Polymer waveguide grating sensors for composite airframe monitoring

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Counsellors: Dr. ir. Bram Van Hoe, Dr. ir. Jeroen Missinne

Master's dissertation submitted in order to obtain the academic degree of
Master of Science in de ingenieurswetenschappen: fotonica

Department of Electronics and Information Systems
Chairman: Prof. dr. ir. Jan Van Campenhout
Faculty of Engineering and Architecture
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Preface

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Anton Vasiliev, June 2014

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Summary

Optical based sensors are a settled value and known for their ultra-small size, immunity to electromagnetic interference, sensitivity, cost and other properties making them the ideal candidates for a large variety of high-demanding sensing applications. Polymers are becoming an increasingly important material class among this type of sensors because they have a variety of advantages compared to their silica counterpart. They are much more cheaper, tougher, bio-compatible, more flexible, etc...

In this work several fabrication methods and materials were evaluated in order to fabricate planar polymer Bragg grating sensors. Two major techniques are investigated experimentally in-depth. The first one is based on a mechanical imprinting method where the pattern of a Si-master stamp is transferred to silicone and then subsequently to a low-loss optical material such as OrmoClad/EpoClad. The second method relies on the interference pattern formed from diffraction of a phase mask. Volume and surface dielectric gratings were fabricated in several materials such as epoxies, methacrylates and hybrid materials. A sensor was produced by transferring the grating formed in PMMA to EpoClad by means of a Reactive Ion Etching process and defining EpoCore single-mode waveguides on top. The produced grating features a Bragg reflection sensor signal of -31dB @ 1581 nm.

Keywords

Planar polymer Bragg grating sensor, phase mask, soft lithography, imprinting, refractive index modification, PMMA
Fabrication and characterisation of planar polymer waveguide grating sensors

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Abstract—Several fabrication methods and materials are evaluated in order to fabricate planar polymer Bragg grating sensors. Two major techniques are investigated experimentally in-depth. The first one is based on a mechanical imprinting method where the pattern of a Si-master stamp is transferred to a soft material such as PDMS and then subsequently to a low-loss optical material such as OrmoClad/EpoClad. The second method uses a UV-lamp and phase mask to produce a sinusoidal interference pattern of required period. Volume and surface dielectric gratings were fabricated in several materials such as epoxies EpoCore/Clad, methacrylates PMMA and hybrid materials OrmoCer. A sensor was produced by transferring the grating formed in PMMA to EpoClad by means of a Reactive Ion Etching process and defining EpoCore single-mode waveguides on top. The produced second order Bragg grating with period 1.01µm features a Bragg reflectivity of -31dB @ 1581 nm and FWHM of 90nm.

Keywords—Planar polymer Bragg grating sensor, phase mask, soft lithography, imprinting, refractive index modification, PMMA

I. INTRODUCTION

Optical based sensors are a settled value and known for their ultra-small size, immunity to electromagnetic interference, sensitivity, cost and other properties making them the ideal candidates for a large variety of high-demanding sensing applications. Polymers are becoming an increasingly important material class among this type of sensors because they have a variety of advantages compared to their silica counterpart. They are much more cheaper, tougher, bio-compatible, more flexible and have larger strain sensitivity.

This work pursues a planar polymeric Bragg grating sensor. The planar structure allows for ease of fabrication and a large variety of functionalities can be implemented on a single chip. Additionally, the planar structure can be easily implemented in-between composite slabs which facilitates assembly and does not degrade the structural properties of the composite. An envisioned application is to monitor the structural health a plane airframe. The Bragg grating sensors are ideal for such applications as they are lightweight, compact and robust. A Bragg structure consists of a waveguide in which a grating is integrated by a periodic refractive index modulation. Such a structure lets all the wavelengths pass except for the one matching the reflection condition \( \lambda = 2n_{eff}\Lambda \) where \( n_{eff} \) is the effective refractive index of the propagating mode and \( \Lambda \) is the grating period. The wavelength reflected by the sensor is called the Bragg wavelength and features a narrow dip in the transmission spectrum or a peak when measured in reflection. From this equation one can easily understand that changes in the period of the grating due to strain will result in a shift of the Bragg wavelength. This type of sensors has been widely used to measure temperature and deformations (strain) [1], [2]. By focusing on planar waveguides, multiple functionalities can be embedded on the same chip such as Arrayed Waveguide Gratings (AWG) [3].

II. OVERVIEW FABRICATION METHODS

There are numerous ways to produce a grating in a polymer. One of the most widely used techniques is to illuminate a photosensitive polymer such as PMMA to induce a refractive index change producing a volume grating. To achieve the required periodicity an interference pattern must be achieved. This can be done by splitting a UV-laser beam and letting them add up coherently on the sample. By varying the angle between the two beams, the interference pattern period can be adjusted to the required value. The laser source must have enough spatial coherence.

Another method is to use a phase mask with a periodic surface relief grating such that light passing perpendicular to it is diffracted into different orders. By suppressing all orders except the +1/-1 diffraction directions one achieves the same interference pattern as with a split uv-laser beam but now the angle between the orders is fixed and so the period that can be obtained is fixed. The advantage to this method is that a large area can be illuminated at once using a low coherence-source such as a Hg-lamp. The setup for fabrication is also less demanding in terms of beam alignment, polarization control, power distribution among beams.... The big disadvantage is that the period of the grating is fixed to one value and cannot be changed. It is this approach that was further investigated with a quartz Ibser phase mask with 1010 nm period.

Another method to produce the grating is to write the grating point-by-point using e-beam lithography in a photosensitive material such as PMMA. Biggest advantage here is that extremely high resolutions are possible (5nm lines [4]) and one can produce arbitrary grating periods. The disadvantage is that it requires a lot of time per sample and is very expensive.

It is also possible to use a femtosecond-laser to write gratings in 3D. By adjusting the focus distance it should be possible to modify the refractive index of some materials point-by-point in the whole volume. Direct laser inscription methods are also possible, where the surface is ablated with a fs-laser or an excimer laser. [5],[6], [7]

Other methods involves soft lithography techniques. All these methods involve a soft material such as Polydimethylsiloxane (PDMS) as an elastomeric stamp. When placed on a curable polymer such as EpoClad or OrmoClad the capillary force pushes the material into the grooves and is subsequently cured. The PDMS stamp has a low surface energy, meaning that it is easily peeled off the sample after curing. To produce the stamp several fabrication processes can be employed but the most common one involves e-beam lithograph on a Si-wafer which is then subsequently used as a stamp for the curable PDMS. Cured
PDMS has low adhesion to Si when cured and is easily peeled off. This approach was investigated in order to fabricate polymeric Bragg gratings. [8]

A. Soft Lithography gratings

A commercial master Si-stamp was used from LightSmyth. Two different stamps were investigated, a 500 nm period with 44% duty cycle and 350 nm depth and a 278nm period 50% DC, 110 nm deep. The periods correspond to an envisioned Bragg wavelength region of 1550 nm and 850 nm for the material systems OrmoCer and EpoClad/Core. To fabricate the PDMS stamp Sylgard184 liquid PDMS was mixed with the curing agent and poured on top of the master grating which was glued on a glass substrate. The reason for this is that it was proven to be hard to remove cured PDMS if it attached to the backside of the master stamp without damaging it. A small ridge structure was put around the stamp to prevent spilling and spreading of the PDMS. The sample is put in a vacuum chamber until all the bubbles have left sample. The sample is then cured over weekend in the oven at 60 °C. Different temperatures could be used to tune the shrinking of the PDMS stamp [9], this way the period could be varied. After peeling off the PDMS layer, a residual layer is visible on the Si-stamp. It is not clear if this affects the grating transfer, but some papers suggest the use of a thin protective layer to be coated on the Si master stamp. [10] The transferred patterns are far from ideal. The period is correctly reproduced but the transfer is non-conformal and very shallow as was observed with the SEM, Figure 1. There are also defects present in the lines. The major problem with this printing method is that when the PDMS stamp is further used for imprinting on spincoated photospolymers such as EpoClad or OrmoClad the stamp soaks up the solvent material, leaving a ridge after UV-curing. This ridge will pose a problem in the path of the future waveguides. Figure 2.

![Fig. 1: SEM picture of transferred grating to S186 PDMS silicone. The period is accurately reproduced, but the grating is shallow and non-uniform.](image1)

Fig. 2: Tencor stylus depth measurement of the formed ridge due to soaking of the solvent into the PDMS after release on the EpoClad sample. The grating is formed on the right side of the figure.

A 5 μm cladding would block the light for hundreds of micrometers. It was not possible to get rid of this unwanted effect. Spin coating thinner layers reduced the soaking but was still not ideal. This is why the phase mask approach was pursued in forming a Bragg grating sensor. To improve the pattern quality it is suggested in ?? to use composite hPDMS which is stiffer making a higher aspect-ratio possible.

