2.74a)$$

$$\nabla \times \mathbf{E}'(\mathbf{r}) = \mathrm{i}k_0 \mathbf{H}'(\mathbf{r}), \qquad (2.74b)$$

in which the permittivity tensor  $\hat{\epsilon}_R$  is a periodic function of the *y* coordinate,  $\hat{\epsilon}_R = \hat{\epsilon}(y)$  with the period  $\Lambda$ . Components of the permittivity tensor are expanded in a Fourier series:

$$\epsilon_{ij}(y) = \sum_{n=-\infty}^{\infty} \epsilon_{ij,n} \exp\left(i n \frac{2\pi}{\Lambda} y\right), \qquad (2.75)$$

where  $\epsilon_{ij,n}$  is *n*-th Fourier coefficient defined using the integral:

$$\epsilon_{ij,n} = \frac{1}{\Lambda} \int_{0}^{\Lambda} \epsilon_{ij}(y) \exp\left(-i n \frac{2\pi}{\Lambda} y\right) dy.$$
(2.76)

Using the Floquet theorem, the electric and magnetic field components are also expanded into Fourier series in each layer in the structure, including homogeneous layers [73,77–79]:

$$\mathbf{E}'(\mathbf{r}) = \sum_{n=-\infty}^{\infty} \mathbf{e}_n(z) \exp\left[\mathrm{i}k_0\left(\nu_x x + \nu_y y\right)\right] \exp\left(\mathrm{i}n\frac{2\pi}{\Lambda}y\right), \qquad (2.77a)$$

$$\mathbf{H}'(\mathbf{r}) = \sum_{n=-\infty}^{\infty} \mathbf{h}_n(z) \exp\left[\mathrm{i}k_0\left(\nu_x x + \nu_y y\right)\right] \exp\left(\mathrm{i}n\frac{2\pi}{\Lambda}y\right).$$
 (2.77b)

#### 2.5.2 Solution in finite Fourier domain

For numerical implementation it is necessary to truncate the Fourier image of the field components. Symmetrical truncation is given by 2N + 1 members of infinite Fourier image. Putting of the equations (2.77a) and (2.77b) into the Maxwell equation (2.30a) and (2.30b) the Fourier image has the form:

$$\nabla \times \sum_{n=-N}^{N} \mathbf{h}_{n}(z) \exp\left[\mathrm{i}k_{0}\left(\nu_{x}x+\nu_{y}y\right)\right] \exp\left(\mathrm{i}n\frac{2\pi}{\Lambda}y\right) =$$

$$= -\mathrm{i}k_{0}\sum_{n=-N}^{N}\sum_{m=-N}^{N}\widehat{\epsilon}_{n-m}\mathbf{e}_{m}(z) \exp\left[\mathrm{i}k_{0}\left(\nu_{x}x+\nu_{y}y\right)\right] \exp\left(\mathrm{i}n\frac{2\pi}{\Lambda}y\right), \quad (2.78)$$

$$\nabla \times \sum_{n=-N}^{N}\mathbf{e}_{n}(z) \exp\left[\mathrm{i}k_{0}\left(\nu_{x}x+\nu_{y}y\right)\right] \exp\left(\mathrm{i}n\frac{2\pi}{\Lambda}y\right) =$$

$$= \mathrm{i}k_{0}\sum_{n=-N}^{N}\mathbf{h}_{n}(z) \exp\left[\mathrm{i}k_{0}\left(\nu_{x}x+\nu_{y}y\right)\right] \exp\left(\mathrm{i}n\frac{2\pi}{\Lambda}y\right), \quad (2.79)$$

where  $\hat{\epsilon}_n$  is a tensor of *n*-th Fourier component. Following a compact notation, Eq. (2.78) and (2.79) are further calculated and implemented in the form:

$$\nabla \times \{ \mathbf{F} \left[ \mathbf{h} \left( z \right) \right] \exp \left[ \mathrm{i}k_0 \left( \nu_x x + \nu_y y \right) \right] \} = -\mathrm{i}k_0 \mathbf{F} \left[ \left[ \widehat{\epsilon} \right] \right] \left[ \mathbf{e} \left( z \right) \right] \exp \left[ \mathrm{i}k_0 \left( k_x x + k_y y \right) \right],$$
(2.80a)
$$\nabla \times \{ \mathbf{F} \left[ \mathbf{e} \left( z \right) \right] \exp \left[ \mathrm{i}k_0 \left( \nu_x x + \nu_y y \right) \right] \} = \mathbf{F} \left[ \mathbf{h} \left( z \right) \right] \exp \left[ \mathrm{i}k_0 \left( \nu_x x + \nu_y y \right) \right],$$
(2.80b)

where the matrix F is a matrix with the Fourier exponents on its diagonal and has the size  $(2N + 1) \times (2N + 1)$ :

$$F_{ij} = \delta_{ij} \exp\left[i\left(j - N - 1\right)\frac{2\pi}{\Lambda}y\right].$$
(2.81)

The symbol  $\lceil . \rceil$  stands for the amplitudes vector of truncated Fourier expansion (in the *y* direction) and symbol  $\lceil . \rceil$  stands for the Toeplitz amplitude matrix of expanded permittivity tensor function  $\hat{\epsilon}(y)$ . This notation helps to express otherwise very complicated formulas in rather compact forms. In the following text we will use these symbols in places, where we believe it could simplify equations and clarify the used algorithms.

Using the same approach like in (2.31) we first evaluate the curl operator in (2.80b). Then the matrix F is eliminated by multiplication of both sides of equations with  $F^{-1}$  from the left. This cancels out the exponential factors and equations are particularly derived with respect to tangential components:

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ 0 & 0 & 0 & -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \\ 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} & 0 & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} & 0 & 0 & 0 \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \begin{bmatrix} e_x(\mathbf{r}) \\ e_y(\mathbf{r}) \\ e_z(\mathbf{r}) \\ \begin{bmatrix} h_x(\mathbf{r}) \\ h_y(\mathbf{r}) \\ \end{bmatrix} \\ \begin{bmatrix} h_y(\mathbf{r}) \\ h_z(\mathbf{r}) \end{bmatrix} \end{bmatrix} =$$

$$= ik_{0} \begin{bmatrix} \begin{bmatrix} -\epsilon_{xx} \end{bmatrix} & \begin{bmatrix} -\epsilon_{xy} \end{bmatrix} & \begin{bmatrix} -\epsilon_{xz} \end{bmatrix} & 0 & 0 & 0 \\ \begin{bmatrix} -\epsilon_{yx} \end{bmatrix} & \begin{bmatrix} -\epsilon_{yy} \end{bmatrix} & \begin{bmatrix} -\epsilon_{yz} \end{bmatrix} & 0 & 0 & 0 \\ \begin{bmatrix} -\epsilon_{yx} \end{bmatrix} & \begin{bmatrix} -\epsilon_{yy} \end{bmatrix} & \begin{bmatrix} -\epsilon_{yz} \end{bmatrix} & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} \begin{bmatrix} e_{x} (\mathbf{r}) \end{bmatrix} \\ \begin{bmatrix} e_{y} (\mathbf{r}) \end{bmatrix} \\ \begin{bmatrix} h_{x} (\mathbf{r}) \end{bmatrix} \\ \begin{bmatrix} h_{y} (\mathbf{r}) \end{bmatrix} \\ \begin{bmatrix} h_{y} (\mathbf{r}) \end{bmatrix} \\ \begin{bmatrix} h_{y} (\mathbf{r}) \end{bmatrix} \end{bmatrix}.$$
(2.82)

And after derivation:

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\partial}{\partial z} & \mathrm{i}k_{0}\mathbf{q} \\ 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & -\mathrm{i}k_{0}\mathbf{p} \\ 0 & 0 & 0 & -\mathrm{i}k_{0}\mathbf{q} & \mathrm{i}k_{0}\mathbf{p} & 0 \\ 0 & -\frac{\partial}{\partial z} & \mathrm{i}k_{0}\mathbf{q} & 0 & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & -\mathrm{i}k_{0}\mathbf{p} & 0 & 0 & 0 \\ -\mathrm{i}k_{0}\mathbf{q} & \mathrm{i}k_{0}\mathbf{p} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \begin{bmatrix} e_{x}\left(\mathbf{r}\right) \\ e_{y}\left(\mathbf{r}\right) \\ \begin{bmatrix} e_{z}\left(\mathbf{r}\right) \\ h_{x}\left(\mathbf{r}\right) \\ \begin{bmatrix} h_{y}\left(\mathbf{r}\right) \\ h_{y}\left(\mathbf{r}\right) \\ \begin{bmatrix} h_{z}\left(\mathbf{r}\right) \end{bmatrix} \end{bmatrix} \end{bmatrix} =$$

$$= ik_{0} \begin{bmatrix} \begin{bmatrix} -\epsilon_{xx} \end{bmatrix} & \begin{bmatrix} -\epsilon_{xy} \end{bmatrix} & \begin{bmatrix} -\epsilon_{xz} \end{bmatrix} & 0 & 0 & 0 \\ \begin{bmatrix} -\epsilon_{yx} \end{bmatrix} & \begin{bmatrix} -\epsilon_{yy} \end{bmatrix} & \begin{bmatrix} -\epsilon_{yz} \end{bmatrix} & 0 & 0 & 0 \\ \begin{bmatrix} -\epsilon_{yx} \end{bmatrix} & \begin{bmatrix} -\epsilon_{zy} \end{bmatrix} & \begin{bmatrix} -\epsilon_{zz} \end{bmatrix} & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} \begin{bmatrix} e_{x} (\mathbf{r}) \\ e_{y} (\mathbf{r}) \\ e_{z} (\mathbf{r}) \\ \begin{bmatrix} h_{x} (\mathbf{r}) \\ h_{y} (\mathbf{r}) \\ \end{bmatrix} \\ \begin{bmatrix} h_{y} (\mathbf{r}) \\ h_{z} (\mathbf{r}) \end{bmatrix} \end{bmatrix}.$$
(2.83)

The matrices p and q are diagonal with elements representing the tangential component of the normalized wave vector,  $p_{ij} = \delta_{i,j}\nu_x$  and  $q_{ij} = \delta_{ij} \left[\nu_y + (j - N - 1)\frac{\lambda}{\Lambda}\right]$ , for  $i, j \in \{1, 2, ..., 2N + 1\}$ . From the equation (2.83) the normal components can be separated and expressed with the tangential components. Finally after some calculation the vector of tangential components is defined as :

 $\left[ \mathbf{F}(z) \right] = \left[ \left[ e_x(z) \right], \left[ h_y(z) \right], \left[ e_y(z) \right], \left[ h_x(z) \right] \right]^T,$ (2.84)

and the same type of eigenvalue problem is obtained:

$$\frac{\partial}{\partial z} \left[ \mathbf{F}(z) \right] = \mathrm{i}k_0 \mathrm{C} \left[ \mathbf{F}(z) \right].$$
(2.85)

The size of the matrix C is now  $4(2N+1) \times 4(2N+1)$  and has the following form:

$$\begin{bmatrix} -p \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zx} \right] \right] & \mathbb{I} - p \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \\ -q^{2} + \left[ \left[ \epsilon_{xx} \right] \right] - \left[ \left[ \epsilon_{xz} \right] \right] \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zx} \right] \right] & - \left[ \left[ \epsilon_{xz} \right] \right] \left[ \left[ \epsilon_{zz}^{-1} \right] \right] p \\ -q \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zx} \right] \right] & -q \left[ \left[ \epsilon_{zz}^{-1} \right] \right] p \\ pq - \left[ \left[ \epsilon_{yx} \right] \right] + \left[ \left[ \epsilon_{yz} \right] \right] \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zx} \right] \right] & \left[ \epsilon_{yz} \right] \right] \left[ \left[ \epsilon_{zz}^{-1} \right] p \\ \vdots & -p \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zy} \right] \right] & p \left[ \left[ \epsilon_{zz}^{-1} \right] \right] q \\ \vdots & -p \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zz} \right] \right] & \left[ \epsilon_{zz} \right] \right] \left[ \left[ \epsilon_{zz}^{-1} \right] \right] q \\ \vdots & -q \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \left[ \epsilon_{zy} \right] \right] & q \left[ \left[ \epsilon_{zz}^{-1} \right] \right] q - \mathbb{I} \\ \vdots & p^{2} - \left[ \left[ \epsilon_{yy} \right] \right] + \left[ \left[ \epsilon_{yz} \right] \right] \left[ \left[ \epsilon_{zz}^{-1} \right] \right] \left[ \epsilon_{zy} \right] ] - \left[ \left[ \epsilon_{yz}^{-1} \right] \right] q \end{bmatrix}$$

$$(2.86)$$

Resulting system is a set of coupled first degree differential equations with constant coefficients and the solution g(z) can be written in the form:

$$\left[\mathbf{g}\left(z\right)\right] = \exp\left[\mathrm{i}k_{0}z_{i}\mathrm{V}\right]\mathbf{A},\tag{2.87}$$

where **A** is the vector of amplitudes of each wave mode and V denotes diagonal matrix of the propagation constants.

#### 2.5.3 S-Matrix algorithm

As was discussed at the end of Sec. 2.4.1 the T-matrix algorithm is not numerically stable for grating calculations. The instability comes from the finite numerical precision of computers. When highly evanescent modes is calculated in the same direction as it propagates, amplitudes of its fields exponentially decreases. But in case of calculation in opposite direction that mode propagation, field are exponentially increased. Total field in any point in the structure is a sum of fields of all *up* an *down* modes, i.e. modes with large and low amplitudes. The idea of the S-matrix algorithm is to separate *up* and *down* modes in the structure and let them propagate in a direction of exponential damping.



Figure 2.6: Differences between input (solid red) and output (dashed blue) arguments in T-matrix and S-matrix algorithms.

Figure 2.7: Separated *up* and *down* propagating modes in medium

Figure 2.6 shows different calculation approach in the T-matrix and S-matrix algorithm. The T-matrix propagates the amplitude vector  $\mathbf{A}_{down}^{(0)}$  through the structure and relates amplitudes in the superstrate with amplitudes in the substrate. The S-matrix algorithm on the other hand relates the amplitudes of incoming waves  $(\mathbf{A}_{down}^{(0)}, \mathbf{A}_{up}^{(n+1)})$  to those of outgoing waves  $(\mathbf{A}_{up}^{(0)}, \mathbf{A}_{down}^{(n+1)})$ . The following calculations show the basic steps of the S-matrix algorithm. the first step is the

separation of the *up* and *down* modes. Starting from a known T-matrix description at a single interface, the relation between amplitudes  $\mathbf{A}^{(i)}(z_i)$  and  $\mathbf{A}^{(i+1)}(z_i)$  is:

$$\mathbf{A}^{(i)}(z_i) = \underbrace{\left(\mathbf{T}^{(i)}\right)^{-1} \mathbf{T}^{(i+1)}}_{\mathbf{T}} \mathbf{A}^{(i+1)}(z_i), \qquad (2.88)$$

or in compact T-matrix notation:

$$\begin{bmatrix} \mathbf{A}_{up}^{(i)} \\ \mathbf{A}_{down}^{(i)} \end{bmatrix} = \begin{bmatrix} T_{11}^{(i)} & T_{12}^{(i)} \\ T_{21}^{(i)} & T_{22}^{(i)} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(i+1)} \\ \mathbf{A}_{down}^{(i+1)} \end{bmatrix}.$$
 (2.89)

In the next step the *up* and *down* modes are separated:

$$\begin{bmatrix} \mathbf{A}_{up}^{(i)} \\ \mathbf{A}_{down}^{(i+1)} \end{bmatrix} = s^{(i)} \begin{bmatrix} \mathbf{A}_{up}^{(i+1)} \\ \mathbf{A}_{down}^{(i)} \end{bmatrix},$$
(2.90)

where the matrix  $s^{(i)}$  comes from T matrix:

$$\mathbf{s}^{(i)} = \begin{bmatrix} s_{11}^{(i)} & s_{12}^{(i)} \\ s_{21}^{(i)} & s_{22}^{(i)} \end{bmatrix} = \begin{bmatrix} T_{11}^{(i)} - T_{12}^{(i)} T_{22}^{(i)^{-1}} T_{21}^{(i)} & T_{12}^{(i)} T_{22}^{(i)^{-1}} \\ T_{22}^{(i)^{-1}} T_{21}^{(i)} & T_{22}^{(i)^{-1}} \end{bmatrix}.$$
 (2.91)

The next step is the description of the field propagation through a layer. The propagation matrix  $P^{(i+1)}$  can be written separately for *up* and *down* modes:

$$\mathbf{A}_{up}^{(i+1)}(z_i) = \mathbf{P}_{up}^{(i+1)} \mathbf{A}_{up}^{(i+1)}(z_{i+1}), \qquad (2.92a)$$

$$\mathbf{A}_{down}^{(i+1)}(z_{i+1}) = \mathbf{P}_{down}^{(i+1)} \mathbf{A}_{down}^{(i+1)}(z_i) \,.$$
(2.92b)

The propagation matrices are diagonal with the eigenvalues as arguments in the exponential factors:

$$P_{up}^{(i+1)} = \exp\left[-ik_0 d_{i+1} V_{up}^{(i+1)}\right],$$
(2.93a)

$$P_{down}^{(i+1)} = \exp\left[ik_0 d_{i+1} V_{down}^{(i+1)}\right],$$
(2.93b)

where  $d_{i+1}$  is the thickness of a layer with index i + 1. The relations (2.93) used in (2.90) lead to relation between waves in the upper medium and waves propagated through the interface and a single layer:

$$\begin{bmatrix} \mathbf{A}_{up}^{(i)}(z_i) \\ \mathbf{A}_{down}^{(i+1)}(z_{i+1}) \end{bmatrix} = \tilde{\mathbf{s}}^{(i)} \begin{bmatrix} \mathbf{A}_{up}^{(i+1)}(z_{i+1}) \\ \mathbf{A}_{down}^{(i)}(z_i) \end{bmatrix},$$
(2.94)

and  $\tilde{s}^{(i)}$  is a matrix describing the continuity on interface and the propagation through layer:

$$\tilde{\mathbf{s}}^{(i)} = \begin{bmatrix} \tilde{\mathbf{s}}_{11}^{(i)} & \tilde{\mathbf{s}}_{12}^{(i)} \\ \tilde{\mathbf{s}}_{21}^{(i)} & \tilde{\mathbf{s}}_{22}^{(i)} \end{bmatrix} = \begin{bmatrix} \mathbf{s}_{11}^{(i)} \mathbf{P}_{up}^{(i+1)} & \mathbf{s}_{12}^{(i)} \\ \mathbf{P}_{down}^{(i+1)} \mathbf{s}_{21}^{(i)} \mathbf{P}_{up}^{(i+1)} & \mathbf{P}_{down}^{(i+1)} \mathbf{s}_{22}^{(i)} \end{bmatrix}$$
(2.95)

If the structure has only one planar interface, the problem is solved with matrix (2.95) for  $d_{i+1} = 0$ . The matrix  $\tilde{s}^{(i+1)}$  is calculated for all interfaces [for example  $(z_{i+1})$ , see Figure 2.7.]. In the next step all the  $\tilde{s}^{(k)}$ ,  $k = 1, 2, \dots, n < N$  matrices are recursively added. The result is the  $S^{(n)}$ -matrix relating incoming and outgoing waves:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)}(z_0) \\ \mathbf{A}_{down}^{(n+1)}(z_{n+1}) \end{bmatrix} = \mathbf{S}^{(n)} \begin{bmatrix} \mathbf{A}_{up}^{(n+1)}(z_{n+1}) \\ \mathbf{A}_{down}^{(0)}(z_0) \end{bmatrix},$$
(2.96)

where matrix  $S^{(n)}$ :

$$\mathbf{S}^{(n)} = \begin{bmatrix} \mathbf{S}_{11}^{(n)} & \mathbf{S}_{12}^{(n)} \\ \mathbf{S}_{21}^{(n)} & \mathbf{S}_{22}^{(n)} \end{bmatrix}.$$
 (2.97)

Components of  $S^{(n+1)}$  are recurrently defined:

$$S_{11}^{(n+1)} = S_{11}^{(n)} \left[ \mathbb{I} - \tilde{s}_{12}^{(n+1)} S_{21}^{(n)} \right]^{-1} \tilde{s}_{11}^{(n+1)},$$

$$S_{12}^{(n+1)} = S_{12}^{(n)} + S_{11}^{(n)} \left[ \mathbb{I} - \tilde{s}_{12}^{(n+1)} S_{21}^{(n)} \right]^{-1} \tilde{s}_{12}^{(n+1)} S_{22}^{(n)},$$

$$S_{21}^{(n+1)} = \tilde{s}_{12}^{(n)} + \tilde{s}_{22}^{(n+1)} S_{21}^{(n)} \left[ \mathbb{I} - \tilde{s}_{12}^{(n+1)} S_{21}^{(n)} \right]^{-1} \tilde{s}_{11}^{(n+1)},$$

$$S_{22}^{(n+1)} = \tilde{S}_{22}^{(n)} \left[ S_{21}^{(n)} \left[ \mathbb{I} - \tilde{s}_{12}^{(n+1)} S_{21}^{(n)} \right]^{-1} \tilde{s}^{(n+1)} \right] S_{22}^{(n)}.$$
(2.98)

After applying recursive formula to all layers in structure one obtains the global scattering matrix S:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)}(z_0) \\ \mathbf{A}_{down}^{(N)}(z_N) \end{bmatrix} = \mathbf{S} \begin{bmatrix} \mathbf{A}_{up}^{(N)}(z_N) \\ \mathbf{A}_{down}^{(0)}(z_0) \end{bmatrix}$$
(2.99)

#### 2.5.4 Condition for guided modes

Calculation of guided modes is an important issue in structure design and optimization. A waveguiding structure could be for example a classical dielectric waveguide where a high-refractive index material is surrounded by a lowrefractive index cladding. Advanced waveguiding structures can be bases on guiding via excitation of surface plasmon resonance or by system periodicity, i.e. photonic crystal waveguides [80,81]. By the analysis of the S matrix it is possible to distinguish between propagating guided modes and localized resonant modes.