B. Phase Mask

The formed surface relief grating in PMMA was fabricated by spincoating a 2 μm MicroChem PMMA A1 950 layer on glass and exposing through the phase mask in direct hard contact with the substrate. The exposure parameters are: 365nm UV-light @ 70mW/cm² for 9min. Then the sample is developed in a solution of (7:3) IPA:H₂O for 10s. This developer-system was chosen due to its optimal parameters as explained in [12], [4]. The interference of the higher order diffraction of the phase mask leads to doubling of the desired period : 1 μm. This can be resolved by using a more coherent source and putting the sample at an optimal distance away from the phase mask. [14] Notice the clear grating formed in the PMMA layer using the phase mask, Figure 3.

![Fig. 3: SEM picture of developed grating by phase mask illumination of a spincoated PMMA sample on glass](image2)
III. PLANAR BRAGG SENSOR

A hard-baked EpoClad sample was prepared using the steps as provided by the manufacturer MicroResist GmbH. Next a 2 μm MicroChem PMMA A1 950 layer is spincoated and exposed through the phase mask. The parameters had to be reoptimized for PMMA layer on top of EpoClad and are: 20 min UV exposure and 35s development time. The grating pattern in PMMA was transferred with Reactive Ion Etching to EpoClad with the following parameters: 5scm:15scm (CHF3:O2, 150mTorr, 150W, 6 min). These parameters were not ideal, as the grating had become worse, further optimization is required. Waveguides with the dimensions 5x[5,8,10,15,20] μm² were produced by lithographic means in EpoCore using a Direct Laser Imaging equipment from Heidelberg 66fs+. An upper EpoClad layer was applied. A protective glass layer was glued on top of the structure using NOA86H adhesive. This was necessary to avoid delamination and facet damaging when the samples are diced. This step was proven to be crucial to achieve optically flat end-facets and prevent delamination of the polymer layers.[13] The minimum achieved insertion loss of the Bragg sensor is -5.7dB @ 635 nm and -7.2dB @ 1554nm. The reflection spectra were measured with an Optical Spectrum Analyzer Agilent 86142B.

Bragg reflection signals were observed for different waveguides in the wavelength region of 1580-1584nm. The highest Bragg reflectivity that was achieved is -30.8dB @ 1583.44nm with a FWHM of 90pm for a single-mode 5x8μm² waveguide. The observed peaks come in pairs, this is due to the two orthogonal polarization modes with a slightly different effective index.

Two major methods to fabricate planar polymer bragg grating sensors were evaluated. The soft lithography technique poses some technological issues that need to be resolved. The phase mask method allows for the fabrication of single-mode bragg grating sensors with a reflectance of ~30dB. Further optimization of the RIE transfer parameters is believed to greatly improve the sensor. A surface relief grating in PMMA was produced with an amplitude > 200nm.

V. CONCLUSION

The Rigorous Coupled-Wave Theory was implemented in Matlab and extended to include multiple layered structures to link the diffraction measurements to the formed sine grating amplitude. The simulation were compared for a sample, measured with the Atomic Force Microscope to good agreement. This allows to quickly estimate the quality of the formed grating by performing a simple measurement.

REFERENCES

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Abstract— Verschillende methodes en materialen werden onderzocht voor het fabriceren van planaire polymere Bragg golfgeleidersensoren. Twee grote technieken zijn in meer detail onderzocht geweest. De eerste is een mechanische imprint methode waarbij een master Silicium patroon is overgezet in een zacht PDMS materiaal. Vervolgens wordt het overgezet naar een optische materialen systeem met lage optische verliezen zoals OrmoClad/EpoClad. De twee methode steunt op het diffractie patroon van een fasemasker, belicht met UV. Een interferentiepatroon is geproduceerd van het gewenst periode. Volume en oppervlakte periodieke structuren werden geproduceerd in epoxy-gebaseerde materialen, methacrylaten en hybride materialen zoals OrmoCer. Een sensor werd geproduceerd door de periodieke structuur of ‘grating’ over te zetten van PMMA door middel van Reactive Ion Etching naar de EpoClad ‘cladding’. Enkelvoudige-mode golfgeleiders worden gemaakt bovenop de actieve grating. Een tweede orde Bragg-reflectie gratings was geproduceerd met een periode van 1.01µm een reflectiviteit van -31dB @ 1581nm en FWHM van 90pm.

Keywords— Planaire polymeer Bragg reflectie sensoren, fasemasker, zachte lithographie, imprinting, brekingsindex modificatie, PMMA

I. INTRODUCTIE


In dit werk wordt een planaire polymeer golfgeleider Bragg sensor beoogd. De planaire structuur laat toe om deze sensoren gemakkelijker te implementeren in een composiet lagenstructuur. Veel verscheidene functionaliteiten kunnen op dezelfde chip dan verwezenlijkt worden. De structurele integriteit van de composietlagen wordt niet beïnvloed. Een beoogde applicatie is het monitoren van de rek van de mechanische componenten van een luchtdoorgang. De Bragg grating structuur is ideaal voor zulke applicaties omdat ze vederlicht, compact en robuust zijn. De structuur bestaat uit een golfgeleider waarin een periodieke structuur is verwezenlijkt door middel van brekingsmodificatie. Deze structuur laat ideaal alle golfglenstrengs door behalve degene die voldoen aan de reflectie Bragg-conditie: \( \lambda = 2n_{eff} \Lambda \) waar \( n_{eff} \) is de effectieve brekingsindex van de propagerende mode en \( \Lambda \) is de grating periode. De golfglenstrengs die gereflecteerd wordt door de sensor wordt de Bragg golfglenstreng genoemd. Het spectrum heeft een dip in transmissie en een reflectiepiek. Uit de Bragg conditie is het duidelijk dat rek van de structuur veroorzaakt een shift in de geobserveerde golfglenstrengs. Dit type van sensoren is wijd in gebruik voor het meten van rek en temperatuur[1], [2]. Door te focussen op planaire sensoren, meerdere functionaliteiten kunnen op dezelfde chip verwezenlijkt worden, zoals een ‘Arrayed Waveguide Gratings’ demultiplexer. (AWG) [3].

II. OVERZICHT FABRICATIE METHODES

Er zijn meerdere manieren om de periodieke structuur te produceren. Een van de meest gebruikte is het belichten van een fotosensitief polymeer zoals PMMA om een brekingsindexmodificatie te verwezenlijken. Op die manier bekomt men een volume-grating. Om het gewenst periode \( \Lambda \) vast te leggen, moet er een interferentiepatroon gecreëerd worden. Dit kan door een UV-laser straal te splitsen en terug te laten samenkomen op het sample onder een hoek. Door deze hoek te veranderen, kan de periode getuned worden. De laserbron moet een voldoende hoge spatiale coherente hebben.

Een andere methodes is om een fasemasker te gebruiken met een periodieke structuur in zich waardoor het fasefront van het licht gediffracteerd wordt in verschillende richtingen. Door het fase-masker loodrecht te belichten en ervoor te zorgen dat het design van het fasemasker zodanig is dat er enkel 2 symmetrische stralen gediffracteerd worden, kan men een interferentie-patroon vormen. Dit is dan gelijkaardig aan het geval waarbij een uv-laser gebruikt wordt. Maar nu ligt de periode vast door het design van het masker en kan niet meer veranderd worden. Het voordeel van deze methode is dat een groot oppervlak kan belicht worden tegelijk met een laag-coherente bron zoals een kwik-lamp. Het setup is ook minder moeilijk dan wanneer zelf-interferentie schema gebruikt wordt. Een quartz fasemasker was gebruikt met een periode van 1010nm van Ibsen.

Een andere methodes om de grating te produceren is door middel van e-beam lithographie in een fotosensitief materiaal als PMMA. Grootste nadeel hier is de hoge kost en de tijd nodig om een sample te verwerken. Extreem hoge resolutie kan verwezenlijkt worden: 5nm lijntjes [4]) en de vorm van de periodieke structuur mag arbitrair zijn.

Het is ook mogelijk een femtoconde-laser te gebruiken om roosters te schrijven in 3D . Door de brandpuntsafstand te veranderen kan het mogelijk zijn om een grating te produceren. Dit is door middel van e-beam lithographie in een fotosensitief materiaal als PMMA. Grootste nadeel hier is de hoge kost en de tijd nodig om een sample te verwerken. Extreem hoge resolutie kan verwezenlijkt worden: 5nm lijntjes en de vorm van de periodieke structuur mag arbitrair zijn.
gepast, maar de meest gebruikelijke zijn e-beam lithografie op een Si-wafer die vervolgens wordt gebruikt als een stempel voor de uithardbare PDMS. Uitgeharde PDMS heeft een lage hechting aan Si en is gemakkelijk af te pellen. Deze aanpak werd onderzocht om polymere Braggroosters fabriceren. [8]

A. Zachte lithographie roosters

Een commerciële master Si-stempel werd gebruikt van LightSmyth. Twee verschillende stempels werden onderzocht, een 500 nm periode met 44% duty cycle en 350 nm diepte en een 278 nm periode van 50% DC , 110 nm diep. De perioden komen overeen met een beoogde Bragg-golflengtegebied van 1550 nm en 850 nm voor de materiaal-systemen ORMOCER en EpoClad/Core. Om de PDMS-stempel te fabriceren wordt er Sylgard 184 vloeibaar PDMS gemengd met een curing agens en vervolgens gegoten op de top van de master-stempel die gelijmd werd op een glazen substraat. De reden hiervoor is dat het moeilijk gebleken was om uitgehard PDMS te verwijderen zonder Si te beschadigen indien er contaminatie was aan de achterzijde van de master stempel. Een kleine nok-structuur werd gezet rond de stempel om te voorkomen dat PDMS zich verspreid tot onderaan het monster. Het monster wordt in een vacumkamer geplaatst tot dat alle bellen het monster hebben verlaten. Het monster wordt vervolgens uitgehard gedurende een weekend in de oven op 60 °C. Verschillende temperaturen kunnen worden gebruikt om het krimpen van de PDMS stempel te controleren [9], op deze manier kan de periode worden gevarieerd. Na het afpellen van de PDMS-laag, is er een resterende laag achtergebleven op het Si master-stempel. [10] De overgedragen patronen zijn verre van ideaal. De periode wordt correct weergegeven maar de overdracht is niet-conform en zeer ondiep als werd waargenomen met de SEM, figuur 1. Er zijn ook defecten zichtbaar. Het grootste probleem met deze imprint methode is dat wanneer de PDMS stempel verder wordt gebruikt voor het stampen van spincoating fotopolymeren zoals EpoClad of OrmoClad, de stempel het oplosmiddel-materiaal absorbeert, waardoor de oppervlakte vervormd achterblijft na UV-uitdaging. Dit vormt een probleem voor als men golfgeleiders er zou op plaatsen. Figure 2.

Een 5 µm obstakel zou het licht voor honderden micrometers blokkeren. Het was niet mogelijk om dit ongewenst effect te omzeilen. Het Spincoaten van dunnere lagen vermindert het zuieffect maar was nog steeds niet ideaal. Daarom is de methode met het fasemasker verder uitgepluist.

B. FaceMasker

De gevormde oppervlak-relief grating in PMMA werd vervaardigd door het spincoaten van een 2 µm MicroChem PMMA A1 950 laag en dan bloot te stellen via fasemasker aan UV licht. Er moet direct contact zijn met van het masker met de harde substraat. De blootstelling parameters zijn: 365nm UV-licht @ 70mW/cm² voor 9min. Vervolgens wordt het monster ontwikkeld in een oplossing van (7:3) IPA: H₂O voor 10s. De optimale ontwikkel-paramaters zijn beschreven in [12], [4]. De ingemenging van de hogere diffractie-ordes van de fase masker leidt tot een verdubbeling van de gewenste periode: 1 µm. Dit kan worden opgelost worden door een meer coherente bron te gebruiken en het monster op een optimale afstand van het fasemasker te plaatsen. [?] De grating is veel beter gevormd dan met de zachte imprint methodes. Figure 3.
III. PLANÆRE BRAGG SENSOR

Een hard-gebakken EpoClad monster werd bereid met behulp van de stappen zoals die door de fabrikant MicroResist GmbH beschreven zijn. Vervolgens werd er een 2 µm MicroChem PMMA A1 950 laag gespincoat en bloeotgesteld aan de fase masker. De optimale parameters zijn anders voor PMMA bovenop EpoClad en zijn gelijk aan: 20 minuten UV-bloeotstelling en 35s ontwikkeltijd. De grating in PMMA wordt overgezet in EpoClad met Reactive Ion Etching met de volgende parameters: 5sccm :15sccm (CHF₃ O₂, 150mTorr, 150W, 6 min.) Deze parameters bleken niet ideaal te zijn en kunnen nog verbeterd worden. Golfgeleiders met de afmetingen 5x [5,8,10,15,20] µm² werden geproduceerd door lithografische middelen in EpoCore met behulp van een Direct Laser Imaging apparatuur van Heidelberg 66fs +. Een bovenste EpoClad laag werd aangebracht. Een beschermende glaslaag is gelijmd op de top van de structuur met behulp van NOA86H lijm. Dit was nodig om delaminatie en facet-beschadiging te voorkomen bij het dienen. Deze stap bleek cruciaal te zijn om optisch vlakke uiteinde-facetten te bekomen en delaminatie van de polymeer lagen te voorkomen. [?] De minimum bereikte verliezen van de Bragg sensor waren -5.7dB @ 635nm en -7.2dB @ 1554nm. De reflectie spectra werden gemeten met een Optical Spectrum Analyser Agilent 86142B. Bragg reflectie signalen werden waargenomen voor verschillende golfgeleiders in het golflengtegebied van 1580 - 1584nm. De hoogste Bragg reflectie dat werd benoemen voor verschillende golfgeleiders in het golflengtegebied van 1580 - 1584nm. De hoogste Bragg reflectie dat werd bereikt is -30.8dB @ 1583.44nm met een FWHM van 90pm voor een single-mode 5x8 µm² golfgeleider. De waargenomen pieken komen in paren voor, dit komt door de twee orthogonale polarisatie modi met een iets andere effectieve brekingsindex.

IV. DIFFRACTIE EFFICIETIE SIMULATIE

De Rigorous Coupled-Wave-theorie werd in Matlab gementeerd en uitgebreid naar gelaagde structuren om de diffractie metingen te koppelen aan de gevormde grating amplitude. De simulaties werden vergeleken voor een monster gemeten met de Atomic Force Microscope. Met deze methode kan men snel de kwaliteit van de gevormde grating schatten door het uitvoeren van een eenvoudige meting.

Fig. 4: Bragg reflectiviteit in dB. OSA parameters: sensitivity -82.34dBm, resolution bandwidth 0.06nm, averaging 20 sweeps

PMMA-op-glas simulatie vergeleken met de AFM meting (d=210 nm). X duidt het gemeten diffractierendement aan.

V. CONCLUSIES


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based sensors are a settled value and known for their ultra-small size, immunity to electromagnetic interference, sensitivity, cost and other properties making them the ideal candidates for a large variety of high-demanding sensing applications. Polymers are becoming an increasingly important material class among this type of sensors because they have a variety of advantages compared to their silica counterpart. They are much more cheaper, tougher, bio-compatible, more flexible and have larger strain sensitivity.

This work pursues a planar polymeric Bragg grating sensor. The planar structure allows for ease of fabrication and a large variety of functionalities can be implemented on a single chip. Additionally, the planar structure can be easily implemented in-between composite slabs which facilitates assembly and does not degrade the structural properties of the composite. An envisioned application is to monitor the structural health a plane airframe. The Bragg grating sensors are ideal for such applications as they are lightweight, compact and robust.

A Bragg structure consists of a waveguide in which a grating is integrated by a periodic refractive index modulation. Such a structure lets all the wavelengths pass except for the one matching the reflection condition \( \lambda = 2n_{eff}\Lambda \) where \( n_{eff} \) is the effective refractive index of the propagating mode and \( \Lambda \) is the grating period. The wavelength reflected by the sensor is called the Bragg wavelength and features a narrow dip in the transmission spectrum or a peak when measured in reflection. From this equation one can easily understand that changes in the period of the grating due to strain will result in a shift of the Bragg wavelength. This type of sensors has been widely used to measure temperature and deformations (strain) [1], [2]. By focusing on planar waveguides, multiple functionalities can be embedded on the same chip such as Arrayed Waveguide Gratings (AWG) [3].

1.1 Overview fabrication methods

There are numerous ways to produce a grating in a polymer. One of the most widely used techniques is to illuminate a photosensitive polymer such as PMMA to induce a refractive index change producing a volume grating. To achieve the required periodicity an interference pattern must be achieved. This can be done by splitting a UV-laser beam and letting them add up coherently on the sample. By varying the angle between the two beams, the interference pattern period can be adjusted to the required value. The laser source must have enough spatial coherence.

Another method is to use a phase mask with a periodic surface relief grating such that light passing perpendicular to it is diffracted into different orders. By suppressing all orders except the +1/-1 diffraction directions one achieves the same interference pattern as with a
split uv-laser beam but now the angle between the orders is fixed and so the period that can be obtained is fixed. The advantage to this method is that a large area can be illuminated at once using a low coherence-source such as a Hg-lamp. The setup for fabrication is also less demanding in terms of beam alignment, polarization control, power distribution among beams,... The big disadvantage is that the period of the grating is fixed to one value and cannot be changed. It is this approach that was further investigated with a quartz Ibsen phase mask with 1010 nm period.

Another method to produce the grating is to write the grating point-by-point using e-beam lithography in a photosensitive material such as PMMA. Biggest advantage here is that extremely high resolutions are possible (5nm lines [4]) and one can produce arbitrary grating periods. The disadvantage is that it requires a lot of time per sample and is very expensive.