The guided modes condition using the T-matrix algorithm (Sec. 2.4.1) has been originally derived by Yeh [73, 82]. In the S-matrix notation resonant or guided modes can be described as follows:

$$\begin{bmatrix} (A)_{up}^{(0)} \\ (A)_{down}^{(N)} \end{bmatrix} = S \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$
(2.100)

where the left vector of outgoing amplitudes corresponds to evanescent waves and right zero vector represent situation without incomming modes from suband superstrate. The nontrivial solution for the inverse S-matrix needs to be find:

$$S^{-1} \begin{bmatrix} (A)_{up}^{(0)} \\ (A)_{down}^{(N)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$
 (2.101)

Such a problem can easily be solved via the *singular value decomposition* (SVD) [83]. The S-matrix can be decomposed into product of three matrices:

$$S = U\Sigma V^T \quad \Rightarrow \quad S^{-1} = V\Sigma^{-1}U^H,$$
 (2.102)

where U is the matrix of the *left* singular vectors, V is the matrix of the *right* singular vectors, both are unitary matrices, and  $U^H$  denotes the conjugate transpose of the matrix.<sup>2</sup> The matrix  $\Sigma$  is a diagonal matrix of singular values. The SVD can be rearranged according to ascending order of singular values:

$$\sigma_{max} = [\Sigma]_{1,1} \ge [\Sigma]_{2,2} \ge \ldots \ge [\Sigma]_{n,n}, \qquad (2.103)$$

then the problem of guided mode can be solved from relation:

$$S^{-1}U = V\Sigma^{-1}.$$
 (2.104)

Relation (2.104) represents a solution of the original problem (2.101). For the  $[\Sigma^{-1}]_{1,1} = 0$  the first column of the matrix  $V^T$  is the vector of outgoing modes  $\left[\mathbf{A}_{up}^{(N+1)}(z_{n+1}), \mathbf{A}_{down}^{(0)}(z_0)\right]^T$ .

In design and optimization of a wave-guiding structure the value  $1/\sigma_{max}$  is minimized in order to optimize waveguiding properties. Numerical minimization of  $1/\sigma_{max}$  together with condition (2.103) lead the diagonal matrix  $\Sigma^{-1}$  to be zero. Therefore it leads to zero matrix on the right side of (2.104) and waveguiding condition (2.101) is fulfilled.

The optimization procedure is done over free parameters (x), which typically are the real and imaginary parts of the propagation constant, geometry, wavelength, etc. [82]. The optimization process can be described:

$$\frac{1}{\sigma_{max}} \to 0: \quad \mathbf{x} \to \mathbf{x}_{optim}, \quad \left[\mathbf{V}^T\right]_{1,:} \to \left[\begin{array}{c} (A)_{up}^{(0)}\\ (A)_{down}^{(N+1)} \end{array}\right], \tag{2.105}$$

or in the compact form:

$$\mathbf{x}_{optim.} = \arg\min_{\mathbf{x}} \frac{1}{\sigma_{max}\left(\mathbf{x}\right)}.$$
(2.106)

<sup>2.</sup> A square complex matrix U is unitary if  $UU^H = U^H U = I$ .

# 2.6 Li-Factorization rules for 1D gratings

The S-matrix algorithm presented in the previous section completely eliminates problems with the numerical stability, theoretically for a infinite Fourier series. But there is a problem with convergence for *p*-polarized waves, especially for structures with high dielectric contrast (for instance metallic grating). For truncated Fourier series the instability problem is a serious issue. Problem comes from situation when the product of two discontinuous functions at the same point is a continuous function, h(y) = f(y) g(y). In other words the problem is that the tangential field components (*x* and *y*) are continuous at the plane interfaces, but they are not continuous inside the periodical layer, Fig. 2.8. On the other hand, the normal field components are continuous inside the grating layer. L. Li shows how the Fourier image of the components of the permittivity tensor must be rearranged for sufficient convergence of the problem [76, 78, 79, 84].



Figure 2.8: Discontinuity of field component  $E_y$  and continuity of  $D_y$  in the periodic layer is shown schematically as well as continuity of  $E_x$  and  $E_z$  fields.

If all functions have the same period  $\Lambda$  then the Fourier image of equation is in the form  $h(y) = f(y) \cdot g(y)$ :

$$\sum_{\infty}^{j=-\infty} h_j \exp\left[ij\frac{2\pi}{\Lambda}y\right] = \sum_{\infty}^{k=-\infty} f_k \exp\left[ik\frac{2\pi}{\Lambda}y\right] \cdot \sum_{\infty}^{l=-\infty} g_l \exp\left[il\frac{2\pi}{\Lambda}y\right].$$
 (2.107)

The right hand side of the equation can be simplified using Laurent's rule: prod-

uct of two function is the discrete convolution of their Fourier images:

$$\forall j \in \mathbb{Z}: \quad h_j = \sum_{\infty}^{k=-\infty} f_k g_{j-k} = \sum_{\infty}^{k=-\infty} f_{j-k} g_j. \tag{2.108}$$

The electric field and the electric displacement vectors are related by the permittivity tensor:

$$\begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}.$$
 (2.109)

This permittivity tensor is discontinuous and the field and flux components  $E_y$ ,  $D_x$  and  $D_z$  are discontinuous too. The components  $E_x$ ,  $E_z$  and  $D_y$  are due to boundary conditions continuous. For correct application of the Laurent rule it is necessary to reorganize equation (2.109) into form *discontinuous* = *discontinuous* × *continuous*:

$$\begin{bmatrix} D_x \\ D_z \\ E_y \end{bmatrix} = \mathbf{B} \begin{bmatrix} E_x \\ E_z \\ D_y \end{bmatrix}, \qquad (2.110)$$

where:

$$B = \begin{bmatrix} \epsilon_{xx} - \epsilon_{xy}\epsilon_{yy}^{-1}\epsilon_{yx} & \epsilon_{xz} - \epsilon_{xy}\epsilon_{yy}^{-1}\epsilon_{yz} & \epsilon_{xy}\epsilon_{yy}^{-1} \\ \epsilon_{zx} - \epsilon_{zy}\epsilon_{yy}^{-1}\epsilon_{yx} & \epsilon_{zz} - \epsilon_{zy}\epsilon_{yy}^{-1}\epsilon_{yz} & \epsilon_{zy}\epsilon_{yy}^{-1} \\ -\epsilon_{yy}^{-1}\epsilon_{yx} & -\epsilon_{yy}^{-1}\epsilon_{yz} & \epsilon_{yy}^{-1} \end{bmatrix}.$$
(2.111)

At this point components of the matrix B (2.111) can be expanded into the finite Fourier series (according to required number of the Fourier harmonics). Each Fourier series of each component is transformed into Toeplitz matrix. Field components are also expanded into finite Fourier series:

$$\begin{bmatrix} \begin{bmatrix} D_x \\ \\ D_z \end{bmatrix} \\ \begin{bmatrix} E_y \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} \begin{bmatrix} \epsilon_{xx} - \epsilon_{xy}\epsilon_{yy}^{-1}\epsilon_{yx} \end{bmatrix} & \begin{bmatrix} \epsilon_{xz} - \epsilon_{xy}\epsilon_{yy}^{-1}\epsilon_{yz} \end{bmatrix} & \begin{bmatrix} \epsilon_{xy}\epsilon_{yy}^{-1} \end{bmatrix} \\ \begin{bmatrix} \begin{bmatrix} e_{xx} - \epsilon_{zy}\epsilon_{yy}^{-1}\epsilon_{yx} \end{bmatrix} & \begin{bmatrix} \epsilon_{xz} - \epsilon_{zy}\epsilon_{yy}^{-1}\epsilon_{yz} \end{bmatrix} & \begin{bmatrix} e_{xy} \\ \begin{bmatrix} e_{xy} \\ e_{yy} \end{bmatrix} \end{bmatrix} \\ \begin{bmatrix} e_{xy} \\ \begin{bmatrix} e_{xy} \\ e_{yy} \end{bmatrix} & \begin{bmatrix} e_{xy} \\ e_{yy} \end{bmatrix} \end{bmatrix} & \begin{bmatrix} e_{xy} \\ \begin{bmatrix} e_{xy} \\ e_{yy} \end{bmatrix} \end{bmatrix} \\ \begin{bmatrix} e_{xy} \\ \begin{bmatrix} e_{xy} \\ e_{yy} \end{bmatrix} \end{bmatrix} \\ \begin{bmatrix} e_{xy} \\ e_{xy} \end{bmatrix} & \begin{bmatrix} e_{xy} \\ e_{yy} \end{bmatrix} \end{bmatrix}$$
(2.112)

The next step is rearrangement of the system (2.112) into the form used in the approach:  $\mathbf{D} = \hat{\epsilon} \mathbf{E}$  [Eq. (2.109)]. The system of equation (2.112) is reassembled into previous form with the following result:

$$\begin{bmatrix} \begin{bmatrix} D_x \\ D_y \end{bmatrix} \\ \begin{bmatrix} D_z \\ D_z \end{bmatrix} = Q \begin{bmatrix} \begin{bmatrix} E_x \\ E_y \end{bmatrix} \\ \begin{bmatrix} E_z \\ E_z \end{bmatrix}, \qquad (2.113)$$

where:

$$Q = \begin{bmatrix} \left[ \left[ \epsilon_{xx} - \epsilon_{xy} \epsilon_{yy}^{-1} \epsilon_{yx} \right] - \left[ \left[ \epsilon_{xy} \epsilon_{yy}^{-1} \right] \right] \left[ \left[ \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yx} \right] \right] \\ - \left[ \left[ \epsilon_{yy}^{-1} \right] \right]^{-1} \left[ \left[ \epsilon_{yy}^{-1} \epsilon_{yx} \right] \right] \\ \left[ \left[ \epsilon_{zx} - \epsilon_{zy} \epsilon_{yy}^{-1} \epsilon_{yx} \right] \right] - \left[ \left[ \epsilon_{zy} \epsilon_{yy}^{-1} \right] \right] \left[ \left[ \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy} \right] \right] \\ \vdots \\ \vdots \\ \left[ \left[ \epsilon_{xz} - \epsilon_{xy} \epsilon_{yy}^{-1} \right] \\ \vdots \\ \vdots \\ \left[ \left[ \epsilon_{zz} - \epsilon_{zy} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \right] \right] \\ \vdots \\ \left[ \left[ \epsilon_{zz} - \epsilon_{zy} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yz}^{-1} \epsilon_{yy}^{-1} \epsilon_{yy}^{-1} \epsilon_{yz}^{-1} \epsilon_{yz}^{-1} \epsilon_{yz}^{-1} \epsilon_{yy}^{-1} \epsilon_{yz}^{-1} \epsilon_{yz}^{$$

The matrix Q is now used instead of the Toeplitz permittivity tensor matrix with significantly improved convergence as a result.

# 2.7 Experimental observables

#### 2.7.1 Reflection and transmission coefficients

The elements in S-matrix (2.99) directly represent the transmission and the reflection coefficients. For the Fourier expansion of the field components into NFourier harmonics, each of the blocks  $S_{11}$  -  $S_{44}$  has the size  $(2N + 1) \times (2N + 1)$ . The eigenmodes in the superstrate (0) and substrate (N + 1) are chosen to be *s*and *p*-polarized modes. The components in the block represent refection or transmission coefficients for each Fourier order (diffracted radiative order, evanescent modes). The global S-matrix is defined as:

$$\begin{bmatrix} \mathbf{A}_{S_{up}}^{(0)} \\ \mathbf{A}_{P_{up}}^{(0)} \\ \mathbf{A}_{S_{down}}^{(N+1)} \\ \mathbf{A}_{P_{down}}^{(N+1)} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{S_{up}}^{(N+1)} \\ \mathbf{A}_{P_{up}}^{(0)} \\ \mathbf{A}_{S_{down}}^{(0)} \\ \mathbf{A}_{P_{down}}^{(0)} \end{bmatrix}.$$
(2.115)

which defines the following forward complex reflection and transmission coefficients:

$$\begin{array}{rcl} r_{\rm ss} &=& S_{13} & t_{\rm ss} &=& S_{33}, \\ r_{\rm ps} &=& S_{14} & t_{\rm ps} &=& S_{34}, \\ r_{\rm sp} &=& S_{23} & t_{\rm sp} &=& S_{43}, \\ r_{\rm pp} &=& S_{24} & t_{\rm pp} &=& S_{44}, \end{array}$$

$$\begin{array}{rcl} (2.116) \\ \end{array}$$

and the backward complex reflection and transmission coefficients:

$$\vec{r}_{ss} = S_{31} \quad t_{ss} = S_{11}, 
 \vec{r}_{ps} = S_{32} \quad \tilde{t}_{ps} = S_{12}, 
 \tilde{r}_{sp} = S_{41} \quad \tilde{t}_{sp} = S_{21}, 
 \tilde{r}_{pp} = S_{42} \quad \tilde{t}_{pp} = S_{22},$$
(2.117)

The S matrix relation (2.115) can be also written in the block form as:

$$\begin{bmatrix} \mathbf{A}_{up}^{(0)} \\ \mathbf{A}(N+1)_{down} \end{bmatrix} = \begin{bmatrix} \tilde{T}_{uu} & R_{du} \\ \tilde{R}_{ud} & T_{dd} \end{bmatrix} \begin{bmatrix} \mathbf{A}_{up}^{(N+1)} \\ \mathbf{A}(0)_{down} \end{bmatrix}$$
(2.118)

In most cases the specular reflection coefficients corresponding to zero diffraction order are needed. Their absolute position in the S-matrix is:

$$r_{ss} = [S]_{N+1,5N+3}, \qquad (2.119)$$

$$r_{ps} = [S]_{N+1,7N+4}, \qquad (2.120)$$

$$r_{sp} = [S]_{3N+2,5N+3}, \qquad (2.121)$$

$$r_{pp} = [S]_{3N+2,7N+4} \,. \tag{2.122}$$

#### 2.7.2 Ellipsometric angles

Ellipsometry is a powerful method for optical characterization. It brings important information about the amplitude and phase change upon reflection of a polarized plane wave from a sample. Due to phase shift detection, ellipsometry is more sensitive to some geometrical properties (like layer thickness) than reflectivity or transmission measurements. The measured quantities are the ellipsometric angles  $\psi$  and  $\Delta$  which are related to the complex ratio of the reflected (or transmitted) TM and TE waves:

$$\tan\psi\exp\left[\mathrm{i}\Delta\right] = \frac{r_{pp}}{r_{ss}}.$$
(2.123)

Relation (2.123) is valid only for isotropic non-depolarizing structures. In case of anisotropy the Jones matrix of a structure contains off-diagonal components:

$$\mathbf{J} = \begin{bmatrix} r_{ss} & r_{ps} \\ r_{sp} & r_{pp} \end{bmatrix} \propto \begin{bmatrix} 1 & \frac{r_{ps}}{r_{ss}} \\ \frac{r_{sp}}{r_{ss}} & \frac{r_{pp}}{r_{ss}} \end{bmatrix}.$$
 (2.124)

and for the ellipsometry it is necessary to introduce so called generalized ellipsometric angles  $\psi_{sp}, \psi_{ps}, \Delta_{sp}, \Delta_{ps}$ , [85–89].

#### 2.7.3 Mueller matrix

The interaction of a light beam with depolarizing sample cannot be fully described by the Jones formalism and more general  $4 \times 4$  Mueller matrix formalism has to be used. The Mueller matrix describes transformation of the Stokes vector

upon reflection (or transmission) from a sample. Most widely used definition of the Stokes vector is [90]:

$$\mathbf{S} = \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = \begin{bmatrix} I_p + I_s \\ I_p - I_s \\ I_{45^\circ} - I_{-45^\circ} \\ I_L - I_R \end{bmatrix}$$
(2.125)

The popularity of the four dimensional real Stokes vector is certainly due to its immediate relationship with the directly measurable quantities  $I_p$ ,  $I_s$ ,  $I_{+45^\circ}$ ,  $I_{-45^\circ}$  i.e. the intensities which would be measured through ideal linear polarizers oriented along the p, s,  $p+45^{\circ}5$  and  $p-45^{\circ}$  in the plane perpendicular to the direction of propagation, while  $I_L$  and  $I_R$  would be the intensities transmitted by left and right circular polarizers. Within the Stokes formalism, the *degree of polarization*  $\rho_s$  related to a given Stokes vector **S** is defined as:

$$\rho_s = \frac{\sqrt{Q^2 + U^2 + V^2}}{I} \tag{2.126}$$

Upon interaction with a sample the Stokes vector is transformed by Mueller the matrix:

$$\mathbf{S}^{out} = \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix}^{out} = \mathbf{M}\mathbf{S}^{in} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix}^{in}$$
(2.127)

The Mueller matrix has generally sixteen independent components, which is much more than six independent parameters from the Jones matrix (or generalized ellipsometry). On the other hand in the case of non-depolarizing systems the Mueller matrix and Jones matrix formalism are equivalent [91] and the Mueller matrix can be directly calculated from Jones matrix [92,93]:

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} = A (J \otimes J^*) A^{-1},$$
(2.128)

where the symbol  $\otimes$  denotes the Kronecker product, matrix  $J \otimes J^*$  is called the Coherence matrix, and A is defined as:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & -\mathbf{i} & \mathbf{i} & 0 \end{bmatrix}.$$
 (2.129)

The full Jones-Mueller matrix of non-depolarizing structure is in the form:

$\frac{1}{2} \left(  r_{ss} ^2 +  r_{sp} ^2 +  r_{ps} ^2 +  r_{pp} ^2 \right)$	$\frac{1}{2} \left( - r_{ss} ^2 +  r_{sp} ^2 -  r_{ps} ^2 +  r_{pp} ^2 \right)$	$\operatorname{Re}\left(r_{ps}r_{pp}^{*}+r_{ss}r_{sp}^{*}\right)$	$-\mathrm{Im}\left(r_{ps}r_{pp}^{*}+r_{ss}r_{sp}^{*}\right)$
$\frac{1}{2} \left( - r_{ss} ^2 -  r_{sp} ^2 +  r_{ps} ^2 +  r_{pp} ^2 \right)$	$\frac{1}{2} \left(  r_{ss} ^2 -  r_{sp} ^2 -  r_{ps} ^2 +  r_{pp} ^2 \right)$	$\operatorname{Re}\left(r_{ps}r_{pp}^{*}-r_{ss}r_{sp}^{*}\right)$	$\operatorname{Im}\left(-r_{ps}r_{pp}^{*}+r_{ss}r_{sp}^{*}\right)$
$\operatorname{Re}\left(r_{sp}r_{pp}^{*}+r_{ss}r_{ps}^{*}\right)$	$\operatorname{Re}\left(r_{sp}r_{pp}^{*}-r_{ss}r_{ps}^{*}\right)$	$\operatorname{Re}\left(r_{ss}r_{pp}^{*}+r_{sp}r_{ps}^{*}\right)$	$\operatorname{Im}\left(-r_{ss}r_{pp}^{*}+r_{sp}r_{ps}^{*}\right)$
$\operatorname{Im}\left(r_{sp}r_{pp}^{*}+r_{ss}r_{ps}^{*}\right)$	$\operatorname{Im}\left(r_{sp}r_{pp}^{*}-r_{ss}r_{ps}^{*}\right)$	$\operatorname{Im}\left(r_{ss}r_{pp}^{*}+r_{sp}r_{ps}^{*}\right)$	$\operatorname{Re}\left(r_{ss}r_{pp}^{*}-r_{sp}r_{ps}^{*}\right)$
			(2.130)

In the case of an isotropic structure without depolarization effects, the reflection Mueller matrix has a block-diagonal form:

$$\mathbf{M} = \begin{bmatrix} 1 & -N & 0 & 0 \\ -N & 1 & 0 & 0 \\ 0 & 0 & C & -S \\ 0 & 0 & S & C \end{bmatrix}.$$
 (2.131)

The Mueller matrix (2.131) is normalized with respect to the element  $M_{11}$ , which describes the total reflected intensity. The elements N, C, and S are related to the classical ellipsometric angles  $\psi$  and  $\Delta$ :

$$N = \cos 2\psi, \quad C = \sin 2\psi \cos \Delta, \quad S = \sin 2\psi \sin \Delta.$$
 (2.132)

For a totally polarized wave the projection of the endpoint of the electric field E is an ellipse characterized by its azimuth  $\theta$  and ellipticity  $\varepsilon$ . If for some reason, this azimuth of ellipticity varies (spatially, spectrally and/or temporally), the light become partially polarized. This is shown on Fig. 2.9 schematically [90]. In such a case, the classical ellipsometric measurements [as defined by Eq. (2.123)] looses their physical meaning and Mueller matrix approach is needed to characterize and describe the depolarization phenomena. The depolarization index is calculated from Mueller matrix as follows [94]:

$$P_q = \sqrt{\frac{\sum_{ij} M_{ij}^2 - M_{11}^2}{3M_{11}^2}} = \sqrt{\frac{\operatorname{Tr}\left(\mathbf{M}^T\mathbf{M}\right) - M_{11}^2}{3M_{11}^2}},$$
(2.133)

where Tr indicates algebraic trace operator. The quadratic depolarization index  $P_q$  varies from 0, for a perfect depolarizer (only  $M_{11}$  is nonzero) to 1, for non-depolarizing matrices.



Figure 2.9: Examples of electric field trajectories in the plane perpendicular to the propagation direction for fully polarized (left) or partially polarized (right) light waves.

# 2.8 Conclusion of the chapter

In the first part of this chapter we have introduced the fully anisotropic RCWA approach for the modeling of optical response from 1D periodic layered structures. The second part was focused on definition of the experimental observables. The RCWA method is further discussed in the Appendix A, where we introduce our parallel implementation of the method for spectral simulations.

# 3 Sample preparation and characterization

In this chapter we describe technological fabrication process of the samples and the optical and magneto-optical characterization methodology, process of samples fabrication and used method for optical and MO characterization. For the MO activity of the plasmonic gratings we choose to work with garnet substrate, namely a substitutes bismuth yttrium iron garnet.