It is also possible to use a femtosecond-laser to write gratings in 3D. By adjusting the focus distance it should be possible to modify the refractive index of some materials point-by-point in the whole volume. Direct laser inscription methods are also possible, where the surface is ablated with a fs-laser or a excimer laser. [5],[6], [7]

Other methods involve soft lithography techniques. All these methods involve a soft material such as Polydimethylsiloxane (PDMS) as an elastomeric stamp. When placed on a curable polymer such as EpoClad or OrmoClad the capillary force pushes the material into the grooves and is subsequently cured. The PDMS stamp has a low surface energy, meaning that it is easily peeled off the sample after curing. To produce the stamp several fabrication processes can be employed but the most common one involves e-beam lithograph on a Si-wafer which is then subsequently used as a stamp for the curable PDMS. Cured PDMS has low adhesion to Si when cured and is easily peeled off. This approach was investigated in order to fabricate polymeric Bragg gratings. [8]

1.1.1 Soft Lithography gratings

A commercial master Si-stamp was used from LightSmyth. Two different stamps were investigated, a 500 nm period with 44% duty cycle and 350 nm depth and a 278nm period 50% DC, 110 nm deep. The periods correspond to an envisioned Bragg wavelength region of 1550 nm and 850 nm for the material systems OrmoCer and EpoClad/Core. To fabricate the PDMS stamp Sylgard184 liquid PDMS was mixed with the curing agent and poured on top of the master grating which was glued on a glass substrate. The reason for this is that it was proven to be hard to remove cured PDMS if it attached to the backside of the master stamp without damaging it. A small ridge structure was put around the stamp to prevent spilling and spreading of the PDMS. The sample is put in a vacuum chamber until all the bubbles have left sample. The sample is then cured over weekend in the oven at 60 ° C. Different temperatures could be used to tune the shrinking of the PDMS stamp [9], this way the period could be varied. After peeling off the PDMS layer, a residual layer is visible on the Si-stamp. It is not clear if this affects the grating transfer, but some papers suggest the use of a thin protective layer to be coated on the Si master stamp. [10] The transferred patterns are far from ideal. The period is correctly reproduced but the transfer is non-conformal and very shallow as was observed with the SEM, Figure 1.1. There are also defects present in the lines. The major problem with this imprinting method is that when the PDMS stamp is further used for imprinting on spincoated photopolymers such as EpoClad or OrmoClad the stamp soaks up the solvent material, leaving a ridge after UV-curing. This ridge will pose a problem in the path of the future waveguides. Figure 1.2.
Figure 1.1: SEM picture of transferred grating to S186 PDMS silicone. The period is accurately reproduced, but the grating is shallow and non-uniform.

Figure 1.2: Tencor stylus depth measurement of the formed ridge due to soaking of the solvent into the PDMS after release on the EpoClad sample. The grating is formed on the right side of the figure.

A 5 μm cladding would block the light for hundreds of micrometers. It was not possible to get rid of this unwanted effect. Spin coating thinner layers reduced the soaking but was still not ideal. This is why the phase mask approach was pursued in forming a Bragg grating sensor. To improve the pattern quality it is suggested in ?? to use composite hPDMS which is stiffer making a higher aspect-ratio possible.

1.1.2 AFM measurements
Figure 1.3: Ridge forming in different samples due to the soaking of EpoClad by PDMS stamps. Measured using the Tencor-stylus.
Figure 1.4: Atomic Force Microscope measurement of gold coated PMMA grating sample.
Chapter 2

Simulations

2.1 Diffraction efficiency

In order to directly assess the formed gratings, a simple setup was built which measures the diffraction efficiencies as described in ???. The gratings fabricated with the phase mask are proven to have a period of $\approx 1\mu m$. The depth measurement tools at our disposal such as the (TENCOR-stylus and WYKO-interferometer) at the time of writing are incapable of measuring small depth variation of such periods. Some samples were measured with an Atomic Force Microscope at TU/e 1.1.2. The idea is to link the relatively easy diffraction efficiency measurements to the formed grating depth. This provides a fast way to examine the formed grating in a quantitative way without the time-consuming AFM-measurements. The estimated grating depths are further used as input for the FDTD-simulations of the Bragg structure in Lumerical.

The intuition that the diffraction efficiency depends strongly on the grating depth and profile is confirmed by the Rigorous Coupled-Wave Theory.[16]

2.1.1 Rigorous Coupled-Wave Analysis

There are different methods to analyze the diffraction of light from a dielectric structure. Today, Finite Difference Time Domain numerical software such as Lumerical, are gaining increasing popularity because they are versatile and can be applied to almost any 2D/3D problem. The key disadvantage is that it requires a large amount of computational time for large structures, which is common for most modern approximate simulations. It is therefore interesting to consider exact methods to solve the grating diffraction problem. There are two prominent but similar approaches: the first one is the Modal Approach [17] and the second one is the Rigorous Coupled-Wave Analysis. The latter one was implemented in Matlab as it is more intuitive and has been extensively studied over the past years [16],[18],[19],[20],[21],[22].

This theory accurately describes the diffraction of a plane wave on an arbitrary dielectric surface grating without approximations. The key idea is to discretize the grating region into N thin slabs where the electromagnetic field is expanded into an infinite sum of coupled allowed modes. The coefficients of this expansion in each slab are determined by imposing the continuity conditions for the electric and magnetic field at each boundary. The first and last interface then provide respectively, the reflection and transmission coefficients of the semi-infinite structure. The analysis solves the Maxwell equations without approximations and is therefore called ’rigorous’. The number of terms $s$ retained in the expansion, together with the number of slabs N, determine the accuracy of the simulation.
Figure 2.1: Schematic representation of various parameters for the RCWA-simulation of diffraction-efficiency. The sign convention for the angles is denoted by the coloured plus and minus signs.

The analysis is performed in the plane of incidence where the space is subdivided into 3 regions as in figure 2.1. An incident TE-polarized plane wave (the electric field is along the y-axis) is incident on the lossless surface grating. Region I is the incident semi-halfspace with dielectric constant $\epsilon_1$, region II contains the arbitrary dielectric surface grating with period $\Lambda$ and region III is the output semi-halfspace with $\epsilon_2$. The grating region is divided into $N$ planar grating slabs perpendicular to the $\hat{z}$-axis. The permittivity in each slab $n$ is then expanded in a Fourier-series as

$$\epsilon_n = \epsilon_1 + (\epsilon_2 - \epsilon_1) \sum_{h=-\infty}^{\infty} \tilde{\epsilon}_{h,n} \exp(jhKx)$$ (2.1)

$$\tilde{\epsilon}_{h,n} = \frac{1}{\Lambda} \int_{0}^{\Lambda} f_n(x, z) \exp(-jhKx) dx$$ (2.2)

where $f_n(x, z)$ is equal to 1 for the portion of the grating inside material with $\epsilon_2$ and equal to 0 inside material $\epsilon_1$. $K = \frac{2\pi}{\Lambda} \hat{x}$ is the grating periodicity vector with magnitude $K$. The total
electric field in each region can be written as:

\[ E_1(r) = \exp(-j k_1 \cdot r) + \sum_{i=-\infty}^{\infty} R_i \exp(-j k_{1i} \cdot r) \] (2.3)

\[ E_{2,n}(r) = \sum_{i=-\infty}^{\infty} S_{i,n}(z) \exp(-j \sigma_{i,n} \cdot r) \] (2.4)

\[ E_3(r) = \sum_{i=-\infty}^{\infty} T_i \exp(-j k_{3i} \cdot (r - d\hat{z})) \] (2.5)

where \( k_1 \) is the incident-field wave vector with magnitude \( k_1 = \frac{2\pi \epsilon_1^{1/2}}{\lambda} \) and \( \lambda \) is the free-space wavelength, \( k_{1i} \) and \( k_{3i} \) are the \( i \)-th order reflected and transmitted wave vectors and \( \sigma_{i,n} \) is \( i \)-th order wave vector in the \( n \)-th slab. \( R_i, T_i \) are the normalized amplitudes of the \( i \)-th reflected and transmitted wave in region I and III. \( S_{i,n}(z) \) is the normalized complex amplitude of the allowed \( i \)-th order plane wave solution in the \( n \)-th grating slab. Due to the Floquet-Bloch theorem [15] the wave vectors \( \sigma_{i,n} \) in each periodic slab must satisfy the following condition, these orders are therefore sometimes called the Floquet-Bloch modes.

\[ \sigma_{i,n} = \mathbf{k}_{2,n} + i \mathbf{K} \quad \forall i \in [-\infty, +\infty], \quad \forall n \in [1, \ldots, N] \] (2.6)

Where \( \mathbf{k}_{2,n} \) is the zero-order \((i = 0)\) wave vector with magnitude defined by the average refractive index in slab \( n \): \( k_{2,n} = \frac{2\pi}{h_{0,n}/\lambda} \).

Due to continuity conditions, each diffracted \( i \)-th order must be phase matched at all boundaries. This implies that the \( x \)-components of the \( k \)-vectors satisfy:

\[ k_{1i} \cdot \mathbf{x} = k_{3i} \cdot \mathbf{x} = \sigma_{i,n} \cdot \mathbf{x} \] (2.7)

The \( k \)-vectors are then uniquely determined by calculating the \( z \)-component using the magnitude of the \( k \)-vector in each material:

\[ k_{1i} \cdot \mathbf{z} = [k_1^2 - (k_{1i} \cdot \mathbf{x})^2]^{1/2} \] (2.8)

\[ k_{3i} \cdot \mathbf{z} = [k_3^2 - (k_{3i} \cdot \mathbf{x})^2]^{1/2} \] (2.9)

The \( k \)-vectors in the grating region \( \sigma_{i,n} \) do not need to be fixed because the effective \( k \)-vector is yet to be determined and is concealed in the complex amplitude term \( S_{i,n}(z) \). A choice, though not explained, was made in [16]:

\[ \sigma_{i,n} \cdot \mathbf{z} = [k_{2,n}^2 - (k_1 \cdot \mathbf{x})^2]^{1/2} \] (2.10)

A different definition would of course not affect the end result. One must be vigilant to take the right complex square root when the right hand side of the previous equations is negative: for \( k_{1i} \cdot \mathbf{z} \) it has to be positive imaginary, so that the wave is evanescent in region I, for \( k_{3i} \cdot \mathbf{z} \) and \( \sigma_{i,n} \cdot \mathbf{z} \) one must take the negative imaginary root.

### Coupled wave equations

Next step is to determine the form of the complex amplitude mode terms \( S_{i,n}(z) \). In region II, the solution must satisfy the wave equation [15]

\[ \nabla^2 E_{2,n} + k_0^2 S_{2,n}(x, z) E_{2,n} = 0 \] (2.11)

\(^{1}\)The Electric field is expressed in the common phasor notation: \( E(r, t) = \Re\{E_{\text{phasor}} e^{j\omega t}\} \). Bold letters and symbols are vectors in \( \mathbb{C}^3 \).
Now by substituting the Fourier-series expansion of $\epsilon_n$ (eq. 2.1 and 2.4) a second-order differential equation is produced:

$$\frac{d^2S_{i,n}(z)}{dz^2} - 2j(\sigma_{i,n} \cdot z) \frac{dS_{i,n}(z)}{dz} + K^2i(m-i)S_{i,n}(z) + k^2(\epsilon_2 - \epsilon_1) \sum_{h=1}^{\infty} \tilde{\epsilon}_{h,n} S_{i-h,n}(z) + \tilde{\epsilon}_{h,n} S_{i+h,n}(z) = 0 \quad (2.12)$$

with $m$ defined as $2\Lambda c_1^1/2 sin\theta_{in}/\lambda$ and $\tilde{\epsilon}_{h,n} = \tilde{\epsilon}_{-h,n}$ because $f_n(x,z)$ is real. When $m$ is an integer this expresses a Bragg condition. The derivation of the above equation is straightforward and is not reproduced here. The most important feature from this equation is that each order $i$ is coupled to all other modes $i \pm h$ through the Fourier coefficients $\tilde{\epsilon}_{h,n}$. This infinite set of second-order equations can be transformed to the state-space representation of first order equations by defining the state variables $S$ as:

$$S_{1,i,n}(z) = S_{i,n}(z) \quad (2.13)$$

$$S_{2,i,n}(z) = \frac{dS_{i,n}(z)}{dz} \quad (2.14)$$

The state-space equation is then concisely written in matrix form $\dot{\mathbf{S}} = \mathbf{A}_n \mathbf{S}_n$ with coefficients determined by eq. 2.14 and 2.12. Note that these matrices are infinite in size. In practice, one truncates the matrices by considering only a limited amount of orders $s$. One takes $(s+1)/2$ orders symmetrically distributed around $i = 0$. For example for $s=5$:

$$i \in [-2, -1, 0, 1, 2]$$

For clarification, the form of the state-space system of equation for $n$-th slab $\dot{\mathbf{S}}_n = \mathbf{A}_n \mathbf{S}_n$ is given for $s=3$:

$$\begin{bmatrix}
\dot{S}_{1,-1,n} \\
\dot{S}_{1,0,n} \\
\dot{S}_{1,1,n} \\
\dot{S}_{2,-1,n} \\
\dot{S}_{2,0,n} \\
\dot{S}_{2,1,n}
\end{bmatrix} =
\begin{bmatrix}
a_n & b_n \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
-2j(\sigma_{-1,n} \cdot z) & 0 & 0 & 0 \\
0 & 0 & 0 & 2j(\sigma_{0,n} \cdot z) \\
0 & 0 & 0 & 0 \\
2j(\sigma_{1,n} \cdot z) & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{S}_{1,-1,n} \\
\mathbf{S}_{1,0,n} \\
\mathbf{S}_{1,1,n} \\
\mathbf{S}_{2,-1,n} \\
\mathbf{S}_{2,0,n} \\
\mathbf{S}_{2,1,n}
\end{bmatrix} \quad (2.15)$$

$$\mathbf{a}_n = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \mathbf{b}_n = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{d}_n = \begin{bmatrix} 2j(\sigma_{-1,n} \cdot z) & 0 & 0 \\ 0 & 2j(\sigma_{0,n} \cdot z) & 0 \\ 0 & 0 & 2j(\sigma_{1,n} \cdot z) \end{bmatrix}$$

$$\mathbf{c}_n = \begin{bmatrix}
-k^2(-1)(m - (-1)) & -k^2(\epsilon_3 - \epsilon_1)\tilde{\epsilon}_{1,n} & -k^2(\epsilon_3 - \epsilon_1)\tilde{\epsilon}_{2,n} \\
-k^2(\epsilon_3 - \epsilon_1)\tilde{\epsilon}_{1,n} & -k^2(0)(m - (0)) & -k^2(\epsilon_3 - \epsilon_1)\tilde{\epsilon}_{1,n} \\
-k^2(\epsilon_3 - \epsilon_1)\tilde{\epsilon}_{2,n} & -k^2(\epsilon_3 - \epsilon_1)\tilde{\epsilon}_{1,n} & -K^2(+1)(m - (+1))
\end{bmatrix} \quad (2.16)$$

The solution to $\dot{\mathbf{S}}_n = \mathbf{A}_n \mathbf{S}_n$ is of the following form [?]:

$$\mathbf{S}_n = \sum_{q=1}^{2s} C_{q,n} \mathbf{w}_{q,n} exp(\lambda_{q,n} z) \quad (2.17)$$

with $\mathbf{w}_{q,n}$ and $\lambda_{q,n}$ the eigenvectors and eigenvalues of the state-matrix $\mathbf{A}_n$. The enumeration is now such that the first $s$ components of $\mathbf{S}_n$ correspond to $S_{1,i,n}$ and components $[s+1,...,2s]$
correspond to \( S_{2,i,n} \). The eigenvalues/vectors are found using Matlab’s eigensolver.

Now that the \( z \)-dependence of the modes is found, one must impose continuity conditions on the electric and magnetic field to find the coefficients \( R_i, T_i, C_i, n \). For a grating subdivided into \( N \)-layers, there will be \( s + s + 2^N s = 2(N+1)s \) unknowns. The boundary continuity conditions produce \( 2s \) equations for each interface; one for the electric field and one for the magnetic, with \( N+1 \) interfaces, this totals up to \( 2(N+1)s \) as well. For TE-polarization the Electric field only has a component along the \( y \)-axis and thus the tangential E-field is given by eq. 2.5. The tangential magnetic field \( H_x \) follows directly from Maxwell’s equations and is given by \( H_x = -j/\omega \mu \frac{dE_y}{dz} \) [15]. Given eq.2.5 and 2.17 the boundary conditions for the first interface between region I and II at \( z=0 \) become:

\[
\begin{align*}
\delta_{i0} + R_i &= \sum_{q=1}^{2s} C_{q,1} w_{i,q,1} \\
\hat{j}|\mathbf{k}_i\cdot\mathbf{z}|(R_i - \delta_{i0}) &= \sum_{q=1}^{2s} C_{q,1} w_{i,q,1}(\lambda_{q,1} - \hat{j}(\sigma_{i,1} \cdot \mathbf{z}))
\end{align*}
\]  

(2.18)  

(2.19)

\( \forall i \in [1, s] \) and \( \delta_{i0} \) the Kronecker delta function. The top equations are for the E-field and bottom ones are for the magnetic field. At the interface between the \( n \)-th and \( n+1 \)-th slab the following equations are valid \( \forall i \in [1, s] \):

\[
\sum_{q=1}^{2s} C_{q,n} w_{i,q,n} \exp(\{\lambda_{q,n} - j(\sigma_{i,n} \cdot \mathbf{z})\} nd/N) = \sum_{q=1}^{2s} C_{q,n+1} w_{i,q,n+1} \exp(\{\lambda_{q,n+1} - j(\sigma_{i,n+1} \cdot \mathbf{z})\} nd/N)
\]

\[
\sum_{q=1}^{2s} C_{q,n} w_{i,q,n} \lambda_{q,n} - j(\sigma_{i,n} \cdot \mathbf{z}) \exp(\{\lambda_{q,n} - j(\sigma_{i,n} \cdot \mathbf{z})\} nd/N)
\]

\[
= \sum_{q=1}^{2s} C_{q,n+1} w_{i,q,n+1} \lambda_{q,n+1} - j(\sigma_{i,n+1} \cdot \mathbf{z}) \exp(\{\lambda_{q,n+1} - j(\sigma_{i,n+1} \cdot \mathbf{z})\} nd/N)
\]