In Sec. 3.1 the fabrication process of this Gd-Pr-Bi-Lu-substituted yttrium iron aluminum garnet garnet (Bi:GIG) on a Ca, Mg and Zr doped gallium-gadolinium garnet (CaMgZr-GGG or sGGG) substrate is described.

Knowledge of the optical functions of the used materials is essential for the design of structure. Mueller matrix spectroscopic ellipsometry was used for optical characterization. In Sec. 3.2 the Mueller matrix ellipsometric setup and measured quantities are introduced. In addition depolarization effects caused by the optical configuration of the apparatus are analyzed and discussed. The main part of this chapter, the optical characterization of optical functions of the sGGG substrate, the Bi:GIG layer, and the gold for the grating fabrication, is presented in Sec. 3.2.3. Optical functions of sGGG and Bi:GIG were fitted from ellipsometric and transmission spectra. Optical functions of the gold were fitted using the Kramers–Kronig consistent B-spline (basis spline) function. The magneto-optical properties of Bi:GIG for in-plane magnetic field were fitted from the Mueller matrix data. The process of MO characterization is presented in Sec. 3.3. At the end, the fabrication of 1D periodic gold grating by electron-beam lithography is described in Sec. 3.4.

# 3.1 Fabrication of MO Bi:GIG layer by liquid phase epitaxy

Single crystal films of Bi-substituted iron garnets were grown by Liquid Phase Epitaxial (LPE) procedures onto doped sGGG (111) oriented substrates. The exact composition of the sGGG substrate is  $Gd_{2.7}Ca_{0.3}Ga_{4.1}Mg_{0.3}Zr_{0.6}O_{12}$ . For magneto-optical devices, both the optical figure of merit and the magnetic properties such as magnetization and anisotropy must be controlled. We prepare rare earth (RE) substituted films by combination of Gd, Pr, Lu on CaMgZr-GGG substrates with large lattice parameter ( $a_S = 12.498$  Å) in order to incorporate a large content of Bi and thus induce a large Faraday rotation. Low in-plane anisotropy is necessary to obtain an easy switching of the magnetization. By the electron micro probe analysis (EPMA) the chemical composition of the Bi:GIG was determined as:  $Gd_{1.24}Pr_{0.48}Bi_{1.01}Lu_{0.27}Fe_{4.38}Al_{0.6}O_{12}$ . The role of each ion is the following: substituted-gadolinium garnet has been selected since large Bi content can

be introduced in such a host [95–97]. Praseodymium ions have high contribution to the Faraday rotation but their main contribution remains the reduction of the anisotropy constant [98]. A similar result can be obtained with Nd<sup>3+</sup> ions. The saturation magnetization is reduced to the selected value by the substitution of Fe<sup>3+</sup> by non-magnetic ions. The best choice is obtained with Al<sup>3+</sup> ions with a smaller content compared to Ga3+ in order to match the lattice parameters of the film and substrate. A perfect surface with a low roughness is obtained with this substituted garnet grown at a low  $\Delta T$ , where  $\Delta T = T_s - T_g$  is the supercooling temperature, T<sub>s</sub> is the saturation temperature and T<sub>g</sub> a growth temperature. For good surface quality films, a low T<sub>g</sub> and generally low growth rates are common features of all melts for incorporation of larger Bi content.

# 3.2 Mueller matrix ellipsometry

The Mueller matrix ellipsometer Woollam RC2-Di was used for the optical and magneto-optical characterization of raw materials and fabricated structures. The ellipsometer uses a combination of a halogen bulb and deuterium lamp as a light source and it operate in the spectral region from 0.74 eV to 6.42 eV (193-1700 nm). The PCSCA (Polarizer-Compensator-Sample-Compensator-Analyzer) configuration with dual rotating compersators is used to obtain the full Mueller matrix [99]. Figure 3.1 shows the ellipsometric configuration schematically. In reflection configuration the angle of incidence can be varied in a wide range, from 19° to 85°. The transmission can be measured in normal incidence configuration and with rotated sample as well. For optical characterization of small samples, as our grating samples are, focusing optics can be installed. The focal length of the lenses is 27 mm and the diameter of the spot is 150  $\mu$ m. With the focusing probes the angle of incidence can be varied from 19° to 70° and to 60° with installed inplane magnet. The *x-y* motorized mapping stage was used for precise aliment of the sample to area of the beam spot and mapping measurements.



Figure 3.1: Dual-rotating compensator ellipsometer configuration and orientation of external in-plane magnetization components are shown schematically.

#### 3.2.1 Analysis of spectroscopic data

In the inverse analysis (fitting procedure) a difference between experimental and simulated data is minimize by a model optimization. Depending on the data, the expression of the  $\chi^2$  function is different. For ellipsometry we have used the Poincaré sphere representation [100]:

$$\chi^2 = \frac{1}{K} \sum_{i=1}^{K} \left[ \arccos\left(\sin 2\psi_i^C \sin 2\psi_i^M \cos\left(\Delta_i^C - \Delta_i^M\right) + \cos 2\psi_i^C \cos 2\psi_i^M\right) \right]^2, \quad (3.1)$$

where *K* is the number of spectral points, and the superscripts *C* and *M* represent the calculated and measured quantities. For normalized Mueller matrix data the  $\chi^2$  is defined as follows:

$$\chi^{2} = \frac{1}{15K} \sum_{k=1}^{K} \sum_{(i,j)\neq(1,1)} \left| M_{ijk}^{C} - M_{ijk}^{M} \right|^{2}, \qquad (3.2)$$

where 15K denotes fifteen components on the Mueller matrix. A local minimum of the differen  $\chi^2$  functions is search for using a combination of Levenberg-Marquardt least square algorithm [101] and SIMPLEX [102].

## 3.2.2 Depolarization effects due to focused beam and finite spectral resolution

Depolarization originates from incoherent superposition of different polarization states transmitting or reflecting from the sample. The depolarization effects could come from the apparatus itself or/and from a measured structure. We can summarize the physical phenomena that generate partially polarized light as follows [103]:

- (a) incident angle variation originating from focusing of the probe light,
- (b) wavelength variation caused by the finite bandwidth of the monochromator,
- (c) surface light scattering caused by a large surface roughness of a sample,
- (d) thickness inhomogeneity of layers in the structure,
- (e) backside reflection in a thick substrate.

In analysis of our experimental data we had to deal with depolarization originating from focusing of the incident light (a) and the finite spectral bandwidth (b). To analyze and separate the origin of the depolarization we performed experiments and data analysis measured on a reference sample of a 1000 nm thick thermal  $SiO_2$  layer on a silicon substrate. To fit experimental data a model of the sample containing surface roughness (air/SiO<sub>2</sub>), a SiO<sub>2</sub> layer, and an intermixing layer (SiO<sub>2</sub>/Si) on a silicon substrate was used. Optical functions of these materials were taken as constants [104]. Surface roughness and intermixing layer used in models have been simulated using the Bruggeman effective medium approximation (BEMA) with the fixed volume fraction f = 0.5 [105].

#### Depolarization from finite bandwidth:

The light diffracted by a grating monochromator has a finite bandwidth and thus different wavelengths are measured simultaneously by the single light detector element. If the bandwidth of the monochromator is too broad, depolarization occurs due to the wavelength dependence of the optical properties of the sample. The normalized Gaussian distribution of the wavelengths around a chosen spectral point  $\lambda_0$  with standard deviation  $\sigma_w$  is assumed [106]. Modeling of the finite spectral resolution requires discretization of the spectral range around  $\lambda_0$  and calculation of the optical response at all specific wavelengths weighted by corresponding distribution. For the tabulated optical functions of the used materials we have used a linear spline to obtain proper values at any wavelength. By numerical test we found, that the use of only three spectral points is sufficient to describe depolarization effect from the finite bandwidth. The use of only three spectral points, namely  $\lambda_0 - \sigma_w$ ,  $\lambda_0$ , and  $\lambda_0 + \sigma_w$  significantly reduces calculation time.

To determine the bandwidth of our apparatus we perform Mueller matrix measurement of the calibration sample of 1000 nm thick thermal SiO<sub>2</sub> at the incident angle of 60° and using collimated beam. In the model we fit the thickness of the surface roughness  $t_{surf}$ , the thicknesses of the SiO<sub>2</sub> layer  $t_{SiO_2}$ , the thickness of the intermixing layer  $t_{intermix}$  together with the angle of incidence  $\varphi_0$  and spectral bandwidth parameter  $\sigma_w$ . Table 3.1 summarizes the best-fit parameters. The obtained thicknesses are in good agreement with the values provided by the manufacturer. Figure 3.2 shows on the left subplot the comparison between measured and fitted depolarization. The right subplot shows very good agreement between measured and modeled ellipsometric quantities  $\psi$  and  $\Delta$  [defined from Mueller matrix (2.131) and relations (2.132)].

Table 3.1: Fitted parameters

$t_{surf}$	=	6.2 nm	$\varphi_0$	=	$60.017^{\circ}$
$t_{\rm SiO_2}$	=	1004.9 nm	$\sigma_w$	=	1.2 nm
$t_{intermix}$	=	1.1 nm			



Figure 3.2: Fit of SiO<sub>2</sub> layer on Si substrate with simulation of the effect of finite spectral bandwidth. Left subplot shows comparison between measured and calculated depolarization after fit. Right subplot shows fit of ellipsometric quantities  $\psi$  and  $\Delta$ ,

#### Depolarization from focused beam:

In the next step the depolarization effect caused by a focused incident beam is analyzed. If a beam of the apparatus is focused, then the measured Mueller matrix is a superposition of all angles of incidence around the central angle  $\varphi_0$ weighted by the spatial intensity distribution of the beam. In order to be able to simulate the effect we assume discretization of partial angles of incidence and weight by the normalized Gaussian distribution with standard deviation  $\varphi_s$ , which is expected to be distribution of the light intensity. According to our numerical experiments a assumption of 11 partial beams within the interval  $\varphi_0 - \varphi_s$  to  $\varphi_0 + \varphi_s$  is sufficient to describe depolarization effect from the focused beam. The weight coefficients  $w_i$  related to each partial perturbation of the incident angle  $\varphi_i \in \langle -\varphi_s, \varphi_s \rangle$  are defined as:

$$w_i\left(\varphi_i\right) = \exp\frac{-\varphi_i^2}{2\varphi_s}.$$
(3.3)

To determine the depolarization effect caused by a divergent incident beam, the same calibration sample of 1000 nm thick SiO<sub>2</sub> layer was measured with the focusing optics with focal length of 27 mm and a spot size of  $150\mu$ m. With the focusing optics the central angle  $\varphi_0$  is not exactly defined and it had to be fitted as well. Measured Mueller matrix data were fitted to the model containing previously determined finite bandwidth. Table 3.2 summarizes the fitted parameters. The obtained values corresponds to values obtained with collimated beam (Tab. 3.1). The results of fitting procedure are shown on Fig. 3.3. The left subplot shows

very good agreement between measured and calculated depolarization. Comparing to the depolarization plot on Fig. 3.2, the assumption of depolarization from angular spread can describe depolarization for lower photon energies.

Table 3.2: Fitted parameters						
$t_{surf}$	=	6.7 nm	$arphi_0$	=	$60.207^{\circ}$	
$t_{\rm SiO_2}$	=	1004.2 nm	$\varphi_s$	=	$2.577^{\circ}$	
$t_{intermix}$	=	1.5 nm				

T....



Figure 3.3: Fit of SiO<sub>2</sub> layer on Si substrate with simulation of the effect of finite spectral bandwidth together with focused incident beam. Left subplot shows comparison between measured and calculated depolarization after fit. Right subplot shows fit of ellipsometric quantities  $\psi$  and  $\Delta$ ,

#### 3.2.3 Optical functions of GGG substrate and Bi:GIG layer

In this section we show the procedure to obtain the optical functions (diagonal permittivity tensor components) of the sGGG substrate and Bi:GIG layer using a combination of the Mueller matrix ellipsometry and transmission spectroscopy.

The critical step involved in fitting spectroscopic ellipsometric data to a given structural model is the proper parametrization of the dispersion of the unknown optical functions. We have used a Kramers-Krönig (KK) consistent Tauc-Lorentz (TL) model and its extension with an Urbach tail (TLU). The imaginary part of

54

the complex dielectric function  $\epsilon = \epsilon_1 - i\epsilon_2$  is defined:

$$\epsilon_{2}(E) = \begin{cases} \frac{1}{E} \frac{AE_{0}C(E - E_{g})^{2}}{(E^{2} - E_{0}^{2})^{2} + C^{2}E^{2}} & E \ge E_{c} \\ \frac{A_{u}}{E} \exp\left(\frac{E}{E_{u}}\right) & 0 \le E \le E_{c} \end{cases},$$
(3.4)

where the first term  $(E \ge E_c)$  is identical with Tauc-Lorentz function [107] and the second term  $(0 \le E \le E_c)$  represents the exponential Urbach tail. Parameters  $E_g$ , A,  $E_0$ , and C denote the band gap energy, the amplitude, the Lorentz resonant frequency, and the broadening parameter, respectively. Parameters  $A_u$ and  $E_u$  are chosen with respect to continuity of first derivatives. The real part  $\epsilon_1$ of the dielectric function is obtained using analytical integration of KK relations. For more details of derivation of the TLU model see Ref. [108]. To fit the spectroscopic data of sGGG and Bi:GIG the combination of the TL and TLU model were used to describe shape of absorptions near the band gap. The advantage of the TLU model is, that it is parametrized by five parameters instead of seven as the (common) Cody-Lorentz model [109].

In our work, the Bruggeman effective medium approximation (BEMA) of the mixture of hosting material ( $\epsilon$ ) with void was used to simulate surface roughness as a thin layer with effective permittivity  $\epsilon_{\text{eff}}$  defined [105, 110]:

$$0 = (1 - f) \frac{\epsilon - \epsilon_{\text{eff}}}{\epsilon + 2\epsilon_{\text{eff}}} + f \frac{1 - \epsilon_{\text{eff}}}{1 + 2\epsilon_{\text{eff}}},$$
(3.5)

where f is the volume fraction.

#### Ellipsometric and transmission spectra on sGGG substrate

Figure 3.4 shows experimental data obtained on a 0.5 mm thick sGGG planar substrate. For these measurements a collimated beam instead of a focussed beam has been used. This is more suitable for the detection of fine spectral features in the absorption of the bulk substrate. Both sides of the substrate have been polished, therefore incoherent reflections from the back-side of the substrate have been included in the model. Ellipsometric data were measured at the incidence angle of  $\varphi_0 = 45^\circ$ , while the transmission was measured at normal incidence. Surface roughness from both sides of the substrate was represented by a thin film with thickness to be fitted and a permittivity given by the BEMA [Eq. (3.5)] with a fixed volume fraction f = 0.5 (mixture of both media in ratio 50 %–50 %). The optical functions of the sGGG were parametrized using two Tauc-Lorentz absorptions [111] with the same band-gap energy  $E_g$  extended by Urbach absorption



Figure 3.4: Measured spectra (dots) of ellipsometric angles  $\psi$  (top left),  $\Delta$  (bottom left) and transmitance (right subplot) are compared with the model (lines).

tail [Eq. (3.4)] and one damped harmonic oscillator (DHO) as follows:

$$\epsilon_{\rm sGGG} = \epsilon_{TL} + \epsilon_{TLU} + \epsilon_{DHO}, \qquad (3.6)$$

where  $\epsilon_{TL}$  and  $\epsilon_{TLU}$  are contributions from TL and TLU functions with common band gap energy and  $\epsilon_{DHO}$  is the damped harmonic oscillator defined :

$$\epsilon_{DHO}(E) = \frac{AE_0^2}{E_0^2 - E^2 + iCE},$$
(3.7)

where A is the amplitude,  $E_0$  is the central energy, and C is the damping parameter.

The best fit parameters are summarized in Table 3.3 and the modeled ellipsometric and transmission spectra are presented by solid lines in Fig. 3.4. Figure 3.5 shows resulting dielectric function of the sGGG substrate. Note that even the very small contribution of the DHO at 4.49eV is visible in ellipsometric and transmission spectra due to long propagation length in transparent material. Precise knowledge of the substrate optical functions is crucial for precise characterization of the MO Bi:GIG layer and the further data fit from the magnetoplasmonic grating structure.

	$\varepsilon_{\infty}$	$E_g$ [eV]	A	$E_0$ [eV]	<i>C</i> [eV]	$E_c$ [eV]
TLU:	1.90	5.35	105.48	7.93	0.54	5.89
TL:	0	5.35	173.39	5.67	1.08	
DHO:			$2.52 \cdot 10^{-6}$	4.49	0.0392	
surf. roughness - BEMA: $t = 2.89 \text{ nm}$ $f = 0.5$						

Table 3.3: Parameters of model of sGGG substrate



Figure 3.5: Optical function of sGGG substrate. The real part  $\Re{\epsilon_{11}}$  and the imaginary part  $\Im{\epsilon_{11}}$  of the function is plotted using solid and dashed lines, respectively.

#### Ellipsometric spectra on Bi:GIG layer

Figure 3.6 shows the ellipsometric spectra ( $\varphi_0 = 45^\circ$ ) measured on an approximately  $4\mu$ m thick Bi:GIG layer, grown by LPE on a sGGG substrate as explained in Sec. 3.1. The observed strong interference oscillations indicate the presence of an absorption gap close to 2.5 eV. Because of these it is difficult to obtain a good fit to an analytical material model over the whole measured spectrum. The optical functions of Bi:GIG were therefore determined in a two-step procedure. In the first step, only the data in the range below 2.5 eV were fitted to a model describing the dispersion of Bi:GIG using Tauc-Lorentz-Urbach parametrization. Again surface roughness at the top of the epitaxial Bi:GIG layer and a possible intermixing layer at the Bi:GIG/sGGG interface were included and described using BEMA with a volume fraction f = 0.5 (mixture of both media in ratio 50%–50%) (3.5). Using a focused beam, the sGGG substrate could be considered as a semi-infinite substrate with a permittivity as determined in the previous section. The thickness of the Bi:GIG layer was fitted. The focusing probes introduce a certain angular spread on the incidence angle. In the transparent region this can have a profound impact on the spectral position and the finesse of the interference fringes. This spread  $\varphi_s$  was therefore also considered as a fitting parameter. Table 3.4 shows the best fit parameters for this TLU model of the Bi:GIG film (below 2.5eV). In the second step, the permittivity of Bi:GIG in the absorbing spectral range was calculated by a point-by-point fitting procedure using the surface roughness and the thickness obtained in the first step. Figure 3.7 shows total dielectric function of Bi:GIG layer in the whole spectral range.



Figure 3.6: Measured ellipsometric angles of Bi:GIG layer on sGGG substrate (dots) are compared with model (lines).Upper and lower subplot corresponds to  $\psi$  and  $\Delta$  respectively.

Table 3.4: Parameters of model of Bi:GIG layer on sGGG substrate, 0.74 - 2.5 eV.

$\varepsilon_{\infty}$	$E_g$ [eV]	A	$E_0$ [eV]	C	$E_c$ [eV]
TLU: 3.39	0.21	8.62	3.64	0.48	3.39
surf. roughness - BEMA:	t = 2.89  nm	f = 0.5			
Bi:GIG thickness:	t = 3988.4  nm				
sGGG/Bi:GIG intermix -	BEMA: $t = 3.94$ nm	f = 0.5			
angular spread:	$\varphi_s = 1.70^{\circ}$				

## 3.2.4 Optical functions of gold

A Sample of reference gold from IEMN has been characterized by the Mueller matrix ellipsometry. A Kramers–Kronig consistent B-spline (basis-function spline) formulation, based on the standard B-spline recursion relation was used to describe optical function of gold [112]. Ellipsometric spectra obtained for 45° and 50° of incidence were fitted together using Woollam software CompleteEASE. Figure 3.8 shows comparison between measured and calculated ellipsometric angles  $\psi$  (left subplot) and  $\Delta$  (right subplot). Fits of optical functions are shown on Fig. 3.9 and compared with the tabulated optica; functions presented in the Palik handbook [113].



Figure 3.7: Optical functions of Bi:GIG layer. The real part  $\Re{\epsilon_{11}}$  and the imaginary part  $\Im{\epsilon_{11}}$  of the function is plotted using solid and dashed lines, respectively.



Figure 3.8: Comparison between calculated and measured ellipsometric angles  $\psi$  (left) and  $\Delta$  (right) at angles of incidence of 45° and 50°.

## 3.2.5 Extension of Mueller matrix ellipsometer for magnetooptical measurements

For magneto-optical measurements a servo motor controlled in-plane magnet has been developed. Figure 3.10 shows the magnet and the focusing probes attached to the ellipsometer. The magnet is driven by the servo motor controlled from PC through Thorlabs T-Cube DC Servo Motor Controller. This allows us to control orientation of the magnetic field with high precision and accuracy. For the space width between poles of 20 nm we measured using Hall probe the magnetic



Figure 3.9: Fitted optical functions of reference gold are compared with constants from Palik's Handbook of Optical Constants of Solids.

field  $H \approx 300$  Oe.



Figure 3.10: Left: Photography of developed in-plane permanent magnetic circuit installed in ellipsometric setup. Right: Numerical simulation of magnetization distribution.

# 3.3 Magnetooptical properties of Bi:GIG in transverse and longitudinal MO configuration

In this section we show a procedure to determine the magneto-optical properties of Bi:GIG layer by the Mueller matrix ellipsometer with focusing probes. To be able to characterize MO properties of the Bi:GIG film, the instrument was extended in-plane permanent magnet circuit. The permanent magnet delivered a sufficiently uniform 300 Oe in a volume enclosing the sample holder, 20 mm spacing between magnet poles. This is largely sufficient for in-plane magnetic saturation of the Bi:GIG [114–117], as testified by the M - H hysteresis loop of Faraday effect measured in transmission through the sample with in-plane external magnetic field and the angle of incidence of 45° shown in Fig. 3.11. This underlines also the planar magnetic anisotropy and the softness of the elaborated garnet material ( $H_c = 0.5$  Oe). Figure shows, that magnetic field of 300 Oe used in our MO analysis is high-enough for in-plane magnetic saturation.