And finally for the interface going from region II to III:

\[
\sum_{q=1}^{2s} C_{q,N} w_{i,q,N} \exp(\{\lambda_{q,N} - j(\sigma_{i,N} \cdot \mathbf{z})\} d) = T_i
\]

\[
\sum_{q=1}^{2s} C_{q,N} w_{i,q,N} \lambda_{q,N} - j(\sigma_{i,N} \cdot \mathbf{z}) \exp(\{\lambda_{q,N} - j(\sigma_{i,N} \cdot \mathbf{z})\} d) = -j(\mathbf{k}_{3,i} \cdot \mathbf{z})T_i
\]

This \( 2(N+1)s \times 2(N+1)s \) system of equations is then solved with the Gauss-elimination method using Matlab for the unknown coefficients \( R_i, T_i, S_{i,n} \forall i \in [1, s], \forall n \in [1, N] \). The diffraction efficiencies are the ratios of power densities diffracted to the \( i \)-th order compared to the input power density. The power density is given by taking the real part of the Poynting vector [15].

\[
\langle P(x) \rangle = \text{Re}(\mathbf{S}(x)) = \text{Re}(\mathbf{E} \times \mathbf{H}) = \text{Re}(n) \frac{|E|^2}{2\sqrt{\mu_0/\epsilon_0}}
\]

This power density is expressed per unit area perpendicular to the propagation direction, which equals to the wave vector direction for isotropic media. The wave vector directions are all different, so one has to express the power densities with respect to a common are. The

\[\text{In paper [16], there is a slight typing error for this equation: the absolute value signs on the left hand side.}\]
most logical choice is to project the Poynting vectors to the area parallel to the different slabs and layers. The diffraction efficiencies are then expressed as

\[ DE_{1i} = \text{Re}[\frac{(k_{1,i} \cdot z)}{(k_1 \cdot z)}]|R_i|^2 \]  

\[ DE_{3i} = \text{Re}[\frac{(k_{3,i} \cdot z)}{(k_1 \cdot z)}]|T_i|^2 \]  

with \( DE_{1i} \) the power reflection coefficients of the grating for the \( i \)-th order and \( DE_{3i} \) correspond to power transmission coefficients. For a lossless grating, the sum of all the diffraction coefficients should add up to unity. This is a rough measure to check whether the solution has converged or not. The difference from unity was typically on the order of \( 10^{-12} \). In practice however, it was proven necessary to check the behaviour of the solution for an increasing number of \( N \) and \( s \) and not to rely solely on this convergence parameter:

\[ \eta = \sum_i DE_{1i} + DE_{3i} - 1 \]

To facilitate the input of parameters and interpretation of the results this algorithm was also implemented as a GUI-script in Matlab. Appendix A

### 2.1.2 Validation of the algorithm

A GUI was programmed using Matlab and gives the user the possibility to easily change all the input parameters as can be seen from the screenshot in Figure 2.2

Figure 2.2: Screenshot of the RCWA GUI in Matlab. Input parameters can be changed and plotted on top of the previous ones. Different grating profiles can be evaluated and all the data (angles and diffraction efficiencies) can be exported to an Excel worksheet. Only the +1,0 and -1 diffraction orders are plotted.

The behaviour of the solution was investigated for an increasing number of terms \( s \) (=orders) of the truncated matrix such as in eq. 2.15 for a square (Figure 2.3) and sine profiles (Figure
For a square profile the number of layers $N$ is irrelevant, since the structure does not change in the $z$-direction.

The solution for a square grating profile quickly converges for an increasing number of modes $s$ regardless of the number of layers $N$, which is as expected. It is therefore important to include enough evanescent modes for the truncated matrix approach to be valid. More modes means that the Gaussian Elimination equation-solver has to deal with a much bigger, sparse matrix which is badly conditioned (very large and very small entries in the matrix at the same time). Even though the condition number gets very close to 0 ($10^{-250}$), Matlab still manages to solve the system of equations and the results converge to the same value as in Figure 2.3. The results from paper [16] differ slightly (<5%) from present work.

For example the maximum diffraction efficiency of a square grating (50% duty cycle) to the $+1$ transmission order was found at a relative grating depth of $d=1.53\Lambda$ and amounts to 90.53%, while in [16] this was found for $d=1.55\Lambda$ and is equal to 88.5%. These slight discrepancies in the results are probably due to the fact that computers were much less powerful back in the eighties to compute such large sparse matrices with sufficient numerical precision. In [16] it is stated that the number of Bloch modes is increased until the changes are less than a certain value, but as one can see in Figure 2.3a or 2.5c, a certain overshoot is present when increasing the number of Bloch modes. They mention that typically 8-12 modes were used, which correspond to the extrema in the Figures, but do not correspond to the convergent solution which is found for $s>20$.

Ultimately, the numerical double precision is insufficient for very large and/or badly scaled matrices. This occurs for very large number of Bloch modes $s$ or when the depth of the grating $d$ becomes large. The exponential propagation factors introduce numerical instability, because some terms become exponentially large and others very small. The computational limit was investigated for a square grating in Figure 2.4.
Figure 2.4: Diffraction efficiency simulation in function of the number of Bloch modes $s$ for a very deep square grating profile. Only the first few orders are plotted. The values converge for $s > 20$ but due to limited numerical precision results cannot be calculated for higher number of $s$. The parameters of the simulation are: $\theta_{in} = 30^\circ$, $\lambda = 1\mu m$, $\epsilon_1 = 1$, $\epsilon_2 = 2.5$, $d = 10\mu m$, $\Lambda = 1\mu m$.

For a sine grating profile the remarks are similar: one has to take enough Bloch modes for the solution to converge, but here one must also ensure that enough discrete levels $N$ are taken to approximate the sine profile. As a rough guideline one must take at least $N=50$ slabs and $s \geq 21$ as in Figure 2.5 is investigated. Some numerical anomalies may occur so it is advised to always look how the values change around a particular set of parameters in function of $N$ and $s$. 
A possibility was also implemented to analyze general blazed gratings, with the two angles $\alpha$ and $\beta$ defined as in Figure 2.1. The results also converge and the discussion is similar.

2.1.3 Analysis of the sine grating

Now the implementation has been validated, one can focus on examining the change in diffraction efficiencies in function of the grating depth. To mimic the setup, the following parameters were chosen:

$$\lambda = 632.8 \text{nm}, \epsilon_1 = 1, \epsilon_2 = 2.2201, \Lambda = 1.01 \mu m, \theta_{in} = 0^\circ, s = 41, N = 70$$

The dielectric constant for region II corresponds to the refractive index of 1.49 for PMMA $A11 \ @ \ 633\text{nm}$. The results in Figure 2.6 indicate that the diffraction efficiency to the first
order monotonically grows up to a certain depth where it reaches its maximum. This graph can be used to estimate the depth using the diffraction efficiency measurements.

![Graph](image1)

Figure 2.6: Diffraction efficiency simulation in function of the grating depth $d$ for a sine grating profile. The parameters of the simulation are: $\lambda = 632.8\text{nm}, \epsilon_1 = 1, \epsilon_2 = 2.2201, \Lambda = 1.01\mu\text{m}, \theta_{in} = 0^\circ, s = 41, N = 70$. For large depths one can see that there are more and more anomalies due to numerical round off errors, Figure ?? . The +1 and -1 transmission diffraction should be identical for perpendicular incidence, there are also appearances of peaks and irregularities. If one would increase the number of modes $s$ and number of slabs $s$, the convergence usually improves but is not required here as one is only interested in the shallow depth-region. An advanced numerical scheme is explained in [21] and [22] that improves the numerical stability of the RCWA-method. This is only useful when one is interested in simulating large grating depths $d > 4 \times \Lambda$.

![Graph](image2)

Figure 2.7: Diffraction efficiency simulation in function of the grating depth $d$ for a sine grating profile. The parameters of the simulation are: $\lambda = 632.8\text{nm}, \epsilon_1 = 1, \epsilon_2 = 2.2201, \Lambda = 1.01\mu\text{m}, \theta_{in} = 0^\circ, s = 41, N = 70$. Note that the analysis is not reliable anymore for larger depths due to numerical round-off errors.
2.1.4 Extension of the algorithm

To approximate the real structure more closely, one has to take into account the full layered structure as in 2.8, where PMMA grating is on top of an EpoCore cladding, and this is spincoated on borofloat glass.

To implement this, the boundary equations are slightly changed. We now have to rewrite the Electric field in region III (PMMA layer) and in the new regions IV(EpoClad), V(glass) and the semi-infinite region VI (air) without reflection back towards the interface.

\[
\begin{align*}
E_3(r) &= \sum_{i=-\infty}^{\infty} \exp[-jk_{3i,x}x](T_{3i}\exp[-jk_{3i,z}(z-d)] + R_{3i}\exp[+jk_{3i,z}(z-d-d_3)]) \\
E_4(r) &= \sum_{i=-\infty}^{\infty} \exp[-jk_{4i,x}x](T_{4i}\exp[-jk_{4i,z}(z-d-d_3)] + R_{4i}\exp[+jk_{4i,z}(z-d-d_3-d_4)]) \\
E_5(r) &= \sum_{i=-\infty}^{\infty} \exp[-jk_{5i,x}x](T_{5i}\exp[-jk_{5i,z}(z-d-d_3-d_4)] \\
&\quad + R_{5i}\exp[+jk_{5i,z}(z-d-d_3-d_4-d_5)]) \\
E_6(r) &= \sum_{i=-\infty}^{\infty} \exp[-jk_{6i,x}x](T_{6i}\exp[-jk_{6i,z}(z-d-d_3-d_4-d_5)])
\end{align*}
\]

where the k-vectors in each region are found in the same manner as in eq. 2.9. As in the previous case, one has to take the right imaginary root for the evanescent fields. Each new region now also features unknown amplitude reflection and transmission coefficients \(R_{ki}, T_{ki}\).
\[ \forall k \in [3, 4, 5], \forall i. \text{ The coefficients } T_{6i} \text{ and } R_i \text{ will determine the global reflectance and transmittance of the layer structure. In order to find these the boundary continuity equations have to be adapted accordingly. The interface for region II going to region III (z=d) now satisfies:} \]

\[
\sum_{q=1}^{2s} C_{q,N} w_{i,q,N} \exp(\lambda_{q,N} - j(\sigma_{i,N} \cdot z)) = T_{3i} + R_{3i} \exp(-j k_{3i,z} d_2) \\
\sum_{q=1}^{2s} C_{q,N} w_{i,q,N} \exp(\lambda_{q,N} - j(\sigma_{i,N} \cdot z)) = -j |k_{3i,z}|(T_{3i} - R_{3i} \exp(-j k_{3i,z} d_2))
\]

At the boundaries between region III and IV (z = d + d_3, p = 3), IV and V (z = d + d_3 + d_4, p = 4):

\[
\exp(-j k_{pi,z} d_p) T_{pi} + R_{pi} - T_{(p+1)i} - \exp(-j k_{(p+1)i,z} d_{p+1}) R_{(p+1)i} = 0 \\
|k_{pi,z}| \exp(-j k_{pi,z} d_p) T_{pi} - |k_{(p+1)i,z}| T_{(p+1)i} + |k_{(p+1)i,z}| \exp(-j k_{(p+1)i,z} d_{p+1}) R_{(p+1)i} = 0
\]

and at the last interface (z = d + d_3 + d_4 + d_5):

\[
\exp(-j k_{5i,z} d_5) T_{5i} + R_{5i} - T_{6i} = 0 \\
|k_{5i,z}| \exp(-j k_{5i,z} d_5) T_{5i} - |k_{6i,z}| R_{5i} - |k_{6i,z}| T_{6i}
\]

The boundary conditions for interfaces in region I and II are the same as before.

The key emerging feature of this extension to the algorithm is that now Fabry-Perot interference effects can be observed when varying the angle of incidence, Figure 2.9b. The peaks look irregular due to the relatively large step-size of 0.2 degrees. The diffraction efficiencies change slightly as compared to the simplified previous model, Figure 2.6b. The results are compared in Figure 2.9a where the following parameters were chosen for the different layers:

\[
\lambda = 632.8 \text{nm}, \epsilon_1 = 1, \Lambda = 1.01 \mu m, \theta_{in} = 0^\circ, s = 41, N = 70 \\
\epsilon_2 = 2.2201 \text{ (PMMA)}, d_3 = 1 \mu m, \epsilon_3 = 2.52953 \text{ (EpoClad)}, \\
d_4 = 20 \mu m, \epsilon_4 = 2.16031 \text{ (Borofloat glass)}, d_5 = 700 \mu m
\]

The values are chosen as to represent the actual diffraction measurements as closely as possible.
The diffraction efficiency measurements, together with the AFM results, are now compared to the simulations. Two samples were measured with the AFM, gold-coated PMMA on glass (PMMA2) and PMMA on EpoClad prior to RIE (RIE2). Results are presented in Figure 1.4.

The diffraction efficiencies of the PMMA-on-glass sample was measured before it was coated with gold for the SEM and is equal to

\[ T_{+1} = 65 \mu W/2.97 mW = 0.128, T_0 = 2.7 mW/2.97 mW = 0.663, R_{+1} = 38 \mu W/2.97 mW = 0.037 \]

and the AFM-depth is \( d \approx 210 \text{nm} \).
Figure 2.10: PMMA-on-glass simulation using the extended algorithm as a function of the grating depth to compare with the experimental measurements of the PMMA$_{2.2}$ sample measured with the AFM. The parameters are the same as in Figure 2.9 but without the EpoClad layer. The thin PMMA layer is $\approx 1\mu m$. The step-size is 10nm. X marks the measured diffraction efficiency of PMMA$_{2.2}$.

From the Matlab-simulations Figure 2.10 it follows that the measured diffraction efficiencies should all correspond with a depth of $\approx 260 nm$. This is a fairly good estimate, when with the actual AFM-result of 210nm, Figure 1.4a. The 50 nm deviation might be caused by the non-uniformity of the grating across the sample: some areas are deeper or shallower than others due to the non-conformal contact. When measuring the diffraction efficiency, the laser spot was moved around the sample and only the maximum value was noted.

The expected change in diffraction efficiency after the RIE is given in Figure 2.11. The simulation results can also be explained intuitively: PMMA ($n=1.49$) has a lower refractive index than EpoClad ($n=1.59$) @ 633nm, this means that the spatial refractive index modulation at the interface Air-Grating is now higher when the grating is in the epoxy and this results in a higher reflection $R_0$ and coupling to the diffracted orders $T_{+1}, T_{-1}$.

The measured diffraction efficiencies of the PMMA-on-EpoClad sample are equal to:

$T_{+1} = 0.022, T_0 = 0.909, R_{+1} = 0.013$ and the AFM-depth is $d \approx 20nm$

Note that this sample does not have the best diffraction efficiency that was achieved with PMMA on EpoClad, the exposure and development parameters were optimized for the next batch, containing the final design. From the Matlab-simulations Figure 2.11 $T_0$ then corresponds to $d \approx 70nm$, $T_{+1}$ to 130 nm and $R_{+1}$ cannot be identified with a valid point on the graph. It is not possible to say with confidence that the AFM-measurements match the simulation results. It could be that unfortunately only a bad area of the sample was measured with the AFM. The grating profile also looks very rough and does not have a nice sine-form as the previous one. The grating area is not completely uniform, due to non-conformal contact of the phase mask.
Figure 2.11: PMMA-on-EpoClad simulation using the extended algorithm as a function of the grating depth to compare with the experimental measurements of sample RIE2. The parameters for the dashed lines are the same as in Figure 2.9. The bold lines represent the same grating structure but now directly in EpoClad and without the PMMA layer, This would represent a perfect RIE-transfer of the grating to the cladding.

2.1.6 Phase mask simulation

According to the manufacturer, the nominal design of the phase mask is a square profile with \( d = 430 \text{nm} \) and duty cycle=40%. The mask is made of fused quartz which has a refractive index of 1.47454 @ 365nm. This can now be simulated with the RCWA-model in Matlab, Figure 2.12. The zeroth order is indeed suppressed up to 0.2072% for \( d = 420 \text{nm} \) and 40% duty cycle, as claimed by the manufacturer. However, the higher order terms are not negligible compared to the first order and they are the cause of the unwanted doubling of the grating period. For \( d=420\text{nm} \), the simulation yields:

\[
T_0 = 0.2072\%, T_{+1} = 38.72\%, T_{+2} = 4.673\%, T_{+3} = 2.23\%, T_{+4} = 1.73\%
\]
Figure 2.12: RCWA-simulation of the fused silica phase mask. The simulation parameters are: $\lambda = 365\text{ nm}$, $\epsilon_1 = 1.475^2$, $\epsilon_2 = 1$, $\Lambda = 1.01\mu\text{m}$, $\theta_{in} = 0^\circ$, $s = 51$, $N = 4$, Duty Cycle square grating = 40%. Zeroth order is suppressed for $d=420\text{nm}$.

2.2 Bragg reflectance

The grating depth estimated in the previous section can now be used to estimate the expected reflected spectrum of the Bragg grating sensor. For that purpose a widely used commercial FDTD-solver was used. The program also allows to calculated the mode profiles to determine if whether the waveguides will be single-mode or not.

2.2.1 Lumerical FDTD

The analysis is performed in 2D because the structure is symmetric and otherwise the computational time becomes very large for centimetre-size structures. One is interested in the order of magnitude of the reflectivity and the location of the Bragg peak. The grating structure is constructed with a simple script. The refractive index data as a function of wavelength for EpoCore and EpoClad were imported into Lumerical to make custom materials. This way, the program will automatically adjust the refractive index for different wavelengths.

A $5\times 5\ \mu\text{m}^2$ EpoCore-waveguide is single-mode\textsuperscript{3} at $1.55\ \mu\text{m}$. The mode profile and values can be seen in Figure 2.13a,2.14b and the source spectrum in 2.13b.