Figure 3.11: Hysteresis loop of Faraday effect measured in transmission through the sample for in-plane external magnetic field and the angle of incidence of 45°.

Because the thickness of the Bi:GIG layer is not perfectly uniform and because the MO characterization was performed with focusing probes in different area of the sample, the thickness of the Bi:GIG layer was re-fited from optical measurement performed as the first step. The new obtained thickness of Bi:GIG layer measured with focusing optics was 3973.6 nm. This is close to the previously fitted thickness 3988.4 nm measured with collimated beam. This step was necessary to perform, otherwise even a small difference between interference peaks in calculation and measurement would introduce oscillations into fitted off-diagonal optical functions. In the model we have used the optical functions of Bi:GIG and sGGG determined in Sec. 3.2.3. In the second step the in-plane magnet was installed and the magnetization was applied both in the transverse ( $M_T^{\text{sat.}}$ ) and the longitudinal ( $M_L^{\text{sat.}}$ ) MO configuration (see coordinate system on Fig. 3.1). After each spectrum measurement the orientation of the magnetization was reversed. Each specific MO configuration (transverse or longitudinal, either "up" or "down") was averaged over five measurements in order to reduce random noise and increase measurement sensitivity. Subtraction of the averaged data for opposite magnetization then leads to the differential Mueller matrices:

$$\mathbf{M}_{x}^{\text{diff.}} = \mathbf{M}\left(+M_{x}^{\text{sat.}}\right) - \mathbf{M}\left(-M_{x}^{\text{sat.}}\right), \quad x = T, L.$$
(3.8)

In the next step, the gyrotropy of Bi:GIG was calculated by a point-by-point fitting procedure from the transverse and longitudinal spectra of the difference Mueller matrices. Because the crystalline structure of Bi:GIG is cubic, the MO parameters fitted from TMOKE ( $M_T^{\text{diff.}}$ ) and LMOKE ( $M_L^{\text{diff.}}$ ) difference Mueller matrix spectra are equivalent [118, 119]. In order to increase the quality of the fit the TMOKE and LMOKE data were used in the fitting procedure together.

Figure 3.12 shows comparison of the measured and calculated TMOKE difference data. The TMOKE affects only *p*-reflectivity and does not lead to a polarization conversion. Therefore the difference Mueller matrices must be block-diagonal  $M_T^{\text{diff.}}$ , since these elements contain only the signature of the diagonal Fresnel coefficients,  $r_{ss}$ , and  $r_{pp}$  (Fig. 3.12). On the other hand, the LMOKE response is detected only in off-diagonal blocks, namely the components  $M_{13}$ ,  $M_{14}$ ,  $M_{23}$ ,  $M_{24}$ ,  $M_{31}$ ,  $M_{32}$ ,  $M_{41}$ , and  $M_{42}$ . This corresponds to conversion between *s*- and *p*-polarized light. The block-diagonal elements are zero up to first order due to the substraction of the isotropic part of the LMOKE reflection (Fig. 3.13).

Figure 3.14 shows the obtained off-diagonal permittivity tensor component. The microscopic origin of the off-diagonal permittivity functions is well discussed in the paper of Wittekoek et. al. [117]. In our data shown on Fig. 3.14, the main MO activity is connected with peaks at 2.7 eV and 3.2 eV. The peak at 2.7 eV corresponds to the second type of transition (so called paramagnetic). The paramagnetic peak is over-beaten by the first type of transition (diamagnetic) at 3.2 eV {Chap. 2. in Sec. 2.6.5. in Ref [10]}. The obtained spectral function of MO activity by the Mueller matrix ellipsometry is in very good agreement with results obtained for fully bismuth substituted (x = 1) BIG presented by Wittekoek [117] and with data presented in other papers [24,116,120]. It should also be noted that the observed spectral behavior of the gyrotropy is in agreement with the dielectric loss spectrum observed on the imaginary part of Fig. 3.7. Indeed, hermiticity of the  $\epsilon$ -tensor requires the real part of the off-diagonal permittivity elements to be zero as long as the material is transparent. In accordance with the band gap observed in Fig. 3.14 at around 2.5eV, the real part of off-diagonal permittivity is



seen to be negligible below this photon energy.

Figure 3.12: Measured differences of the Mueller matrix components obtained from MO measurements in transverse MO configuration (blue dots) are compared with the model (red lines).



Figure 3.13: Measured differences of the Mueller matrix components obtained from MO measurements in longitudinal MO configuration (blue dots) are compared with the model (red lines). Reduced number of spectral points is shown in order to distinct the measured data from model.



Figure 3.14: Fitted spectral dependence of off-diagonal tensor component from ellipsometric measurement of Bi:GIG in transverse and longitudinal MO configuration.

# 3.4 Fabrication of the gratings structures

This section describes the fabrication process of samples. The samples were designed according to numerical simulations presented further in Chap. 4, where we analyze optical and magneto-optical response of the structures with various geometry. The result of simulations is need of, ideally identical, gratings which differ only in one geometrical parameter: width of the air gap or thickness of the gold grating. Moreover, the variable parameter should be varied in the monotonous way for all the samples of the fabricated set. To obtain such a set we decide to vary the width of the grating air gap and keep the thickness fixed. The main advantage of this process is, that all the samples are made in one exposition and the gold is evaporated to the whole area of the sample one time. Therefore the gold thickness should be homogeneous around the sample.

The gold grating structure was fabricated by Au evaporation on a mask written by e-beam lithography in the positive poly-methyl metacrylate (PMMA) resist. The spin-coated PMMA resist has been baked for 10 min at 180° C. Instead of conducting resist a 5 nm thick layer of germanium was used.  $300 \times 300 \mu$ m rectangular patches of 1D gratings were written by electron beam lithography with a varying exposure dose 890–1040  $\mu$ C/cm<sup>2</sup> in order to obtain different grating duty cycles. The period of the grating was kept fixed at  $\Lambda = 500$  nm. After e-beam writing, the germanium layer was removed by a 1:1 solution of  $H_2O_2/H_2O$  for 1 min. In the next step the sample was developed in MIBK/IPA (methyl isobutyl ketone/isopropyl alcohol) in ratio 1:2, for 1 minute. Finally, the Au layer with a thickness of approximately 100nm has been evaporated on the developed resist and the grating structure was obtained by lift-off in an ultrasonic bath of SVC14 remover for 1 hour. The thickness of the gold was chosen according to numerical simulations in Chap. 4 and with respect to required dimensions of the samples (by the experimental setup) and fabrication technology (structural stability of the developed photoresist).

Figure 3.16 shows layout of fabricated set of gratings. Scanning electron microscopy (SEM) was used for approximate estimation of the opening of gratings.

The air-gaps *r* estimated by SEM are compared with values obtained by fitting of Mueller matrix data in Chapter 5.



Figure 3.15: Fabrication process of gold grating using positive PMMA photo resist, electron-beam lithography, gold evaporation and lift-off is shown schematically.

# 3.4.1 SEM images of fabricated samples

Figure 3.17 images of fabricated structures obtained with the scanning electron microscope. The sample was fabricated by the same process as was described before. The purpose of the Figure 3.17 is to present quality of the grating fabricated with introduced technology. One can see that quality of edges of the grating is not perfect, therefore it should be taken in account in the modeling. Moreover, the SEM estimation of width of gaps in grating varies and it has to be estimated by numerical modeling.




Figure 3.16: Layout of fabricated samples with opening determined from SEM.



Figure 3.17: Scanning electron microscopy of fabricated samples.

## 3.5 Conclusion of the chapter

The main result of this chapter is characterization of optical and magnetooptical functions materials used for design and fabrication of the magnetoplasmonic gratings. The characterization was done by the Mueller matrix ellipsometer. For the magneto-optical characterization the in-plane magnet was developed and installed to the experimental setup. We have describe process of the magneto-optical garnet and grating samples fabrication. Depolarization effects caused by the finite spectral resolution and focused incident beam were analyzed and results will be used in further characterization of fabricated samples.

# 4 Numerical simulation and fundamentals of nonreciprocal magnetoplasmonic structures

In this chapter we are focused to the following structures and configurations:

We apply *transverse magneto-optic effect*. The advantage of this configuration (discussed in Sec. 2.3.3) is that the nonreciprocal effect appears only in *p*-polarization. Therefore no mode and polarization conversion is present, which is important for further device functionality.

For the enhancement of the magneto-optical effect by the concentration of the local field we attempt to use *surface plasmons*. Generation of plasmons in the structure requires requires interface between dielectric material and noble metal. In our models we use magnetic garnet (with negligible absorptions in infrared) and gold as a noble metal. In models we use optical function of the materials determined in Chapter 3.

Generation of surface plasmon requires high propagation constant, which is obtained as higher diffraction mode in *periodic grating*. We used 1D periodic system (perpendicular to the plane of incidence), which is efficient and optimal to maximize interaction with magneto-optical material.

We propose concept of the waveguiding structure which combines guided modes in a silicon waveguide with magnetoplasmon excitation. The concept is presented in the following steps:

- (i) First we study how the guided mode in the silicon waveguide could couple with the SPP mode via the evanescent field. Here we try to describe different modes in the structure.
- (ii) In the second step we investigate impact of the coupling to effective index of the guided mode and to the shift of the effective index by MO effect.

## 4.1 Simulated structure - 1D grating



Figure 4.1: Coordinate system and schematic representation of the studied structure: gold grating with a period  $\Lambda$  and a thickness  $h_1$  on a magneto-optic garnet substrate in transversal configuration with incident plane wave in y - z plane at the incident angle  $\varphi_0$  and with *s*- or *p*-polarization.

Figure 4.1 shows the typical structure of a magnetoplasmonic TMOKE grating. The one-dimensional (1D) periodic gold grating is deposited on a transversely magnetized magneto-optic dielectric substrate and illuminated by a ppolarized beam. The transverse character refers to the orientation of the magnetization with respect to the plane of incidence [i.e. magnetized along the x-axis, Eq. (2.28)]:

$$\widehat{\epsilon}_{3} = \begin{bmatrix} \epsilon_{xx} & 0 & 0\\ 0 & \epsilon_{yy} & \epsilon_{yz}\\ 0 & -\epsilon_{yz} & \epsilon_{xx} \end{bmatrix}.$$
(4.1)

As the magnetization is assumed to be parallel to the slits, the incidence plane is perpendicular to the latter and only *p*-polarized light can generate SPP's. In this case of the incidence plane perpendicular to the grating slits, we speak about the <u>planar</u> diffraction geometry. If the grating slits are not perpendicular to the plane of incidence the diffraction on the grating is *conical* and the parallel component of the wavevector  $k_y$  is then defined by the incident wavevector and angle of the grating rotation. As the result the conical diffraction also provides conversion between *s*- and *p*- polarizations which affect possible excitation of SPPs modes. The geometry of the grating is described by the period  $\Lambda$ , the air-slit width *r*, and the thickness  $h_1$ .

72

In order to make a simple model only Bi:GIG was taken as a semi-infinite substrate. This eliminates possible interferences in the Bi:GIG layer on the sGGG substrate: the refractive index of Bi:GIG MO layer is higher than the refractive index of the sGGG substrate (see optical function of the sGGG and Bi:GIG at Figures 3.5 and 3.7 in Chapter 3). The effect of a finite thickness of the Bi:GIG layer on the sGGG substrate is discussed further in Sec. 4.1.2.

Note also that from Eq. (4.1) it is clear that the *s*- and *p*- polarizations will not couple as long as  $\mathbf{k}_{inc} \perp \mathbf{M}$  and the response of the structure can therefore be modeled for both polarizations separately. In case where  $\mathbf{k}_{inc} \not\perp \mathbf{M}$  or at conical diffraction the MO response of the structure is given by the combination of the transversal and longitudinal MO effect. In such a case conversion between *s*- and *p*- polarizations appears and more advanced analysis of data is needed.

#### 4.1.1 Operation principle

The transverse MO Kerr effect is usually defined as the relative change of reflected intensity of *p*-polarized light while the magnetization varies its amplitude and orientation [from one saturated state  $(+M_T^{sat})$  to opposite one  $(-M_T^{sat})$ ]:

$$\delta R_p = \frac{R_p \left(+M_T\right) - R_p \left(-M_T\right)}{R_p \left(M_T = 0\right)},\tag{4.2}$$

In our simulations we investigate the behavior of the structure under saturated magnetic state ( $M_T = M_T^{\text{sat}}$ ). This assumption is perfectly fulfilled, for the considered Bi:GIG layers, for an external in-plane magnetic field of 300 Oe (see hysteresis loop in Fig. 3.11) In our case the nonreciprocal optical response manifests itself as a spectral shift of the reflectivity resonances and anomalies. Therefore we do not normalize the difference of reflected intensity in order to avoid artificial enhancement of the TMOKE effect that can appear when  $R_p (M_T = 0) \rightarrow 0$ . The TMOKE is then defined as the difference of reflectivity upon magnetization reversal:

$$\Delta R_p = R_p \left( + M_T^{\text{sat}} \right) - R_p \left( - M_T^{\text{sat}} \right).$$
(4.3)

In other words, the presence of the transverse magnetization in the structure breaks Lorentz reciprocity for the *p*-polarized waves (but it does not break the symmetry for the *s*-polarization). The reciprocity of the system depends (among others) on the symmetry of the reflection matrices upon reversal of the tangential component of the incidence wavevector:

$$\mathbf{R}_{ud}^T(-k_{\mathrm{inc},y}) = \mathbf{R}_{ud}(k_{\mathrm{inc},y}), \tag{4.4}$$

where the matrix of reflection coefficients  $R_{ud}$  represents reflection in the superstrate (see Eq. 2.118 for its definition). The change of sign of the wavevector is equivalent to mirroring the structure of Fig. 4.1 in a plane perpendicular to the *y*-axis. Even though this is a geometrical symmetry of the system, it is <u>not</u> a symmetry of its permittivity profile as:

$$\hat{\epsilon}_3 \neq \hat{\sigma}_y^{-1} \hat{\epsilon}_3 \hat{\sigma}_y \tag{4.5}$$

where:

$$\hat{\sigma}_y = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
(4.6)

A strong TMOKE signature is thus expected for those *p*-polarized grating's resonances that have a pronounced nonreciprocal forward-backward shifting. This is the basic idea behind the plasmonic enhancement of the TMOKE as proposed by Belotelov [55]. As the noble metal/magnetic garnet supports strongly confined *p*-polarized surface waves, these are expected to have a strongly non-reciprocal modal spectrum and therefore a pronounced and enhanced TMOKE response.



Figure 4.2: Specular reflectivity (middle red line), specular transmission (bottom green line) and associated TMOKE spectrum (top red line) of p-polarized light incident on the grating structure in Fig. 4.1 with  $\Lambda = 500$  nm,  $h_1 = 150$  nm and r = 20 nm.

In order to establish the main ideas Fig. 4.2 shows the specular reflectivity of the structure (middle red line) and the corresponding TMOKE spectrum (upper, blue curve) for p-polarized light impinging at  $\varphi_0 = 10^\circ$  on a typical EOT grating configuration ( $\Lambda = 500 \text{ nm}$ ,  $h_1 = 150 \text{ nm}$ , r = 20 nm). From the bottom green line one can observe extra-ordinary optical transmission (EOT) resonances as pronounced dips in the specular reflection peaks in the specular transmission. It should also be noted that these reflection dips are not related to Wood-Rayleigh (WR) anomalies. The positions of these are given by the crossings of the  $\varphi_0$ -line with the light cones of the sub- and superstrate shifted by multiples of the grating wavenumber,  $\frac{2\pi}{\Lambda}$ :

$$E_{\rm ph} = \frac{hc}{\Lambda} \frac{m}{\sqrt{\varepsilon_i \pm \sin \varphi_0}} \qquad i = 1, 3, \quad m \in \mathbb{Z},$$
(4.7)

where *m* is the diffraction order, and the plus resp. minus sign for the negative resp. positive diffraction orders. The spectral position of the lowest order anomalies are indicated by arrows in Fig. 4.2 as  $WR_{\varepsilon_i}^{(m)}$ . The observed dips in the reflection curve originate therefore from the grating's own resonant modes, or in other words its Bloch modes. Depending on their nature these resonances might experience a more or less important MO response (nonreciprocal spectral shift) upon magnetization reversal, as can be seen from the magnitude of the corresponding TMOKE signature for each EOT resonance (see top subplot in Fig. 4.2).

Collin has shown how for 1D metallic gratings (excited under a fixed incidence angle) its high Q-resonances have in general a SPP character while the Fabry-Perot resonances inside the grating slits have a much lower quality factor [121]. The latter, having a negligible interaction with the MO substrate and a low Q-factor on top of that, will leave therefore very little trace in the TMOKE spectrum. In Fig. 4.3 we have plotted field distributions in the grating (in particular  $|H_x|^2$ ) that have been calculated at the different indicated resonances in the EOT spectrum of Fig. 4.2. This confirms that the high-Q resonances with strong TMOKE effect (A) and (B) are indeed Au/MO substrate SPPs coupled to  $\pm 1$  diffraction orders. The proximity of the first order substrate Rayleigh anomalies also reveals their origin. It is also confirmed that (C) is indeed a low Q FP slit resonance. The weaker resonances (D) and (E) close to 1.7 eV and 2.0 eV are too low in energy to be higher order FP resonances. The first one is suspected to be the minus 2<sup>nd</sup> order Au/BIG SPP. It has an extremely low quality factor (as confirmed by intensities of an order in magnitude lower) but experiences a strong enough MO shift to still leave a trace in the TMOKE spectrum. The complete absence of TMOKE for the resonance (F) near 2.1eV and the closeness of  $WR_{\epsilon_1}^{(-1)}$ leaves little doubt that this is the minus  $1^{st}$  order Au/air SPP, having hardly any overlap with the magnetic substrate. The field plots corresponding to (D), (F)and (E) confirm these predictions.



Figure 4.3: Field color map of the magnitude squared of the magnetic field component  $H_x$  at 0.973 eV (A), at 1.097 eV (B), at 1.403 eV (C), at 1.683 eV (D), at 2.053 eV (E), and at 2.077 eV (F). Field distribution is plotted for grating with the period  $\Lambda = 500$  nm, the thickness  $h_1 = 150$  nm, the air-slit width r = 20 nm and the incidence of p-polarization at  $\varphi_0 = 10^\circ$ .

Dispersion diagrams of the optical and magneto-optical response are very useful for a better understanding of the global behavior of the structure. Figure 4.4 shows the specular *p*- reflectivity (left subplot) and MO effect (right subplot) as a function of photon energy and parallel component of the wavevector  $k_y$ . On the other hand, in such dispersion dispersion diagrams the strength of the effects isn't easily distinguished due to the reduced discretization and the limited contrasts of the used colormap. For that reason the Figure 4.2 showing the reflectivity and the MO effect at a fixed angle of incidence of  $10^\circ$  is more useful. The angle of incidence was chosen in order to illustrate the different types of resonant modes without them interacting spectrally.



Figure 4.4: Dispersion diagram photon energy vs.  $k_y$  is shown for specular *p*-reflectivity (left) and TMOKE response (right). The angle of incidence of 10 ° is marked with a black line.

### 4.1.2 Effect of finite thickness of the Bi:GIG layer

In the model of the structure (Fig. 4.1), in the calculated optical and magnetooptical response (Fig 4.2) and in the field plots shown in Fig. 4.3 a semi-infinite Bi:GIG was taken as a substrate. Figure 4.5 shows the optical and MO response of the same structure as before but with a 3988.4 nm thick layer of Bi:GIG on semi-infinite sGGG substrate. The thickness of the Bi:GIG layer was taken from the optical characterization in Chapter 3, Table 3.4. Figure 4.5 shows that the main SPP peaks [(A'), (B')] are still present at the same photon energy. On the other hand the cavity mode peak (C') is strongly modulated. The field plots in Fig. 4.6 show the distribution of the magnetic field intensity  $|H_x|^2$  related to the peaks (A'),(B'), and (C') in the whole structure (top row) and a detailed zoom of it near the grating (bottom row). The position of the grating and the Bi:GIG/sGGG interface is marked by a dashed white line. All subplots show similar field distributions as those obtained for a semi-infinite Bi:GIG substrate. This confirms that the results obtained with a simplified model can be transferred to the structure with a finite thickness of the Bi:GIG on the sGGG.

Figure 4.7 shows that more interesting field distributions appears at new peaks close to main peaks [(A'), (B'), and (C')]. Subplots  $(A'_{1,2})$  were calculated at the position of two tiny peaks for photon energy 1.016 eV and 1.026 eV [close to original peak (A')]. In the same way subplots  $(B'_{1,2})$  were calculated for photon energy 1.078 eV and 1.130 eV. Subplots  $(C'_{1,2})$  were calculated in positions of strongest peaks between (B') and (C') for photon energy 1.255 eV, and 1.282 eV. Subplots show coupling between different grating modes with different orders of interference resonant modes in the Bi:GIG layer. From this small observation we can



Figure 4.5: Specular reflectivity (middle red line), specular transmission (bottom green line) and associated TMOKE spectrum (top red line) of p-polarized light incident on the grating structure in Fig. 4.1 with  $\Lambda = 500$  nm,  $h_1 = 150$  nm and r = 20 nm and with the thickness of the Bi:GIG 3988.4 nm.

conclude that surface plasmon resonances in the periodic structure are not generally affected by this interference resonances in the Bi:GIG layer. However, we have to take into account the finite thickness of the layer during interpretation of experimental data from real prepared samples (discussed later in Chap. 5).



Figure 4.6: Color maps of the magnetic field intensity  $|H_x|^2$  at 0.973 eV (*A*), at 1.097 eV (*B*), and at 1.403 eV (*C*). The field distribution is plotted for a grating with period  $\Lambda =500$  nm, thickness  $h_1 = 150$  nm and the air-slit width r = 20 nm. The incidence angle of *p*-polarization was  $\varphi_0 = 10^\circ$  and a 3988.4 nm thick Bi:GIG layer on sGGG substrate was considered. The top row shows the field distribution in the whole structure, while the bottom row zooms in on the grating region.



Figure 4.7: Distribution of the square of the magnitude of the magnetic field component  $(A'_{1,2})$ ,  $(B'_{1,2})$ , and  $(C'_{1,2})$  calculated for photon energies 1.016, 1.026, 1.078, 1.130, 1.255, and 1.282 eV, respectively. The subplots show coupling between different grating's modes with different orders of guided modes in the Bi:GIG layer.

## 4.2 Analytical formulae of the grating's resonances

Having reminded the typical resonances in magnetoplasmonic TMOKE spectra, we now turn our attention to their dispersion, in particular as a function of the geometrical parameters of the grating. The obvious aim is to identify whether or not an (anti-)crossing of the cavity modes and the SPP modes occurs and how it impacts the TMOKE response (this phenomena will be discussed in Section 4.5). Even though it was argued before that the character of the resonances in an EOT grating can hybridize via coupling [61], the impact of geometrical tuning to enhance the EOT levels has only recently been studied [60, 122, 123]. Of these only d'Aguanno et al. [122] expand considerably on the physics of the coupling of the FP slit resonances with the grating's SPPs and its impact on EOT. Apart from studying a hypothetical free standing Ag grating in air, they moreover study this coupling by tuning the incidence angle rather than the geometry of the grating.

The aim of this section is to show how cavity-plasmon modes coupling occurs in magnetoplasmonic gratings and in particular how it can be tuned geometrically for any angle of incidence. For that purpose we consider the specular reflection spectrum  $R_p$  as a function of the grating period  $\Lambda$ , the grating thickness  $h_1$  and the grating opening r. A strong subwavelength slit (r = 20 nm) ensures a monomodal regime for the Au/air/Au guide governing the FP resonances. Moreover, as will be shown further down, a small slit ensures low energy fundamental cavity resonances, allowing to study its interaction with plasmon modes for reasonable thicknesses. In a last subsection the possibility of geometrical TMOKE tuning shall be studied for varying slit widths r. This configuration has been chosen for the experimental demonstration of anomolous TMOKE switching as will be explained in Chapter 5.

### 4.2.1 SPP mode dispersion

The loci of the minima in the reflectivity spectrum correspond to the resonant modes in the grating. According to the field plots of Fig. 4.3 SPPs both on the air/gold and on the gold/garnet interface can be excited. Intuitively, one would assume the plasmon modes to be independent of the grating thickness  $h_1$ . Except for sufficiently thin metallic layers (i.e. < 50 nm for near-IR and optical frequencies [124]), the grating interfaces can be considered decoupled and the SPP resonance wavelengths become indeed independent of the grating thickness. The resonances are in good approximation determined by the dispersion relation of the SPP on a single interface. The dispersion of the SPP mode can be easily derived using a T-matrix algorithm (introduced in Sec. 2.4.1) as a solution of the waveguiding condition on a single interface. Figure 4.8 shows the situation schematically. The *s*- and *p*- polarization modes in an isotropic system



Figure 4.8: Single interface model for derivation of the dispersion relation of the surface plasmon resonance.

can be described separately. Since the surface plasmon phenomena exist only for *p*-polarization, the T-matrix of media with permittivity  $\epsilon_1$ ,  $\epsilon_2$  takes the form:

$$\mathbf{T}^{(x)} = \begin{bmatrix} \left(\sqrt{\epsilon_x}\right)^{-1} \sqrt{\epsilon_x - \nu_y^2} & \left(\sqrt{\epsilon_x}\right)^{-1} \sqrt{\epsilon_x - \nu_y^2} \\ -\sqrt{\epsilon_x} & \sqrt{\epsilon_x} \end{bmatrix}, \quad x = 1, 2.$$
(4.8)

The single interface system is then described by:

$$\begin{bmatrix} A_{Pdown}^{(1)} \\ A_{Pup}^{(1)} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \sqrt{\epsilon_1} \left( \sqrt{\epsilon_1 - \nu_y^2} \right)^{-1} & -\left(\sqrt{\epsilon_1}\right)^{-1} \\ \sqrt{\epsilon_1} \left( \sqrt{\epsilon_1 - \nu_y^2} \right)^{-1} & \left(\sqrt{\epsilon_1}\right)^{-1} \end{bmatrix} \begin{bmatrix} \left(\sqrt{\epsilon_2}\right)^{-1} \sqrt{\epsilon_2 - \nu_y^2} & \left(\sqrt{\epsilon_2}\right)^{-1} \sqrt{\epsilon_2 - \nu_y^2} \\ -\sqrt{\epsilon_2} & \sqrt{\epsilon_2} \end{bmatrix} \begin{bmatrix} A_{Pdown}^{(2)} \\ A_{Pup}^{(2)} \end{bmatrix}$$

$$(4.9)$$

or in compact form:

$$\mathbf{A}^{(1)} = \underbrace{\left(\mathbf{T}^{(1)}\right)^{-1} \mathbf{T}^{(2)}}_{\mathbf{T}} \mathbf{A}^{(2)}.$$
(4.10)

The final expression for SPP dispersion is then derived assuming a guided mode on a single interface. As was discussed in Sec. 2.5.4, a guided mode is defined as an eigenmode of the structure, i.e. mode that exists without incidence from neither the substrate nor the superstrate,  $A_{Pup}^{(2)} = 0$  and  $A_{Pdown}^{(1)} = 0$ . Using the simple notation (4.10), the waveguiding condition is:

$$T_{11} = 0, (4.11)$$

or in expanded form:

$$T_{11} = \sqrt{\frac{\epsilon_1 \left(\epsilon_2 - \nu_y^2\right)}{\epsilon_2 \left(\epsilon_1 - \nu_y^2\right)}} + \sqrt{\frac{\epsilon_2}{\epsilon_1}} = 0.$$
(4.12)

Solution of the Eq. (4.12) for the effective index of guided mode  $n_{\text{eff}} = \nu_y$  leads to the well-known relation for surface plasmon resonance on a single interface. Assuming the plasmonic material, gold, with permittivity  $\epsilon_2$  and dielectrics materials air ( $\epsilon_1$ ) and Bi:GIG ( $\epsilon_3$ ), the surface plasmon modes in our system are described

by the relation in the form:

$$k_{\rm SP}(E) = k_y = k_0 \nu_y = k_0 n_{\rm eff} = \frac{2\pi}{hc} E \sqrt{\frac{\epsilon_2(E) \epsilon_i(E)}{\epsilon_2(E) + \epsilon_i(E)}}, \qquad i = 1, 3, \qquad (4.13)$$

where *E* is the photon energy and  $\epsilon_2(E)$  represents the permittivity of gold characterized in Sec. 3.2.4, *i* = 1 for the SPP on the air/gold and *i* = 3 for the SPP on the gold/garnet interface. In the 1D periodic structure the SPP is excited by the diffracted wave:

$$k_{W}(E) = \pm k_{\rm SP}(E) + m \frac{2\pi}{\Lambda}, \text{ with } m \in \mathbb{Z},$$
(4.14)

where  $k_W$  denotes the wavevector of the SPP. This SPP excitation is historically known as a *Wood plasmon*, because it was observed close to the Wood-Rayleigh anomalies Eq. (4.7) [125]. Putting thus  $k_W = \frac{2\pi}{hc} E \sin \varphi_0$  and solving Eq. (4.14) for E gives us a first order numerical approximation for the height-independent loci of the SPP resonances.

#### 4.2.2 Cavity mode dispersion

The spectral position of the slit resonances can, with a good accuracy, be predicted by considering the response of an equivalent FP-like slab resonator: a layer with an index  $n_{\text{eff}}$ , the same thickness as the gold grating and sandwiched between air and the garnet substrate. The effective index  $n_{\text{eff}}$  is given by the fundamental TM mode of the Au/air/Au guide. Figure 4.9 shows the symmetrical guide schematically.

$$\begin{array}{cccc} {\rm T}^{(1)}{\bf A}^{(1)} & \epsilon_1 & & \\ & & & & \\ & & & & \\ \hline {\rm T}^{(2)} & {\rm P}^{(2)} & \epsilon_2 & & \\ & & & & \\ \hline {\rm T}^{(3)}{\bf A}^{(3)} & \epsilon_1 & & \\ \end{array}$$

Figure 4.9: Symmetrical gold/air/gold waveguide is shown schematically.

The dispersion of the cavity mode is found as a solution of the gold/air/gold sandwich structure described by the following T matrix:

$$\mathbf{A}^{(1)} = \underbrace{\left(\mathbf{T}^{(1)}\right)^{-1} \mathbf{T}^{(2)} \left(\mathbf{P}^{(2)}\right)^{-1} \left(\mathbf{T}^{(2)}\right)^{-1} \mathbf{T}^{(3)}}_{\mathbf{T}} \mathbf{A}^{(3)}.$$
 (4.15)

84



Figure 4.10: Left: gold/air/gold waveguide and its extension into a resonant cavity by introduction of the garnet and air media is shown schematically. Right: field profile of guided mode for thickness of the air gap r = 20 nm, the photon energy 1.4 eV, and the effective index of guided mode  $n_{\text{eff}} = 1.7371 + 0.0250i$ .

Assuming only *p*-polarized modes and putting  $A_{Pdown}^{(1)} = 0$  and  $A_{Pup}^{(3)} = 0$ , the solution of the waveguiding condition  $T_{11} = 0$  has the following form [122]:

$$\tanh\left(\frac{r}{2}\sqrt{k_0^2 n_{\rm eff}^2 - k_0^2}\right) = -\frac{\sqrt{k_0^2 n_{\rm eff}^2 - k_0^2 \varepsilon_2}}{\varepsilon_2 \sqrt{k_0^2 n_{\rm eff}^2 - k_0^2}}.$$
(4.16)

Figure 4.10 schematically shows the gold/air/gold waveguide and its transformation into resonant cavity. The field plot on the right corresponds to a guide width of 20 nm which is equivalent to the slit width in the grating. At 1.4 eV, i.e. the FP resonance observed in Fig. 4.2, an effective index of  $n_{\text{eff}} = 1.7371 + 0.0250i$ , is obtained for this mode. As known, this plasmonic slot waveguide has no cutoff and this is independent on the slit width (see [126]). An extreme subwavelength confinement and accompanying high effective index is therefore obtained at very small slit widths, thereby allowing low energy FP resonances for moderate thicknesses of the metal grating. Figure 4.11 shows the effective index of the guided mode at 1.4 eV, i.e. the FP resonance observed in Fig. 4.2 as a function of the air layer thickness. Complex effective index was calculated by the numerical optimization introduced in Sec. 2.5.4. For spacing up to 40 nm the effective index shows low dispersion. Note that the imaginary part of the effective index was multiplied by a factor of 100.

The location of the cavity resonances is then found by expressing round-trip resonance:

$$2k_0 n_{\text{eff}} h_1 + \phi_{r_1} + \phi_{r_3} = 2n\pi, \quad n \in \mathbb{Z},$$
(4.17)

where  $\phi_{r_i}$  is the reflection phase shift of the slit mode at both ends of the cavity. The reflection coefficient can be roughly approximated as a normal-incidence



Figure 4.11: Effective index of guided mode in gold/air/gold at  $\lambda = 884$  nm.

reflection:

$$r_i = |r_i| \exp\left[\mathrm{i}\phi_{r_i}\right] = \frac{n_{\rm eff} - \sqrt{\varepsilon_i}}{n_{\rm eff} + \sqrt{\varepsilon_i}},\tag{4.18}$$

where i = 1 for the the permittivity of air and i = 3 for the permittivity of the nonmagnetized garnet [ $\varepsilon_{yz} = 0$  in Eq. (4.1)]. Such a simple approximation is sufficient for a cavity mode in regions where it doesn't interact with the plasmon modes. In case of interaction between modes, the reflection phase shift of the mode at both ends of the cavity can be fitted and described in a more precise way [60].

According to (4.16) and (4.17) we can conclude that it is possible to tune the spectral position of the cavity mode in two ways. The first option of variation of the grating air gap width, when the sight dispersion of the mode effective index (Fig. 4.11) plays the role. The second possible approach is to tune by the grating thickness, when the resonant wavelength is affected by the phase-matching condition (4.17).

### 4.3 Geometrical dispersion of resonant modes

Analytical description of resonant modes in the structure brings important information about their dependence on the grating's geometry. In summary the dispersion relations Eq. (4.14,4.13) and Eq. (4.16,4.17) show that the plasmon resonant modes depend on the grating period  $\Lambda$  and the cavity modes depend on the grating thickness  $h_1$  and on the air-slit width  $r = f\Lambda$ . From Fig. 4.2 one can see that the TMOKE spectrum achieves its extrema in the spectral range from 0.74 eV to 2.5 eV for this particular angle  $\varphi_0 = 10^\circ$ ; it would change considerably with the angle of incidence angle. Therefore, we present specular reflectivity spectra  $R_p$ for various grating thicknesses  $h_1$ , grating periodicities  $\Lambda$ , and air-gaps r in this spectral range.

#### 4.3.1 Grating thickness variation

Figure 4.12 shows the spectral dependence of the specular reflectivity  $R_{p}(E)$ on grating thickness for a fixed grating period  $\Lambda = 500 \text{ nm}$  and an incidence angle of  $\varphi_0 = 10^{\circ}$ . In this configuration, the  $-1^{st}$  plasmon mode [m = -1 in Eq. (4.13)] is excited at a photon energy of 0.97 eV which is close to the wavelength 1.3  $\mu$ m commonly used in optical telecommunication. According to Eq. (4.14) and Eq. (4.17) the plasmon modes (blue lines) are dispersion-less under fixed grating period and the cavity modes (red curves) are dispersive respectively. On the left subplot it can be seen that the interaction of the cavity mode with the  $-1^{st}$ plasmon mode pushes the resonant energy from 1.13 eV (for grating thickness  $h_1 = 100 \text{ nm}$ ) to 0.99 eV ( $h_1 = 330 \text{ nm}$ ), which corresponds to a smooth transformation between  $-1^{st}$  and  $+1^{st}$  plasmon mode. A further increase of the grating thickness (up to 330 nm) leads to interaction between the SPP mode and the higher-order cavity modes. A similar phenomenon appears at photon energies from 1.7 eV to 2 eV where cavity modes interact with  $\pm 2^{nd}$  SPP modes. Finally the effect at 2.1 eV comes from the interaction between the cavity mode and SPP at the gold/air interface (see field plot (E) on Fig. 4.3). The right subplot of Fig. 4.12 shows dispersion curves of four different orders of cavity modes, corresponding to n = 1, 2, 3 and 4 in Eq. (4.17). One can see that relatively good agreement, even from this simple approximation, is obtained.

Figure 4.13 shows dispersion maps of the *p*-reflectivity. The maps have been calculated for a grating with period  $\Lambda = 500$  nm and thicknesses 90, 105, 120, 135, 150, 165, 180, 195, 210, and 225 nm. These maps clearly show how the cavity mode moves to lower energies with increasing grating thickness. For thicknesses from 90 nm to 135 nm we can see, that interaction appears mainly for second order SPP modes. With an additional increase of the thickness, the cavity mode interacts with the first order of SPP modes.



Figure 4.12: Left: Simulated dispersion of the grating's reflection for various thicknesses  $h_1$  from 50 nm to 600 nm and a fixed periodicity  $\Lambda = 500$  nm. Right: spectral position and geometrical dispersion of resonant modes calculated with analytical dispersion models Eqs. (4.14,4.13) and Eqs. (4.16,4.17).



Figure 4.13: Dispersion diagrams of specular reflectivity for grating thickness from 90 nm to 225 nm in steps of 15nm. Note the drift of the flat cavity mode towards lower photon energy for increasing thickness  $h_1$ . The evolution of coupling between modes is shown as bending of the SPPs by cavity modes.

#### 4.3.2 Grating period variation

Figure 4.14 shows the spectral dependence of  $R_p$  on the grating period  $\Lambda$  in a range from 200 nm to 900 nm and for fixed grating thickness  $h_1 = 150$  nm. In this plot the cavity modes are nondispersive for constant thickness  $h_1$  and constant air-slit width  $r = \Lambda f = 20$  nm (note that in our model the change of the filling factor f compensates the change of the grating period  $\Lambda$ ). On the other hand the plasmon modes show clear dispersive behavior, that is compared with the simple models of Eq. (4.13) and Eq. (4.14) on the right subplot. Following Eq. (4.14) we have put  $m = \pm 1, \pm 2$ , and  $\pm 3$  for the plasmon modes at the gold-garnet interface (SPP -  $\varepsilon_3$ , blue curves) and  $m = \pm 1$  for plasmon modes at the gold-air interface (SPP -  $\varepsilon_1$ , green curves). The left subplot shows anticrossing behavior of modes. The  $\pm 1^{st}$  SPP modes and cavity mode are excited separately for a grating period between 450 nm and 550 nm. For longer period the cavity mode is coupled into the  $+2^{nd}$  plasmon mode. For shorter grating periods (less than 300 nm) anticrossing of modes provides a smooth shift from the  $-1^{st}$  plasmon mode to the  $+2^{nd}$ mode ( $\Lambda = 700$  nm). This is accompanied by a full transformation of the  $+2^{nd}$ plasmon mode into the fundamental cavity mode. In addition, the cavity mode at 1.5 eV is becomes less sharp for a grating period  $\Lambda < 500$  nm. The fill-factor of the air gap is higher (the fill-factor varies with the period) and the Q-factor of the cavity mode is decreased. We suppose that this is a result from an increasing diffractive coupling between the grating slits. For longer period the Q-factor of the cavity mode increases due to coupling with hi-Q SPP mode which makes the mode spread narrower.

Note finally, that up to a certain extent periodicity tuning for fixed slit width r and grating height  $h_1$ , allows to shift the mode coupling to higher incidence angle. This is of course limited by the SPP gap forming at  $E_{\rm ph} = \frac{hc}{2\Lambda}$  close to which near grazing incidence would be required if the cavity resonance were to be at this energy. A readjustment of the grating thickness is then necessary.

Figure 4.15 shows dispersion diagrams calculated for a grating with periods from 400 to 850 nm (in steps of 50nm). These subplots show that the position of the cavity mode is almost independent on the grating period. In addition, they show how, at a given angle of incidence, the grating period can be used to achieve coupling of the FP resonance with the desired order of SPP mode. The right subplot of the Fig. 4.14 calculated with analytical models describing Wood-plasmons and cavity modes (derived in Secs. 4.2.1 and 4.2.2) describes positions of modes in good agreement with numerical simulations. Therefore we can directly conclude that a shorter period is useful for the study of low order SPP modes (first, second), hence for a long grating period higher SPP modes play a role. Moreover in a long period domain it is possible to study interaction between different orders of SPP modes.



Figure 4.14: Left: Simulated dispersion of reflection for the grating with various period  $\Lambda$  from 300 nm to 900 nm and fixed thickness  $h_1 = 150$  nm,. Right: spectral position and geometrical dispersion of resonant modes calculated with analytical dispersion models Eq. (4.14,4.13) and Eq. (4.16,4.17).



Figure 4.15: Dispersion diagrams of specular reflectivity are shown for grating periods from 400 nm to 850 nm in steps of 50nm. Note that the cavity mode keeps its spectral position.

### 4.3.3 Grating air gap variation

The last group of simulations considers variations the grating air gap. Figure 4.16 shows on the left subplot the spectral dependence of  $R_p$  on the air gap in the range from 20 nm to 120 nm. The right subplot shows calculated dispersion curves of (dispersive) cavity and (nondispersive) SPPs modes. The calculated map shows that for a wider opening of the air gap the cavity mode is slightly shifted to higher photon energies and its quality factor drops. This observed behavior was used in design of experimental samples. In the design (Chap. 3) the set of samples were fabricated by different exposition, but the gold was evaporated in one shot. Therefore the thickness of the gold is the same for all the samples and only width of the air gap varies.

To complete the study of the geometrical dispersion of modes in a plasmonic grating, Figure 4.17 shows dispersion diagrams calculated for gratings with different widths of air gaps. Gratings with a period  $\Lambda = 500$  nm, a thickness  $h_1 = 150$  nm and an air gap width varying from 20 to 110 nm in steps of 10 nm were simulated. For this particular grating the interaction between cavity and SPP mode becomes stronger for increased air gap width, which is related to decrease of the reflectivity.

The important information from those simulations is, that the coupling effect appears for the second-order of SPP modes. This is given by the relatively low thickness of the grating. The additional advantage of using second-order SPP modes is large MO effect (see dispersion curve on Fig. 3.14 in Chap. 3). To obtain interaction with the fist-order SPP modes, the thickness of the grating should be increase to approximately 200-220 nm. In such a case it would be possible to observe the interaction of the first-order cavity mode with the first-order SPP and the second-order cavity mode with second-order SPP modes. Unfortunately, requirement of strong sub-lambda air gaps and thick grating bring fabrication complications.



Figure 4.16: Left: Simulated dispersion of reflection for the grating with various air-gap r from 20 nm to 120 nm and the fixed period  $\Lambda = 500$  nm and grating thickness  $h_1 = 150$  nm. Right: spectral position and geometrical dispersion of resonant modes calculated with analytical dispersion models Eqs. (4.14,4.13) and Eqs. (4.16,4.17).



Figure 4.17: Dispersion diagrams of specular reflectivity are shown for grating air gaps from 20 nm to 110 nm (steps of 10nm). Note broadening of the cavity mode.

### 4.4 Anticrossing of resonant modes, field plots

Figure 4.18 shows the field distribution (of the transversal magnetic field component  $H_x$ ) close to the points of modal anticrossing. Both field distributions were calculated for the grating period  $\Lambda = 500$  nm and the modes are marked in the dispersion diagram (Figs. 4.12, 4.14). The left subplot shows the field distribution of the  $+1^{st}$  plasmon mode [m = +1 in Eq. (4.14)] coupled with the cavity mode at a photon energy of 0.9 eV and a grating thickness  $h_1 = 200$  nm. The right subplot shows field plot of the  $-1^{st}$  plasmon mode coupled with the cavity mode at a photon energy of 1 eV and a grating thickness  $h_1 = 200$  nm.

From both plots shown on Fig. 4.18 one can recognize that the field component  $H_x$  is much more enhanced than in the case of single resonant mode excitation (Fig. 4.3, note different color scale). In addition the modes coupling decreases reflection significantly. Decrease of reflectivity and strong field enhancement at the interface with MO garnet cause significant increase of the transverse MO effect discussed in the next section.



Figure 4.18: Distribution of square of the magnitude of the magnetic field component  $H_x$ . Left subplot: coupled resonant mode of  $+1^{st}$  plasmon and cavity mode for the photon energy 0.89 eV and the grating thickness 200 nm. Right subplot: coupled resonant mode of  $-1^{st}$  plasmon and cavity mode for the photon energy 0.98 eV and the grating thickness 200 nm.

# 4.5 Nonreciprocal optical response of grating's resonant modes

Up till now we studied the impact of the grating geometry on the dispersion of its EOT resonances. We now move on to see whether a similar impact can be observed in the nonreciprocal response of this EOT system. In Section 4.1.1 it was explained how the MO response of this structure can be easily understood at its grating/garnet SPP resonances.

#### 4.5.1 Dispersion of the magnetoplasmon

In order to describe the shift of the SPP by the transverse magnetooptic Kerr effect we used Yeh's matrix formalism to solve Maxwell's equation for a single interface between gold ( $\epsilon_2$ ) and a MO garnet  $\hat{\epsilon}_3$  in transverse MO configuration with gyrotropy *q*:

$$\widehat{\epsilon_3} = \begin{bmatrix} \epsilon_3 & 0 & 0\\ 0 & \epsilon_3 & \mathrm{i}q\\ 0 & -\mathrm{i}q & \epsilon_3 \end{bmatrix}$$
(4.19)

The structure is shown on Figure 4.19 schematically.



Figure 4.19: Layout of the structure for derivation of the magnetoplasmon dispersion.

To derive the dispersion of the magnetoplasmon the waveguiding problem of a single interface needs to be solved. For *p*-polarization the matrix  $T^{(1)}$  of the semi-infinite gold has the following form:

$$\mathbf{T}^{(1)} = \begin{bmatrix} \left(\sqrt{\epsilon_2}\right)^{-1} \sqrt{\epsilon_2 - \nu_y^2} & \left(\sqrt{\epsilon_2}\right)^{-1} \sqrt{\epsilon_2 - \nu_y^2} \\ -\sqrt{\epsilon_2} & \sqrt{\epsilon_2} \end{bmatrix},$$
(4.20)

The matrix  $T^{(2)}$  of the transverse magnetic medium (introduced in Chap. 2 in Sec. 2.3.3) for *p*-polarization has the form:

$$\mathbf{T}^{(2)} = \begin{bmatrix} \epsilon_3 - \nu_y^2 & \epsilon_3 - \nu_y^2 \\ iq\nu_y - \epsilon_3\sqrt{\epsilon_3 - \nu_y^2 - \frac{q^2}{\epsilon_3}} & iq\nu_y + \epsilon_3\sqrt{\epsilon_3 - \nu_y^2 - \frac{q^2}{\epsilon_3}} \end{bmatrix}, \quad (4.21)$$

The single interface problem is then described in compact form by the relation:

$$\mathbf{A}^{(1)} = \underbrace{\left(\mathbf{T}^{(1)}\right)^{-1} \mathbf{T}^{(2)}}_{\mathbf{T}} \mathbf{A}^{(2)}.$$
 (4.22)

The dispersion of the magnetoplasmon is derived from the waveguiding condition for a single interface:  $A_{Pup}^{(2)} = 0$  and  $A_{Pdown}^{(1)} = 0$ . Using the simple notation (4.22), the waveguiding condition is:

$$T_{11} = 0. (4.23)$$

The expanded form of the waveguiding problem takes the following form:

$$T_{11} = \frac{\epsilon_3 - \nu_y^2}{\epsilon_2 - \nu_y^2} - \frac{iq\nu_y - \epsilon_3\sqrt{\epsilon_3 - \nu_y^2 - \frac{q^2}{\epsilon_3}}}{\epsilon_2\sqrt{\epsilon_2 - \nu_y^2}} = 0,$$
(4.24)

By multiplying by the wavenumber  $k_0$  and considering only linear terms in q, Eq. (4.24) can be linearized as:

$$k_{\rm SP} = k_0 \left[ \sqrt{\frac{\varepsilon_2 \varepsilon_3}{\varepsilon_2 + \varepsilon_3}} + \frac{iq\varepsilon_2^2}{(\varepsilon_3^2 - \varepsilon_2^2)\sqrt{\varepsilon_3 + \varepsilon_2}} \right], \tag{4.25}$$

where the first term corresponds to the standard surface plasmon resonance Eq. (4.13) and the second term represents the shift originating from the magneto-optical effect. Our model of the spectral shift of SPP by TMOKE is equivalent with the previously introduced model for the MO SPP shift [56,63]. Figure 4.20 compares the MO SPP shift calculated (at a photon energy 1 eV) from the exact model Eq. (4.24) with the linear approximation Eq. (4.25) for increasing gyrotropy q.

Together with the relation for the Wood plasmon anomalies (Eq. (4.14)), it describes the phenomena in good agreement with the RCWA calculation. The linear model of magnetoplasmon Eq. (4.25) together with the equation for the Wood plasmon Eq. (4.14) describes the different shift of  $+1^{st}$  and  $-1^{st}$  SPP's resonant frequency. The total wavevector shift of the SPP anomalies in the spectra is then given by two contributions: by multiples of wavevector of the grating [Eq. (4.14)] and by the linear perturbation in Eq. (4.25).

### 4.5.2 TMOKE sign control by optimization of the interaction between modes

We have already seen how MO response is obviously related to field confinement in the MO material as shown in Fig. 4.2 and on the field plots in Fig. 4.3 (A) and (B) (in Sec. 4.1.1). Moreover, the interaction between the plasmon and cavity



Figure 4.20: Shift of SPP by TMOKE: comparison between the exact solution from the Eq. (4.24) (circle dots) and the linear approximation model Eq. (4.25) (dashed line) calculated at the photon energy 1eV. The green line represents pure SPP mode.

mode provides strong field enhancement in the MO substrate (Fig. 4.18), which provides a further enhancement of the MO effect. It is therefore expected that in the previously indicated regions of specific modal crossing and anticrossing, interesting MO responses will appear.

#### Grating thickness variation

Repeating the same simulations as in Sec. 4.3 we present analysis of the TMOKE spectral dependence on the grating geometry. Figure 4.21 shows how the TMOKE is affected by the interaction between the SPP and the cavity modes. Subplots in the left column show details of the dependence of the TMOKE for various grating thicknesses for  $\pm 1^{st}$  (top subplot) and  $\pm 2^{nd}$  (bottom) magnetoplasmon modes. It is clearly visible that TMOKE keeps the same dispersive dependence as already observed on the specular reflection in the non-magneto-optic case (Fig. 4.12). In addition these subplots reveals the parameter combination where coupling occurs efficiently. In this region the coupled modes have characteristic properties of both SPP and cavity modes. The SPP contribution to the coupled mode behavior is mainly responsible for the MO effect. In addition the cavity mode contribution gives the dependence on the grating thickness. Moreover, on the colormap one can see that the modal interaction leads to an enhancement of the TMOKE. This happens due to the fact that coupling of modes leads to an increase of the electromagnetic field concentration in MO layer. The cavity mode in this case contributes as electromagnetic field channel which corresponds to the extraordi-

98

nary optical transmission (EOT). Because of TMOKE splitting of the SPP (and the coupled mode as well), the increase is different for modes excited for different orientation of the magnetization, +M and -M.

The subplots in the right column show TMOKE at a fixed photon energy as a function of the grating thickness (the chosen energies are marked by colored lines on the left subplots). These reveal an interesting new possibility of geometrical switching of the TMOKE. At a photon energy of 0.97eV for instance, TMOKE reaches its maximum for a grating thickness of 210 nm. If the thickness of the grating is increased to 220 nm, the TMOKE is reduced to zero. Further increasing of the thickness to 230 nm switches the sign of the TMOKE effect. The modal anticrossing switches the sign of the TMOKE without change the orientation of the magnetization. The same phenomenon appears for the  $\pm 2^{nd}$  plasmon SPP modes at 1.74 eV and 1.88 eV. The modes at 1.74 eV can be completely switched by the change of the grating thickness from 100 nm to 107 nm. The effect is much more sensitive for the mode at 1.88 eV, when only 3 nm difference in grating thickness leads to the reversion (from 90 nm to 93 nm).

#### Grating air gap variation

In a second step we analyze the impact of increasing the slit openings on the TMOKE response. In Section 4.3.3 we have already seen how "broadening" the cavity mode affects  $-2^{nd}$  SPP mode. This observation together with the following MO analysis has been crucial in further design of samples for experimental observation of the phenomena. Figure 4.22 shows on the left subplot the detail on TMOKE response of the  $-2^{nd}$  SPP mode as a function of various grating air gap. Significant shift of the coupled mode by the air gap width is observed. The left subplot shows that the maximum of the TMOKE can be achieved (for this structure and  $-2^{nd}$  SPP mode) for the grating opening from 20 nm to 60 nm. This information was also very useful in the fabrication process. The right subplot shows TMOKE at 1.74 eV as a function of the air gap width. Clear TMOKE switching phenomena is observed with the air gap variation from 30 nm to 45 nm.



Figure 4.21: Left column: detail of TMOKE spectral dependence  $\Delta R_p$  for the grating thickness  $h_1$  from 50 nm to 600 nm and period  $\Lambda = 500$  nm. Right column: switching of the TMOKE sign at fixed photon energy 0.97 eV, 1.11 eV, 1.74 eV, and 1.88 eV by variation of the thickness of the grating.



Figure 4.22: Left detail of TMOKE spectral dependence  $\Delta R_p$  for the grating air gap  $h_1$  from 20 nm to 120 nm and period  $\Lambda = 500$  nm. Right: switching of the TMOKE sign at fixed photon energy 1.74 eV by variation of the gratin air gap width.

## 4.6 Proposition of waveguiding structure with nonreciprocal dispersion of TM modes

In this section a concept of TM-waveguiding structure is proposed. Figure 4.23 shows the proposed structure of silicon waveguide structure with plasmonic grating and the MO Bi:GIG garnet layer is placed on a top of the grating. Materials used in the structure, namely silicon and  $SiO_2$ , were taken for their high dielectric contrast. Therefore is it possible to achieve waveguiding inside the silicon layer. In this study we seek to determine the nonreciprocal behavior of the guided modes. The main subject is the analysis of a possible coupling between guided modes and plasmon modes on the grating interfaces. The evanescent field of the guided mode in the silicon is used for the excitation of the surface plasmon mode at the grating. To achieve nonreciprocal behavior the Bi:GIG garnet is placed on the top of the grating. Therefore excitation of the SPP and its control by magnetization would lead to the nonreciprocal behavior.

In the following simulations we assume a wavelength  $\lambda = 1300$  nm, refractive indexes of the Bi:GIG layer n = 2.32 + 0.0001i, of Gold n = 0.63 + 10.96i, of Silicon n = 3.5 and of the SiO<sub>2</sub> n = 1.52. Considered parameters of the structure are the grating thickness  $h_1 = 100$  nm, the air gap width r = 20 nm, the grating period  $\Lambda$ , the thickness of the SiO<sub>2</sub> tunneling layer  $h_2 = 60$  nm, and the thickness of the silicon waveguide  $h_3 = 600$  nm. The thickness of the Si waveguide was chosen to obtain multimodal behavior.





The numerical design was done as two step process of S-matrix waveguiding calculation (see Sec. 4.1.2). In the first step the S-matrices calculated from structure with various parameters (grating period, propagation constant  $\nu_y$ ) are decomposed using the singular value decomposition (SVD).<sup>1</sup> Local minima in plot of  $1/\sigma_{max}$  ( $\sigma_{max}$  is the largest singular value of S-matrix) represent positions of

<sup>1.</sup> Propagation constant  $\nu_y$  is the *y*-component of the normalized wavevector, see Chap. 2, Sec. 2.3.1

guided modes. In the second step the complex propagation constant  $\nu_y$  is found by the minimization of  $1/\sigma_{max}$ , [Eq. (2.106)].

The structure was studied for the following ranges of parameters. The pure real propagation constant  $\nu_y$  was varied from 2.32 to 3.5 in order to achieve waveguiding primary in the silicon. Values 2.32 and 3.5 are the refractive indexes of the Bi:GIG and silicon, respectively. The grating period was varied over a large interval from 100 nm to 350 nm. It is important to point out that diffraction effects caused by the grating in the structure could occur. If the assumed parallel wavevector component  $k_y = k_0\nu_y$  is decreased by the grating parallel wavevector  $k_{grat} = 2\pi/\Lambda$ , a diffracted mode may leak out of the structure which could represent losses. Taking in account the interval of propagation constant and refractive indexes of surrounding media, the leakage into the Bi:GIG superstrate may appear for  $\Lambda > 223$  nm, and into the SiO<sub>2</sub> substrate for  $\Lambda > 258$  nm. This effect has to be considered in the analysis of modes in the structure.



Figure 4.24: Left:Dispersion map of guiding indicator  $1/\sigma_{max}$  in logarithmic scale calculated as a function of the effective index  $\nu_y$  and the grating period  $\Lambda$ . Right: Detail on area of modes anticrossing.

Figure 4.24 shows dispersion map of the waveguiding indicator  $1/\sigma_{max}$  calculated for TM modes, dark lines represent guided modes. The map shows dominant mode at  $\nu_y = 2.86$  as the vertical line (the second mode is observed for  $\nu_y = 3.34$ ). The right subplot shows zoom of the area where the vertical mode crosses different modes in the structure and interesting anticrossing behavior occurs. A smooth transformation of the modes is observed. The modes are further study via field plots and by analysis of the effective index of modes.

In the first step we analyze modes which appears as the vertical lines [modes (A) and (B)]. Figure 4.25 shows field plots calculated in the points (A) and (B). Both field plots were calculated for the period of the grating 140 nm, therefore below the level of leakage to the substrate or to the superstrate caused by the


Figure 4.25: Field plot distributions of fundamental and first-order guided modes in the silicon. Field plots were calculated for the structure with grating period 140 nm.

grating. Moreover, both modes shows independence on the grating geometry. Subplot (A) shows field distribution of fundamental guided mode and subplot (B) shows second-order guided mode in the silicon waveguide. The better confinement of the fundamental mode (A), i.e. weaker evanescent field outside the waveguide, leads to the weaker anticrossing effect. Therefore, in our geometry, the anticrossing effect on the fundamental mode is hard to observe. On the other hand, higher evanescent field of the second-order guided mode (B) provides anticrossing as was shown on the right subplot of the Fig. 4.24.

In the second step we have focused on the area of modes anticrossing, points (C) and (D) on the zoom of the Fig. 4.24. Figure 4.26 shows on the left subplot (C) the mode, which is conformable with already discussed firs-order guide mode (shown on subplot (B) on Fig. 4.25). But the observed field profile is being modulated by the periodic grating on the top of the structure. Moreover, partial field enhancement is observed at the top side of the grating, i.e. at the interface between grating and MO Bi:GIG superstrate. The right subplot shows field distribution for the fixed *y*-coordinate at the middle of the grating lamela (marker by vertical dashed line on the left subplot). The field confinement at the top side of the gold is clearly visible. The bottom subplot (D) shows mode with he field confined mostly on the top side of the grating. We can conclude that this mode is a guided along the metal-dielectric interface, i.e. surface plasmon mode. The typical surface plasmon field distribution is present on the right subplot. From the observed evanescent coupling between mode guided in the silicon waveguide and SPP mode in MO BI:GIG material one can expect possible nonreciprocity of guided mode in the silicon. The strength of coupling could be tuned by optimization of the thickness of the SiO<sub>2</sub> layer.

Figure 4.27 shows field plots (E) and (F) almost identical as were already pre-



Figure 4.26: Field plot distributions calculated at the area of the modes interaction.



Figure 4.27: Field plot distributions calculated at positions of expected leaky modes.

sented by Fig. 4.25. Moreover, dispersion of the guided modes shows obvious difference. Modes (E) and (F) are dependent on the grating period and they exist for the grating period above 223 nm, which is the limit of leakage into Bi:GIG superstrate. This is related to remarkably low imaginary part of the effective index (at the level of the guided modes in the Si waveguide), which is 2.509 + 0.00008i and 2.53 + 0.0007i for modes (E) and (F), respectively.



Figure 4.28: Left: Magneto-optic dispersion map of guiding indicator  $1/\sigma_{max}$  in logarithmic scale calculated as a function of the effective index  $\nu_y$  and the grating period  $\Lambda$ . Right: Detail on area of modes anticrossing.

Figure 4.28 shows magneto-optic image of a guiding indicator. The dispersion map was calculated as the difference of between two dispersion maps calculated for opposite magnetization:  $\delta(1/\sigma_{max}) = 1/\sigma_{max}(+\mathbf{M}) - 1/\sigma_{max}(-\mathbf{M})$ . The figure shows how the main MO response is related to the SPP mode on the top side of the grating, at grating/Bi:GIG interface. The right subplot shows zoom on area of modes anticrossing. The subplot shows how the nonreciprocal dispersion of mode guided in the silicon can be achieved by an appropriate grating geometry, namely its period. Figure 4.29 shows how the effective index of mode guided in the silicon waveguide is affected by coupling with the SPP mode near the anticrossing. Top row shows how coupling between modes, achieved by tuning of the grating period, leads to increase of both real and imaginary part of the effective index of guided mode. Bottom subplot shows MO change of the effective index  $(\nu_{y,opt.}(+\mathbf{M}) - \nu_{y,opt.}(-\mathbf{M}))$  as a function of the grating period, i.e. quality of coupling between modes. The bottom subplot shows, that the MO change of the real part of the effective index can be enhanced while the imaginary part (which is related to propagation losses) is unaffected. According to the bottom subplot of Fig. 4.29 this happens for the gratin period around 240 nm.

Proposed theoretical concept of the waveguiding structure based on material with high refractive index separated from magnetoplasmonic structure and



Figure 4.29: Top: The Effective index of guided mode in silicon waveguide as a function of the grating period  $\Lambda$ . Bottom: MO change of effective index.

based on the coupling between evanescent field with magnetoplasmon can be further optimized. By optimization the isolation properties could be improved and enhanced by the cavity mode resonance excitation.

## 4.7 Conclusion of the chapter

In this chapter we have numerically analyzed via a rigorous anisotropic RCWA method the electromagnetic response of a 1D gold grating on a transversely magnetized medium; Bi:GIG layer. In addition the effect of finite thickness of the Bi:GIG layer and presence of the sGGG substrate was discussed. Using straightforward analytical models we have identified geometrical parameter regions where its two basic modes — SPP and FP cavity modes — may potentially couple and interact (Sec. 4.2). By variation of the grating geometry, namely its thickness, air gap, and period, this interaction and anticrossing has been confirmed. In Sec. 4.5 it has been shown that this hybridization of SPP and cavity modes leads surprisingly to significant changes in TMOKE amplitude as well as its spectral position. Moreover, the sign of the TMOKE (under fixed magnetization) can be switched by tuning of the grating thickness and air gap width. A linearized model of the MO shift explains the opposite signs undergone by SPP modes of opposite diffractive coupling. At the end we have proposed concept of the waveguiding structure combined with the magnetoplasmonic grating. We have discuss the change of the effective index of the guided modes and the MO change of the effective index, both introduced by the grating geometry.

## 5 Experiments on real magnetoplasmonic structures

In this chapter we present analysis of the Mueller matrix data measured on fabricated samples. In the first part a development of the structure model is presented. The model is developed in step-by-step process, from the simple description of a perfect structure to the model with surface roughness and residual PMMA photo resist inside the gaps of the grating. The model is fitted to experimental data in each step. Accuracy of each model is evaluated using  $\chi^2$  parameter (3.2). Quality of the developed model is presented in direct comparison between measured and calculated ellipsometric quantities *N*, *C*, and *S* for a wide range of angle of incidence from 20° to 60°.

In the second step the set of 15 Mueller matrix data obtained on 15 different samples is fitted together and the grating opening r of each grating is estimated (for fabrication details see Sec. 3.4). The fitted width of the opening is compared with values obtained by scanning electron microscopy (Fig. 3.16).

Third part is focused on analysis of magneto-optical response of the structure. The measured MO effect is compared with MO response calculated using developed model at the angle of incidence of  $45^{\circ}$ . To analyze global behavior of the sample, the MO response is compared over the interval of the incidence angle from  $20^{\circ}$  to  $60^{\circ}$ .

A good agreement between experimental Mueller matrix magneto-optic spectroscopic data and the grating model increase credibility of the previous models in Chapter 4 and enables us to trust the functionality of the designed magnetoplasmonic structure.

## 5.1 Optical characterization of samples

#### 5.1.1 Measured ellipsometric response of structures

The fabricated 1D periodic gratings were measured with the Mueller matrix ellipsometer Woollam described in Sec. 3.2. The optical response of the samples were measured in a configuration, where the plane of incidence was perpendicular to the lamelas of the grating, the same configuration as was used in theoretical study in Sec. 4.1. This configuration avoid conversion between *s*- and *p*-polarization. Moreover, the transverse MO configuration also do not induce polarization conversion. Thus, Mueller matrix (2.130) is reduced into three pa-

rameters: N, C, and S, [Chap. 2, Sec. 2.7.3, (2.131)]:

$$\mathbf{M} = \begin{bmatrix} 1 & -N & 0 & 0 \\ -N & 1 & 0 & 0 \\ 0 & 0 & C & -S \\ 0 & 0 & S & C \end{bmatrix},$$
(5.1)

In a non depolarizing system, the elements N, C, and S are related to the classical ellipsometric angles  $\psi$  and  $\Delta$ :

$$N = \cos 2\psi, \quad C = \sin 2\psi \cos \Delta, \quad S = \sin 2\psi \sin \Delta.$$
 (5.2)

For further analysis of the optical response of the structure (4.3) we define the relative reflectivity  $R_p/R_s$  as follows:

$$\frac{R_p}{R_s} = \tan \Psi, \tag{5.3}$$

which is directly related to the measured data and will allow us to quantify the MO response of the structures (see further in Sec. 5.3).

#### 5.1.2 Development of the structure model

In the theoretical study of the magnetoplasmonic structure we already discussed the effect of a finite thickness of the MO Bi:GIG layer (Sec. 4.1.2), and the depolarization effects due to beam focusing (Sec. 3.2.2). To be able to reproduce the experimental results, a generalization of the model is needed. The step-bystep process of model adjustment is described in this section. Quantities N, C, S, and depolarization are used to compare models and experimental data. The  $\chi^2$ value [defined by (3.2)] is used as an indicator of the fit quality.

To model optical response of the structures 30 Fourier harmonics (N = 30, see Sec. 2.5.2) were assumed and the experimental data were fitted by our parallel RCWA code described in Sec. 2.5.

In the following text we use sample code in the format  $p500_X$ , where p500 denotes the grating with period 500 nm fabricated and the electron exposition dose equal to X. The dose varies from 900 to 1040 as was described in the Section 3.4 in Chapter 3.

#### A. Model of expected structure vs. experimental data

In the firs step we compare simple model of the structure with the experimental data. The cross section of the model is shown on Fig. 5.1. The nominal parameters of the sample are: the grating period  $\Lambda = 500$  nm, the grating thickness  $t_1 = 100$  nm, the width of air-gap r = 63 nm, the dose of 1040  $\mu$ C/cm<sup>2</sup>, and the thickness of the Bi:GIG  $t_2 = 3988.4$  nm (from Tab. 3.4). In the model we use the nominal parameters. Parameters used in model are summarized in tab. 5.1. Figure 5.2 shows comparison between model and experimental data measured on sample p500\_1040 (Fig. 3.16). One can see, that model does not fit the data well and more advanced model is needed.

Note that the simplest model does not describe attenuation of the interferences in Bi:GIG layer (at about 700 nm and 1400 nm), position of plasmon peaks (at about 886 nm). The model does not describe depolarization at all. The origin of the interference phenomena was already discussed in Sec. 4.1.2 in Chapter 4.



Figure 5.1: Cross-section of the grating structure.

Table	e 5.1:	No	minal pai	rame	eters	s of simple model
			$\chi^2 =$	0.0	103	
	$arphi_0$	=	$45^{\circ}$			
	Λ	=	$500~\mathrm{nm}$	r	=	63 nm
	$t_1$	=	100 nm	$t_2$	=	3988.4 nm



Figure 5.2: Comparison between simple model with nominal parameters and experimental data.

#### B. Model with focused beam

In the next step the divergence of the focused beam was introduced into the model. As was discussed in Sec. 3.2.2 to model data obtained with focusing probes, it is necessary to fit the angle of incidence  $\varphi_0$  and the beam divergence  $\varphi_s$ . Moreover, we also allow the geometrical parameters of the grating, namely the period  $\Lambda$ , the grating thickness  $h_1$ , and the grating opening r, to be fitted. The cross section of the model is shown on Fig. 5.3. Figure 5.4 shows fitted quantities N, C, S and comparison between measured and calculated depolarization. Subplots show that the model matches significant peaks in data with sufficient precision, but the amplitudes of peaks are not well modulated. The  $\chi^2 = 0.0053$  is much better than for the previous model. Parameters obtained by the fit are summed in Tab. 5.2, in which fitted parameters values are emphasized by bold numbers.



Figure 5.3: Cross-section of the grating structure.

ubic	0.2.	r nace paran	ie te i t	5.01	ompre mode		
	$\chi^2 = 0.0053$						
$\varphi_0$	=	$45.64^{\circ}$	$\varphi_s$	=	$2.84^{\circ}$		
Λ	=	$506.94\mathrm{nm}$	r	=	$86.52\mathrm{nm}$		
$t_1$	=	99.59 nm	$t_2$	=	3988.4 nm		

Table 5.2: Fitted parameters of simple model



Figure 5.4: Comparison between simple model and experimental data.

#### C. Model with surface roughness

In the next step of modeling, we have introduced a surface roughness on the top of the gold grating. The roughness was simulated as a thin film on the top of the gold with optical functions described using the Bruggeman effective medium approximation (BEMA), see Sec. 3.2.3 for definition. We use fixed volume fraction f = 0.5 [105, 127, 128] and the fitted thickness  $t_3$ . The cross section of the model is shown on Fig. 5.5. Parameters estimated by previous model were used as initial values for the fit. Figure 5.6 shows comparison between experimental data and best fit model. Table 5.3 summarizes fitted parameters. Note that  $\chi^2 = 0.0013$  is much smaller than for previous model, which proves necessity to include roughness.



Figure 5.5: Cross-section of the grating structure with surface roughness.

$\chi^2 = 0.0013$						
$arphi_0$	=	$44.38^{\circ}$	$\varphi_s$	=	$3.11^{\circ}$	
$\Lambda$	=	$502.19\mathrm{nm}$	r	=	<b>76.60</b> nm	
$t_1$	=	$92.59\mathrm{nm}$	$t_2$	=	3988.4 nm	
$t_3$	=	15.01nm				

Table 5.3: Fitted parameters of model with roughness



Figure 5.6: Comparison between model with surface roughness and experimental data.

#### D. Final model of the structure with the residual PMMA

To achieve the best fit of the experimental data, the residual layer of the PMMA photo-resist was introduced in the model. The dispersion of PMMA resist was taken from Ref. [129]. The assumption of residual PMMA leads to further reduction of  $\chi^2$  from 0.0013 to 0.0011, therefore we found model good-enough to describe our experimental data. From the  $\chi^2$  reduction we can conclude, that PMMA was really present. The cross section of the model is shown on Fig. 5.7. Table 5.4 summarizes best-fit parameters (denoted as bold symbols). Note that total thickness of the grating is given as  $t_1 + \frac{1}{2}t_3 + t_4 = 98.74$  nm. The thickness of the layer representing the surface roughness was taken as the  $\frac{1}{2}t_3$  due to the fixed volume fraction f = 0.5 (see Sec. 3.2.3). Figure 5.8 shows very good agreement between model and data. Moreover, calculated and measured depolarization are in very good agreement.



Figure 5.7: Cross-section of the grating structure with surface roughness and residual PMMA.

Table 5.4: Parameters of the best-fit						
$\chi^2 = 0.0011$						
$\varphi_0$	=	$44.33^{\circ}$	$\varphi_s$	=	$2.91^{\circ}$	
$\Lambda$	=	$502.6~{ m nm}$	r	=	<b>78.68</b> nm	
$t_1$	=	<b>68</b> .16 nm	$t_2$	=	3988.4 nm	
$t_3$	=	$13.55~{ m nm}$	$t_4$	=	23.8nm	



Figure 5.8: Comparison between model with surface roughness and residual PMMA and experimental data.

#### Sensitivity on partial sample illumination

Since the size of the spot of the focused beam is approximately  $150 \,\mu\text{m}$  in diameter and the size of the grating is  $350 \times 350 \,\mu\text{m}$ , the analysis of possible partial illumination of the sample has to be done. In order to understand effects of partial illumination of the sample we performed x - y scan over the surface of the sample. It is known, that partial illumination of the sample and the substrate can be observed in the Mueller matrix data as the depolarization [106]. Figure 5.9 shows image of fabricated structures (left subplot), and measured depolarization over surface of the sample (right subplot). The right subplot directly shows, that minimal depolarization is measured on the grating and on the pure substrate. In case of partial illumination of the grating (or labels under gratings), the depolarization increases.



Figure 5.9: Left: Photography of fabricated samples with marked area of x - y scan. Right: measured depolarization at the photon energy of 2.149 eV.

# 5.1.3 Comparison between simulated and measured optical data

In this section we compare measured data on single grating with data calculated from developed model (Fig. 5.7). Best-fit parameters of geometry and angular spread  $\varphi_s$  were used for simulation and the angle of incidence  $\varphi_0$  was varied from 20° to 60°. Figure 5.10 shows a comparison of the calculated and measured N, S, and C quantities.

From both measured and calculated data in Fig. 5.10 we can directly distinguish dispersive modes and dispersionless modes with respect to the angle of incidence or thus parallel k vector (close to wavelength of 500 nm, Sec. 4.2.2). This observation is further used in analysis and estimation of the operational point of the structure; estimation of the angle of incidence where the coupling of cavity and plasmon mode increases the MO effect. But before that, the analysis of all samples and comparison between the measured and calculated MO response should be done. Detailed description of dispersive and non-dispersive grating modes is summarized and discussed in the Chapter 4 in the Sec. 4.2 and will be discussed later in this chapter.



Figure 5.10: Comparison between calculated (left column) and measured (right column) quantities N, S, C.

## 5.2 Global fit of fabricated samples

In Sec. 3.4 we have described the fabrication process of 15 samples (see samples layout on Fig. 3.16). Samples with different opening were fabricated by variation the dose from 900 to  $1040 \ \mu C/cm^2$ . The openings *r* were approximately estimated from SEM observations. Best fit of the Mueller matrix data measured on sample p500\_1040 shows a difference between the gap estimated from the SEM and from the model (63 nm vs. 77.4 nm), therefore it was necessary to perform a fitting procedure of the gaps of all fabricated gratings. To eliminate possible correlations between parameters of the model we performed a global fit. The same parameter coupling approach was used for the angle of incidence, the angular spread, the period, and the thickness of the layer representing surface roughness.

The coupling of parameters leads to increase uniqueness of parameters and eliminates possible correlations between parameters. In the global fit we have used model of the grating with surface roughness (see Sec. 5.1.2). Despite the fact, that model with surface roughness and residual PMMA gives the best fit, we have used model without residual PMMA, because it can describe the structure with good agreement with less free parameters. Assumption of the residual PMMA inside the gap would lead to significant increase of free parameters because the thickness of the PMMA in each grating could be different (i.e. 15 extra free parameters). Since the sample was fabricated at the same time and under the same condition, we can expect the same thickness and period of the each particular grating. Moreover, the Mueller matrix data of all gratings were measured using the x - y mapping stage, therefore the angle of incidence could be taken as a common parameter for all spectra. Those preconditions leads to significant reduction of free parameters. The total number of free parameters of the global fit was 20.<sup>1</sup>

The results of the fit are listed in Tab. 5.5. Fitted angle of incidence, angle of angular spread, grating thickness and period are almost the same as the values obtained by single spectra fits presented in the previous section. All fitted parameters are denoted as bold symbols. The  $\chi^2$  was calculated separately for each sample and it shows values comparable to single sample fits. the fitted air-gap r is compared with SEM observation and comparison with nominal parameters is included. Fitted air-gap shows the same trend as observed. Figure 5.11 shows graphically comparison of air-gap r obtained on all samples by SEM and by the global fit. Figure 5.12 shows the fitted ellipsometric quantity N to the experimental data. The difference of the air-gap width obtained by SEM and by the global fit comes from the fact, that SEM observations are local, but the ellipsometric data represents global response (averaged effect over the size of the spot). The key

<sup>1.</sup> Assuming N = 25 Fourier harmonics (see Sec. 2.5.2) the fitting procedure costs  $\approx 18000$  CPU hours, i.e. three day of parallel computing on 256 CPUs.

information from global fit is, that it shows the same trend of change of the airgap as was observed by the SEM. Moreover, with the fitted parameters we can reproduce each measured spectra as Fig. 5.12 shows.

Table 5.5. I drameters of the global fit								
	common fitted parameters:	$arphi_0=43.33^\circ$	$arphi_s = \mathbf{3.05^\circ}$	$\Lambda = 502.4~nm$				
		$t_1 = 95.3 \ \mathrm{nm}$	$t_2 = 3988.4 \text{ nm}$	$t_3 = 12.7 \ nm$				
	nominal parameters:	$\varphi_0 = 45^\circ$	$\varphi_s = 3^{\circ}$	$\Lambda=500~\mathrm{nm}$				
		$t_1 = 100 \text{ nm}$	$t_2 = 3988.4 \text{ nm}$	$t_3 = 0 \text{ nm}$				
sam	ple:	$r_{ m SEM}$ nm	$r_{ m fit}{ m nm}$	$\chi^2$				
1.	p500_1040	63	77.4	0.002				
2.	p500_1030	66	78.4	0.0015				
3.	p500_1020	72	87.7	0.0016				
4.	p500_1010	96	115.1	0.0018				
5.	p500_1000	92	84.1	0.0020				
6.	p500_990	96	101.5	0.0013				
7.	p500_980	97	115.3	0.0016				
8.	p500_970	110	116.3	0.0014				
9.	p500_960	110	119.0	0.0016				
10.	p500_950	116	120.7	0.0017				
11.	p500_940	130	120.8	0.0016				
12.	p500_930	114	134.5	0.0014				
13.	p500_920	137	137.1	0.0016				
14.	p500_910	142	147.1	0.0017				
15.	 p500_900	145	147.3	0.0016				

Table 5.5: Parameters of the global fit



Figure 5.11: The openings *r* estimated by SEM and by global fitting procedure are compared.



Figure 5.12: Ellipsometric quantity N obtained by global fit procedure on 15 samples is compared with experimental data.

# 5.3 Transverse magneto-optical response of the sample

This section is focused on the analysis of the magneto-optical response of the structure. The magneto-optical response is calculated using the model with residual PMMA described in Sec. 5.1.2 and magnetooptical constants of Bi:GIG determined in Sec. 3.3 (Fig. 3.14). To quantify the MO response in the transverse configuration, we define  $\delta R$  quantity as follows :

$$\delta R = \frac{R_p}{R_s} \left( + M_x^{\text{sat.}} \right) - \frac{R_p}{R_s} \left( - M_x^{\text{sat.}} \right), \qquad (5.4)$$

where ratio  $R_p/R_s$  is directly related to the ellipsometric angle  $\psi$  [Eq. (5.3)] and  $\pm M_x^{\text{sat.}}$  represents saturation magnetization in transverse magneto-optical configuration. For the MO measurements we have used the same in-plane magnet as applied for the MO characterization of the Bi:GIG layer. In order to reduce noise in the data, we averaged three spectra for each orientation of the same magnetization.

### 5.3.1 Comparison between measured and simulated magnetooptical response

In the first step the model is compared with measured MO data. The MO data were obtained for the same configuration of the ellipsometer, therefore we can directly use the already fitted model<sup>2</sup>. Figure 5.13 shows on the left subplot a comparison of the relative reflectivity  $R_p/R_s$  between measured data and model. The calculated *s*-reflectivity flat specrum (green line) is included to demonstrate, that all key-features appear for *p*-polarization. The right subplot shows the calculated and the measured MO quantity  $\delta R$ . This illustrates how the model describes the MO response in a very good agreement. Thus we can use the model to determine the origin of the MO effect by field distribution plots, calculate MO response for different angle of incidence, etc.

Figure 5.14 shows a comparison between measured and calculated MO effect  $\delta R$  as a function of wavelength and incident angle. Experimental data were obtained by a scan over the wide interval of the angle of incidence from 20° to 60° with the step of 0.5°. The experimental data (right subplot) are compared with the model (left subplot). Figure gives an important information about the amplitude of the MO effect as a function of the angle of incidence. Maximal MO effect was measured (right subplot) for the angle of incidence in interval from 40° to

<sup>2.</sup> In the first part of the experiment we performed optical measurements. After that the magnet was installed without any mechanical manipulation of the ellipsometer.



Figure 5.13: Left: comparison between calculated and measured relative reflectivity  $R_p/R_s$ . Right: Comparison between measured and calculated MO effect.

 $50^{\circ}$  and close to  $20^{\circ}$ . For further analysis both interesting points have pros and cons. Disadvantage of the maximum of the MO effect around  $45^{\circ}$  is that different plasmon modes interact at this point. Therefore the analysis of MO behavior is not straightforward. Moreover, we have already noticed (in Sec. 5.1.3) that cavity mode is excited in region of shorter wavelengths, around 500 nm. Thus the MO data measured close to the angle of incidence of  $20^{\circ}$  represent the simple case of this coupling just between the cavity mode with a single plasmon mode. The analysis of coupling is presented in the next section.



Figure 5.14: Measured and calculated MO effect as a function of the wavelength and the angle of incidence are compared.

#### 5.3.2 Incident angle estimation for the maximal coupling effect

In this work we are mainly interested in the coupling between the surface plasmon and cavity mode and more importantly what impact this coupling has on the MO effect. As was shown in the previous section (on the experimental and the numerical data), the maximal MO response is achieved for angles of incidence around 20° and around 45°. Figure 5.15 shows the measured map of the relative reflectivity  $R_p/R_s$  and the MO effect  $\delta R_p/R_s$ . On the left subplot we clearly recognize curved dispersion curves of surface plasmons and flat (dispersionless) cavity modes. The evolution of the relative reflectivity and the MO effect for angles of incidence of 20°, 30°, and 45° is shown on Fig. 5.16 and the spectral position of main peaks are marked.



Figure 5.15: Measured map of the relative reflectivity (left) and the MO effect  $\delta R_p/R_s$  for the angle of incidence from 20° to 60°.

Figure 5.16 shows the different shape of two main MO peaks: blue (for  $20^{\circ}$ ), red ( $45^{\circ}$ ). At the  $20^{\circ}$  the MO effect switches sign from negative to positive when increasing the wavelength starting at the plasmon resonance. For the SPP at  $45^{\circ}$  this switching behavior is reversed. This is explained by different order of plasmon mode. The blue curve represents  $+2^{nd}$  and the red one represents  $-1^{st}$  plasmon mode. For the definition of the order of plasmon mode see (4.14), the opposite sign change is described by (4.25).

Figure 5.17 shows the distribution of the field components  $H_x$  calculated for the three main peaks at 747 nm, 786 nm, 886 nm (marked on Fig. 5.16). The first subplot (left) shows field enhancement both at the grating-Bi:GIG interface and inside the grating cavities. The second subplot shows relatively small field enhancement in Bi:GIG, which is in accordance with weak measured MO response.



Figure 5.16: Relative reflectivity and MO effect measured at angles of incidence of  $20^{\circ}$ ,  $30^{\circ}$ , and  $45^{\circ}$ .



Figure 5.17: Field component  $H_x$  distribution calculated at the wavelength of 741 nm, 786 nm, and 886 nm ad the angle of incidence of 20°, 30°, and 45°, respectively.

Finally, third subplot shows field enhancement at the Bi:GIG and inside the cavity which also leads to significant MO response. Moreover, the fieldplot shows field concentration on at the top side of the grating, which is related to the (partial) plasmon excitation at the top of the grating at the gold-air interface. Thus the field enhancement inside the cavity is not given as resonant cavity mode itself, but as an energy channel. Because of the complicated behavior for  $45^{\circ}$ , we have decided to study the less complicated situation of two modes coupling at the angle of incidence of  $20^{\circ}$ .

# 5.4 Impact of modes coupling to optical and MO response

In this section the impact of interaction between surface plasmon and cavity mode is analyzed. In the first part we experimentally confirm previous theoretical results on coupling between SPP and cavity modes. We demonstrate both experimentally and by the model how the position of the plasmon peak is affected by variation of the width of the air-gap r. The same procedure is then repeated for the analysis of the MO response. The model used for the simulations was based on the real structure parameters obtained from the global fit in Sec. 5.2. Only the angle of incidence  $\varphi_0 = 20^\circ$  was used instead of fitted one and the opening r was varied. By the global fitting procedure we have obtained systematic change of the grating air gap with a good armament with the SEM observation (Fig. 5.11 and Tab. 5.5). Therefore in following simulations we use equidistant change of the value and compare the result with the measured drift of the peaks. As was mentioned in previous section, for the incident angle of  $20^\circ$  (and principally below) only single surface plasmon mode and cavity mode interacts, which makes analysis less complicated.

## 5.4.1 Effect of modes coupling observed in relative reflectivity spectra

Figure 5.18 shows a zoom of the relative reflectivity  $R_p/R_s$  near the  $+2^{nd}$  plasmon peak at 730 nm. A blue shift of the plasmon peak for increasing width of the air gap r. Obtained experimental data are compared with simulations on the right subplot and the same shift is observed. Therefore we can conclude that the shift originates from the change of the grating's geometry and it is not artificial effect from experiment (system alignment etc.).



Figure 5.18: Zoom of the plasmon peak at  $\varphi_0 = 20^\circ$ . Experimental data obtained on samples with different dose (left subplot) are compared with numerical data obtained for different opening *r*. Measured systematic change of the peak width, amplitude, and a blue-shift of spectral position of the plasmon peak is in good agreement with a numerical data (right subplot).

#### 5.4.2 Experimental observation of TMOKE switching

In Chapter 4 in Sec. 4.5 we have predicted possible switching of the TMOKE by optimization of the grating air gap. This was predicted Fig 4.22 (which is repeated below and was calculated for the  $\varphi_0 = 10^\circ$ ). At this point we prove the



Figure 5.19: Left: Detail of the TMOKE spectral dependence  $\Delta R_p$  for the grating air gap  $h_1$  from 20 nm to 120 nm and period  $\Lambda = 500$  nm. Right: Switching of the TMOKE sign at fixed photon energy 1.74 eV (712 nm) by variation of the gratin air gap width.



Figure 5.20: Trend of the MO peak shift measured on 15 samples with various opening r is compared with systematic shift obtained by simulations.

predicted phenomena by the experimental observations. As the firs step we have used developed the model of the structure (described in Sec. 5.1.2) and recalculate MO response as the function of the grating air gap. For the experimental confirmation we have measured MO response of fifteen samples, analyze the drift of the MO peak, and compared with the numerical data. Moreover, the bottom subplot shows the measures switching phenomena at the fixed photon energy 1.68 eV.

Figure 5.21 shows on the left subplot zoom on MO peaks calculated for different widths of the air gap. The blue shift of the MO peak is clearly visible. The right subplot shows zoom on measured MO peaks on different samples (with different width of the air gap). The subplot clearly demonstrate the blue shift of the MO peak by the increasing air gap, which is in good agreement with the predictions.



Figure 5.21: Detail on MO peak at  $\varphi_0 = 20^\circ$ . The numerical data obtained for different opening r (right subplot) are compared with the experimental data obtained on samples with different dose. Measured systematic change of the peak width, amplitude, and a blue-shift of spectral position of the plasmon peak are in good agreement with a numerical data (right subplot).

These magneto-optical observations confirm the presented theory of the TMOKE geometrical tuning in the 1D magnetoplasmonic grating.

## 5.5 Conclusion of the chapter

The main result of this chapter and the main result of this thesis is experimental confirmation of previously predicted TMOKE tuning or even inverting (without magnetization inverting) by a proper adjusting of the grating geometry. For conclusive demonstration of the phenomena we have presented detailed process of optical characterization of the fabricated structures. The developed advanced model assuming the experimental angular spread of the incidence Gaussian beam also contributed to this and allowed to explain the presence of interference fringes in the Mueller spectra. The described technique is a generic tool that can be used to study magneto-optic structures in many different configurations or geometries.

# **Achieved results and Perspectives**

# **Achieved results**

Objective of this work was the study of TMOKE response of the 1D periodic magnetoplasmonic gratings, analysis of resonant modes, and impact of their coupling to the enhancement of the TMOKE. Achieved work and results can be summarized in four groups:

- 1. Coupling of cavity and plasmon modes in magnetoplasmonic structure
- The main result of this work is explanation and experimental confirmation of new observed phenomena of the TMOKE enhancement and it was demonstrated how the sign of the TMOKE can be reversed without change in magnetization. Numerically this phenomena was explained as the effect of interaction between grating resonances (cavity and surface plasmon modes) and it was demonstrated how the TMOKE can be tuned via slight adjustment of the grating geometry (Chapter 4, Section 4.3) – published in [65,66].
- To confirm theoretical results a set of fifteen real magnetoplasmonic grating was fabricated by electron beam lithography and lift off technique. Magnetooptic response of the samples was measured with Mueller matrix ellipsometer and the experimental data prove predicted effect with very good agreement (Chapter 5, Section 5.4).
- 2. Determination of optical and magneto-optical spectra of used materials:
- Optical functions of material used for fabrication of samples were fitted from Mueller matrix reflection and intensity transmission spectra (Chapter 3, Sections 3.2.3 - 3.2.4) – published in [130].
- Depolarization effects introduced by ellipsometric setup, finite spectral resolution, and focusing of the beam were analyzed (Chapter 3, Section 3.2.2).
- Mueller matrix ellipsometer was extended with in-plane permanent magnet controlled by PC. The magnet was used for characterization of MO properties of Bi:GIG and for MO experiments on magnetoplasmonic gratings (Chapter 3, Section 3.2.5 – published in [131].

# 3. Development of advanced models of real fabricated magnetoplasmonic structures:

- Model of the 1D plasmonic grating assuming fabrication imperfections, like a surface roughness on a top of the grating and residual PMMA photo resist inside the grating air gaps and divergence of the focused beam, was developed. The developed model gives very good agreement between measured and calculated MO data (Chapter 5, Section 5.1.2), – published in [131]
- To characterize widths of air gaps over whole set of fifteen fabricated samples, a global fit with coupled common geometrical parameters was per-

formed. Obtained air gaps by fitting show the same trend as air gaps determined by the SEM observations (Chapter 5, Section 5.2).

- 4. Development of software for modeling of grating
- New software program for modeling optical response of the one-dimensional periodic grating based on RCWA was developed in MATLAB and optimized for parallel solution of spectral problems.
- The parallel implementation of the code was optimized and linear scalability up to 256 cpus was achieved for problems of spectral simulations with included divergence of focused beam (using supercomputing center IT4I).

## Perspectives

Though in this thesis we have successfully designed some experiments to confirm aspects of some predicted results, there are indeed a large number of potentially interesting future studies. Here only a small selection of ideas is listed.

For example, in the Chapter 4 we have predicted the coupling between SPP and cavity modes via the grating thickness and air gap width variation. However experimental samples fabricated by method described in Chapter 3 confirm only predictions on grating air gap variation. It would be great to analyze the coupling and compare the magneto-optical response obtained by the grating thickness variation. Samples for this experiments were already fabricated.

In addition the structures studied in this thesis are one dimensional, perfectly rectangular and were studied in the planar diffraction configuration and the transverse magnetization. The most obvious future work is to extend to the conical diffraction configuration, to the 2D periodic structures and to the study of effects for the longitudinal or polar magnetization. The conical diffraction configuration should be promising for precise optical characterization and for study of nonreciprocal mode-conversion. These 2D structures should also have interesting optical properties in both the reflection and the transmission configuration. Study of the structures with conical profile could bring new effects in tuning of the cavity modes and an important information about fabrication process itself.

The next direction of research was opened by the theoretical proposition of the waveguide structure. Further study and optimization of the structure is obvious. The structure should be designed from compatible (from fabrication point of view) materials and it should operate for the fundamental guided mode. The integrated device may operate as an optical isolator or modulator, depending on fixed or modulated magnetization.

At last but not least the transfer of the presented theoretical and experimental results on magnetoplasmonic structures into far infrared and THz domain could be useful in the design of new optical components.

## A Parallel implementation of the RCWA

Our implementation of the RCWA was done in MATLAB software. For parallelization we have used the Matlab Distributed Computing Engine, Matlab Distributed Computing toolbox and OPEN MPI library for communication between nodes over InfiniBand network. The code was optimized for supercomputing cluster Anselm in the frame of software resources of IT4Innovation National Supercomputing Center.

Efficiency of our parallel implementation of the RCWA is demonstrated on the developed model of the plasmonic grating in Chapter 5. Figure A.1 shows the cross-section for the structure used for testing of the code efficiency. In the testing we have consider model with the following parameters:  $\Lambda = 500$  nm, r = 75 nm,  $t_1 = 90$  nm,  $t_2 = 4000$  nm,  $t_3 = 15$  nm,  $\phi_0 = 45^\circ$ , 30 Fourier harmonics (N = 30, see Sec. 2.5.2), and for the spectral domain with 1088 points of wavelength range from 210 nm to 1700 nm.<sup>1</sup>



Figure A.1: Cross-section of the grating structure with surface roughness used for analysis of the parallelization efficiency.

## A.1 Parallelization and scalability

In the spectral simulations each spectral point represents individual and independent eigenvalue problem. Than a proper parallelization of the code may strongly reduce required computing time. Our implementation of the parallel RCWA was done in the sense *divide et impera*, when the spectral problem is split into set of spectral subploblems. Each of subploblems represents a few individual eigenvalue problems which are solved one-by-one on a single core. Figure A.2 shows the parallelization approach schematically. The method of parallelization based on splitting into subproblems reduces required communication time between computing nodes significantly. This approach gives better efficiency than method when each of spectral points is solved separately as a subproblem. We

<sup>1.</sup> Number of the spectral points corresponds to spectral resolution of the used Mueller matrix ellipsometer.


Figure A.2: Single spectrum parallelization.

have test the code for the introduced structure and for spectral domain containing 1088 points. By the numerical testing we found almost linear reduction of computing time up to 64 parallel jobs, i.e. 64 cores. Figure A.3 shows comparison of ideal linear scaling (red line) when computation on 64 cores need 1/64 computing time of a single-core simulation, and measured scaling of our code. Further increase of number of parallel jobs decrease ration between communication and calculation time and the efficiency decreases.



Figure A.3: Scalability of single spectra problem.

In the next step of the code parallelization we have use an advantage of the Mueller matrix simulations of the divergent incident beam described in Sec. 3.2.2. For this type of simulation, the spectrum of Mueller matrix needs to be recalculated for each partial angle from the interval of incident angles. According to our numerical experiments the assumption of 11 partial beams within the interval  $\varphi_0 - \varphi_s$  to  $\varphi_0 + \varphi_s$  is sufficient to describe the depolarization effect originating

from the focused beam. The benefit on the Mueller matrix simulations of the divergent beam comes from the fact, that the result is achieved as a weighted sum of a partial Mueller matrix spectra.

Figure A.4 shows used parallelization approach schematically. In the first step, 11 partial spectral problems are defined. In the second step each spectral problem is split into set of the subproblems. Each subproblem represents part individual part of whole spectrum and one partial angle of incidence. All sub-problem sets are collected and in the next step distributed for parallel execution. With described approach we have improved scalability of our code up to 256



Figure A.4: Multiple spectra parallelization.

cores. Figure A.5 shows comparison between ideal linear and measured scaling of our code.



Figure A.5: Scalability of spectral problem assuming beam divergence.

# Used abbreviations and symbols

RCWA	Rigorous Coupled Waves Analysis
MO	Magneto-Optical
TMOKE	Transverse Magneto-optical Kerr Effect
LPE	Liquid Phase Epitaxy
MZI	Mach-Zender Interferometer
MMI	Multi-Mode Interference
SOI	Silicon-On-Insulator
SEM	Scanning Electron Microscopy
SPP	Surface Plasmon Polarion
FP	Fabry-Perot
TE	Transversal Electric polarization
TM	Transversal Magnetic polarization
KK	Kramers-Krönig
BEMA	Bruggeman Effective Medium Approximation
MIBK	Methyl Isobutyl Ketone
IPA	Isopropyl Alcohol

×	cross product
$\nabla \cdot$	divergence operator
abla  imes	curl operator
[.]	Fourier coefficients vector with respect to <i>y</i> axis
[[.]]	Toeplitz matrix of Fourier coefficients respect to <i>y</i> axis
R	real part
$\mathcal{S}$	imaginary part
$\delta_{ij}$	Kroenecker symbol
$\otimes$	Kronecker product

$\mathbf{E}(\mathbf{r},t)$	electric field vector
$\mathbf{H}(\mathbf{r},t)$	magnetic field vector
$\mathbf{D}(\mathbf{r},t)$	electric displacement
$\mathbf{B}(\mathbf{r},t)$	magnetic flux density
$\rho(\mathbf{r},t)$	charge density
$\mathbf{j}(\mathbf{r},t)$	current density vector
$\mathbf{P}(\mathbf{r},t)$	polarization volume density vector
$\mathbf{M}(\mathbf{r},t)$	magnetization volume density vector
$\mathbf{E}'(\mathbf{r},t)$	normalized electric field vector
$\mathbf{H}'(\mathbf{r},t)$	normalized magnetic field vector
e	electric field polarization vector
h	magnetic field polarization vector
$\mathbf{e}'$	normalized electric field polarization vector
$\mathbf{h}'$	normalized magnetic field polarization vector
$E_0$	electric field vector amplitude
$H_0$	magnetic field vector amplitude
$E_0'$	normalized electric field vector amplitude
$H_0'$	normalized magnetic field vector amplitude
$\hat{\epsilon}$	electric permittivity tensor
$\widehat{\epsilon}'$	complex electric permittivity tensor
$\widehat{\chi_e}$	electric susceptibility tensor
$\widehat{\sigma}$	electric conductivity tensor
$\hat{\epsilon_R}$	relative permittivity
$\epsilon_{i,j}$	components of permittivity tensor
$\epsilon_0$	free space electric permittivity
$\mu_0$	free space magnetic permeability
$\mathbf{M}$	magnetization vector
$K_{ijk}$	components of linear magneto-optic tensor
r	space position vector
x,y,z	space coordinates
t	time
i	imaginary unit
k	wavevector
$k_0$	free space wave vector amplitude
ν	normalized wave vector
$\omega$	angular frequency
$\lambda$	wavelength
f	fill factor
Λ	grating period

Q	vector of linear magneto-optical parameters
$d^{(n)}$	thickness of the n-th laver
$\varphi_0$	angle of incidence
$\sigma_{max}$	maximal singular value
$\psi$	ellipsometric amplitude angle
$\Delta$	ellipsometric phase angle
$r_{ij}$	reflection coefficient
$t_{ij}$	transmission coefficient
$\hat{R}_{ii}$	reflectivity matrix components
T	total transfer matrix
S	total scattering matrix
I	unity matrix
С	matrix of eigenvalues problem
V	eigenvalue matrix
$\mathbf{V}^{(n)}$	eigenvalue matrix in n-th medium
Т	eigenvectors matrix
$\mathbf{T}^{(n)}$	eigenvectors matrix in n-th medium
F	Fourier base vectors diagonal matrix
Р	propagation matrix
$P_{up}$	upwards propagating modes propagation matrix
$\mathbf{P}_{down}^{(n)}$	downwards propagating modes propagation matrix
uoun	matrix of normalized wave vectors x axis tangential
р	components
	matrix of normalized wave vectors y axis tangential
q	components
D	matrix relating continuous and discontinuous components
D	of electric field and electric displacement
0	matrix representing permittivity of the grating after FF
Q	applied in $y$ direction
A	amplitudes vector
$\mathbf{A}_{up}$	upwards propagating modes amplitudes vector
$\mathbf{A}_{down}$	downwards propagating modes amplitudes vector
М	Mueller matrix
$M_{ij}$	Mueller matrix components
$P_q$	depolarization index
M <sup>diff.</sup>	differential Mueller matrix
$E_{ph}$	photon energy
$n_{eff}$	effective index

## List of Figures

1	Illustration schématique de la structure étudiée : réseau en or avec période $\Lambda$ et épaisseur $h_1$ sur substrat de grenat magnéto-optique pour une configuration transversale avec onde au niveau de l'incidence au niveau $u = z_i$ avec angle d'incidence $\varphi_0$ et polarisation <i>s</i> - ou <i>p</i> -, xii
2	Illustration schématique de la configuration de l'ellipsomètre avec deux compensateurs rotatifs et orientation des composantes extérieures d'aimantation dans le plan.
3	Fonction optique du substrat sGGG (graphique à gauche) et de la couche Bi:GIG (graphique à droite). La composante réelle $\Re{\epsilon_{11}}$ et la composante imaginaire $\Im{\epsilon_{11}}$ de la fonction sont illustrées par une ligne pleine et pointillée
4	Dépendance spectrale ajustée de la composante off-diagonale du tenseur obtenue par la mesure ellipsométrique Bi:GIG pour une configuration MO transverse et longitudinale
5	Réflectivité spéculaire et spectre TMOKE correspondant
6	Cartographie du module de la composante du champ magnétique. xix
7	Indice effectif du guide d'onde or/air/or, $\lambda = 884$ nm
8	Illustration schématique du guide d'ondes « or/air/or » xx
9	Le détail à gauche illustre la dépendance spectrale TMOKE par rapport à l'ouverture du réseau
10	Schéma de la structure du guide d'onde silicium avec réseau d'or et Bi:GIG
11	Courbe de dispersion de l'indicateur de guidage d'ondes xxiii
12	Coupe de la structure du réseau avec rugosité de surface et PMMA résiduel
13	Comparaison entre le modèle avec rugosité de surface et PMMA résiduel et les données expérimentales.
14	Comparaison de la réflectivité relative calculée et mesurée $R_p/R_s$ . xxvi
15	Décalage spectral de la réponse MO, extraite des mesures réalisées pour 15 échantillons
1.1	Prism coupling and decoupling of guided forward and backward modes is shown schematically
1.2	Basic principle of free space polarization-dependent optical isola- tor
1.3	Schematic illustration of an integrated GaInAsP MZI optical isola- tor developed by Sobu et. al. [37]

1.4	Structure of the monolithic nonreciprocal optical-resonator-based isolator introduced by L. Bi [39] (left subplot), transverse cross-sectional SEM image of the resonator ring covered with MO garnet layer (middle subplot), and operation principle for optical isolation. Maximum isolation ratio (19.2 dB), corresponding insertion loss and operation wavelength range are shown	6
1.5	Left: Schematic of a three-port Y-junction circulator. The straight arrows indicate the incoming and outgoing waves. The curved arrows represent the two counter-rotating modes in the resonator.	0
	Right: Transmission spectra at the output and isolated ports of a	_
	three-port junction circulator.	7
1.6	Schematic representation of the studied structure	11
2.1	Real part of elliptically polarized vector.	16
2.2	Basic magneto-optic configurations.	20
2.3	System of coordinates for planar structure	21
2.4	Wave propagation through a system of layers.	31
2.5	System of coordinates for 1D grating.	33
2.6	Differences between T-matrix and S-matrix algorithms	37
2.7	Separated <i>up</i> and <i>down</i> propagating modes in medium	37
2.8	Principle of Li-factorization is shown schematically.	41
2.9	Electric field trajectories for fully and partially polarized light	47
3.1	Dual-rotating compensator ellipsometer is shown schematically	50
3.2	Fit of $SiO_2$ layer on Si substrate, simulation of the finite spectral	
	bandwidth.	53
3.3	Fit of $SiO_2$ layer on Si substrate with with focused incident beam.	54
3.4	Fit of measured ellipsometric spectra of sGGG	56
3.5	Optical functions of sGGG.	57
3.6	Fit of measured ellipsometric spectra of Bi:GIG.	58
3.7	Optical functions of Bi:GIG layer.	59
3.8	Fit of ellipsometric spectra of reference Au	59
3.9	Optical functions of reference gold	60
3.10	Developed in-plane permanent magnet.	60
3.11	Hysteresis loop of Faraday effect of Bi:GIG.	61
3.12	Measured transverse difference Mueller matrix.	63
3.13	Measured longitudinal difference Mueller matrix.	64
3.14	Fitted spectral dependence of off-diagonal tensor component of BiGIG	65
3.15	Fabrication process of gold grating is shown schematically	67
3.16	Layout of fabricated samples with opening determined from SEM	68
3.17	Scanning electron microscopy of fabricated samples.	68

4.1	Coordinate system and schematic representation of the studied struc-	
	ture	72
4.2	Optical and magnetooptical response of the grating structure	74
4.3	Field plots of grating resonances.	76
4.4	Dispersion diagram of optical and magnetooptical response	77
4.5	Optical and magnetooptical response of the grating structure, fi-	
	nite thickness of Bi:GIG.	78
4.6	Field plots of grating resonances.	79
4.7	Field plots of grating resonances.	80
4.8	Single interface model for derivation of the dispersion relation of	
1.0	the surface plasmon resonance.	82
49	Symmetrical gold /air/gold waveguide is shown schematically	83
4 10	Model of the gold /air/gold waveguide	84
4 11	Effective index of guided mode in gold/air/gold at $\lambda = 884$ nm	85
<u>4</u> 12	Simulated dispersion of the grating's reflection and MO effect for	00
<b>T</b> .12	various thickness	87
/ 13	Dispersion diagrams of the gratings for various thickness	88
1.15 1 11	Simulated dispersion of the grating's reflection and MO effect for	00
4.14	various period	۵n
1 15	Dispersion diagrams of the grating's reflection for various period	90 01
4.15	Simulated dispersion of the grating's reflection and MO effect for	91
4.10	various air gap	02
1 17	Dispersion of the grating's reflection for various sin can	93
4.17	Even by the provided medical strain of various air gap.	94
4.10	Field plots of coupled modes.	95
4.19	Layout of the structure for derivation of the magnetoplasmon dis-	07
4 00		96
4.20	Shift of SPP by TMOKE: comparison between the exact solution	
	from the Eq. (4.24) (circle dots) and the linear approximation model	
	Eq. (4.25) (dashed line) calculated at the photon energy lev. The	00
4 01	green line represents pure SPP mode.	98
4.21	IMOKE spectra for various grating thickness.	
4.22	IMOKE spectra for various grating air gap.	101
4.23	Layout of the structure of silicon waveguide with gold grating and	
	Bi:GIG.	102
4.24	Dispersion map of guiding indicator.	103
4.25	Field plot distributions of fundamental and first-order guided modes.	104
4.26	Field plot distributions calculated at the area of the modes interac-	
	tion.	105
4.27	Field plot distributions calculated at positions of expected leaky	
	modes.	105
4.28	Magneto-optic dispersion map of guiding indicator.	106

4.29	The Effective index of guided mode in silicon waveguide as a func-	
	tion of the grating period.	107
5.1	Cross-section of the grating structure.	111
5.2	Comparison between simple model with nominal parameters and	
	experimental data.	112
5.3	Cross-section of the grating structure.	113
5.4	Comparison between simple model and experimental data	114
5.5	Cross-section of the grating structure with surface roughness	115
5.6	Comparison between model with surface roughness and experi-	
	mental data.	116
5.7	Cross-section of the grating structure with surface roughness and	
	residual PMMA.	117
5.8	Comparison between model with surface roughness and residual	
	PMMA and experimental data.	118
5.9	Photography of fabricated samples with marked area of $x - y$ scan.	119
5.10	Comparison between calculated (left column) and measured (right	
	column) quantities $N, S, C$	121
5.11	The openings $r$ estimated by SEM and by global fitting procedure	
	are compared.	124
5.12	Ellipsometric quantity $N$ obtained by global fit procedure on 15	
	samples is compared with experimental data.	125
5.13	Comparison between calculated and measured relative reflectivity	
	$R_p/R_s$	127
5.14	Measured and calculated MO effect as a function of the wavelength	
	and the angle of incidence are compared.	127
5.15	Measured map of the relative reflectivity (left) and the MO effect	
	$\delta R_p/R_s$ for the angle of incidence from 20° to 60°	128
5.16	Relative reflectivity and MO effect measured at angles of incidence	
	of $20^{\circ}$ , $30^{\circ}$ , and $45^{\circ}$ .	129
5.17	Field component $H_x$ distribution calculated at the wavelength of	
	741 nm, 786 nm, and 886 nm ad the angle of incidence of $20^{\circ}$ , $30^{\circ}$ ,	100
<b>F</b> 10	and 45°, respectively.	129
5.18	Measured optical data are compared with calculations.	131
5.19	Detail of the IMOKE spectral dependence.	131
5.20	Irend of the MO peak shift measured on 15 samples.	132
5.21	Measured systematic change of the peak width, amplitude, and	
	a blue-shift of spectral position of the plasmon peak are in good	100
A 1	agreement with a numerical data (right subplot).	133
A.I	Cross-section of the grating structure with surface	139
A.2	Single spectrum parallelization.	140
A.3	Scalability of single spectra problem.	140

A.4	Multiple spectra parallelization	141
A.5	Scalability of spectral problem assuming beam divergence	142

## List of Tables

. X	κxv
	52
	54
	56
5	
	58
. 1	111
. 1	113
. 1	115
. 1	117
. 1	123
	. 1 . 1 . 1

### List of publications

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