\textsuperscript{3}There are 2 orthogonal polarization modes which will experience a slightly different effective index.
Figure 2.13: 2D-simulation in Lumerical. The selected source mode is shown in (a), note that only the two first effective indices are above the cladding refractive index 1.5702. This indicates that the waveguide is single-mode @ 1.55 µm. The selected source spectrum is shown in (b). This spectrum is analogous to the experimentally used ASE-FL7002.

The simulated structure is a square grating profile of EpoClad in the EpoCore region with a total length of 1mm, note that the simulation time increases significantly. One has to take small mesh-cells, in order for the grating to be visible to the program. The step-size of the mesh must also be a multiple of half the grating period, otherwise the index profile is not correctly meshed. The simulation time has to be increased beyond 12000fs for the signal to come back to the reflection detector. The depth of the grating was chosen to be 200nm. The square profile should give similar results to a sine profile. The reflected power is shown in Figure 2.14a. The reflectivity is very weak, but is as expected for a low refractive index modulation of only $\Delta n = n_{\text{core}} - n_{\text{clad}} \times \Gamma = 1.5772 - 1.5700 \Gamma = 0.0072 \Gamma$. For a grating depth of 200nm the mode-overlap integral $\Gamma = 0.0186$ is found by integrating the real electric field of the mode, Figure 2.14b, over the grating height of 200nm and referenced to the total electric field. To compare with the simulation one can estimate the reflectance using the well-known low reflectivity approximation equation [15]:

$$R_{\text{max}} = \tanh^2 \left( \frac{2 \Delta n \Gamma L}{\lambda_B} \right) = \tanh^2 \left( \frac{2 \times 0.0072 \times 0.0186 \times 1 \text{mm}}{1.58 \mu\text{m}} \right) = 2.8\% = -15.5\text{dB}$$

(2.23)

which is much higher than the simulated values of -62dB. This large mismatch is strange.

The influence of the order of the grating was also investigated. A deeper grating profile of 2 µm ($\Gamma = 0.249$) was simulated for a sensor length of 50µm. For a first order grating ($\Lambda = 0.5\mu\text{m}$) a reflectivity of 2.55% (-16dB) was obtained which comes close the value if one calculates it using 2.23 (1.27%), second order ($\Lambda = 1\mu\text{m}$) -60dB, third order ($\Lambda = 1.5\mu\text{m}$) 0.3 % (25.2dB) and fourth order ($\Lambda = 2\mu\text{m}$) -55dB. It is strange that Lumerical calculates a much lower reflectance for the even orders (2,4,...)
as compared to the odd ones. Of course for orders $> 1$ there will always be extra scattering. For example, for the second order, light is allowed to scatter upwards, perpendicular to the waveguide. But for the third and higher orders, light can also scatter out of the structure into the cladding. This could be an issue inherent to the FDTD-algorithm or when simulating in 2D. Peak reflectance values from Figure 2.14a may therefore be erroneous and should not be trusted blindly. The Bragg-wavelength 1.581 $\mu m$ appears to be consistent for the different simulations and is used as a guideline for further experimental work.

2.2.2 Other simulation schemes

The FDTD-method proves to be not the ideal choice for simulating large Bragg-sensor structures. First of all, the structure is mostly z-invariant for which a modal propagation approach is much more efficient. Large 3D millimetre-size structures can not be simulated without the help of powerful supercomputers. The solution would be to use a coupled-wave approach where one finds the allowed modes in the structure and propagates them throughout the structure[15]. This type of approach is also commercially available in MODE-solution software. The rest of the work was focused towards the experimental fabrication and characterisation of a proof-of-principle Bragg sensor instead of performing simulations in the new software.

Figure 2.14: 2D-Bragg reflectance simulation in Lumerical for a 1mm and 2mm 2-nd order sensor ($\Lambda = 1\mu m$) for a 5$\mu m$ EpoCore-waveguide with a square EpoClad grating at the bottom with a depth of 200nm (a). The peak wavelength is found @ 1.581 $\mu m$. Since only one polarization mode was excited, only a single peak is observed. The mode profile is shown in (b), together with the position of the core (red).
Chapter 3

Bragg Sensor Fabrication

The fabrication of the sensor itself consists of several steps. The grating is realized with the parameters in mind as described in section ???. The different steps are schematically presented in Figure 3.1 and are described in more detail in Figure 3.2. The first batch of sensors, labeled $RIE1_1$, was made without the protective glass layer of step (h). The parameters that are different for the second and final batch of sensors $RIE3_3$ are denoted with an asteriks * and are greyed out.

3.1 Waveguide geometry

The dimensions of the waveguides for the Bragg sensors are best chosen as large as possible to facilitate coupling of light from and to a single-mode fibre but small enough to be single mode. Using Lumerical’s eigenmode solver, the largest dimensions for which the waveguide is still single-mode was found to be around 7x7,6x8,5x9 $\mu m^2$. Different waveguides were fabricated; 2 single-modes and 3 multimode : 5x(5, 8, 10, 15, 20) $\mu m^2$

To fabricate the waveguides, EpoClad-2 photoresist was spincoated on top of the plasma treated samples and then the common lithography steps were performed to pattern the core: pre-bake to evaporate the solvents, UV-exposure to activate the polymerisation followed by post-bake and development. The UV-exposure of the samples was performed mask-less using the Heidelberg DWL 66fs Laser Direct Imaging equipment. This equipment allows the user to expose the samples with a custom design: in this work these were simple lines spaced 100$\mu m$ apart having the mentioned widths.
Figure 3.1: Schematic representation of the steps in order to fabricate a polymer Bragg sensor in EpoClad/Core material system using a phase mask: processing of EpoClad undercladding (a), processing of PMMA photoresist layer (b), UV-exposure with the phase mask (c), develop PMMA in IPA: \( H_2O \) (d), RIE transfer of grating pattern to undercladding (e), lithographic patterning of EpoCore waveguides with LDI (f), processing of uppercladding (g), glueing of protective top-glass layer and dicing of the sample (h). The steps from Figure 3.1 are explained in detail in Figure 3.2.
Figure 3.2: Detailed description of the fabrication parameters of the EpoClad/Core Bragg sensor. The parameters that are different for the second and final batch of sensors RIE3 are denoted with an asterisk *.

### 3.1.1 Optical microscope characterisation

The produced waveguides were inspected using an optical microscope with the results presented in Figure 3.3. The lateral dimensions are very close to the set parameters. There are no visible defects to the waveguides along the full length of the design. When focussed just
below the waveguides in areas exposed to the phase-mask illumination, the grating lines are visible. The interface region where the grating stops does not seem to affect the waveguides. The vertical direction was measured with the WYKO-interferometer and is equal to 4.92\(\mu m\), which is also close to the set height of 5\(\mu m\). The lateral roughness is negligible. The side-wall roughness is unknown, but parallel work on EpoCore waveguides in CMST shows that the waveguides look very smooth. The samples are further processed by processing a 20\(\mu m\) upper cladding layer of EpoClad and dicing the samples.

![Waveguides' end-view](image1)

![Interface for 5x5 \(\mu m^2\) waveguide](image2)

![Focused on grating, \(\Lambda = 1.02\mu m\)](image3)

![Focused on the waveguide 5 \(\mu m\) higher](image4)

Figure 3.3: Optical microscope picture of EpoCore-waveguides lithographically fabricated on EpoClad using LDI. The waveguides are without visible defect throughout the full length of the sample (not shown), at the end of the sample (a) and at the interface of the grating region (b). The transferred gratings with 1\(\mu m\) period are visible in EpoClad after RIE with EpoCore waveguides patterned on top. (c) and (d)

### 3.2 Sensor characterisation

The diced samples can now be optically characterised by coupling light into the waveguides and observing the reflected and transmitted spectra.
3.2.1 Setup

A motorized-stage was used with submicron precision to control the X,Y and -Z positions of the input and output fibre. A schematic of the setup and picture of light coupling into a sensor are shown in Figure 3.4. The laser-diode sources in the visible and infrared are used together with the detector and power meter to determine the losses. The alignment of the input fibre to the sensor is achieved in two steps. First, the scattering of 635nm light is monitored along the sample by using a microscope camera. When the light couples into the waveguide, scattering is strongly visible only inside the waveguide as in Figure 3.4b. The coupling is then optimized further by measuring the transmitted power with a detector and adjusting the stage until a maximum is achieved. This alignment is easiest for the largest waveguide $5 \times 20\mu m$ and once coupled it can be shifted laterally by the exact distance of $100\mu m$ to the next waveguide. This way only minor readjustments of the translation stage have to be performed after each waveguide. 9$\mu m$ single-mode fibre was used to couple the light into the waveguide. At the output end, a multimode 50$\mu m$ diameter fibre was used.

![Schematic representation of the connections for the different measurements](image)

**Figure 3.4:** Schematic representation of the connections for the different measurements. (a) Red lines are spectrum-measurements and blue connections are for insertion loss measurements. Microscope photo of light coupled into the waveguide. (b)
3.2.2 Beam-profile measurements

A lensed beam-profile camera *Spiricon BeamGage* was used to characterize the beam coming out of the sensor. The results for the first batch of sensors *RIE₁* is presented in Figure 3.7. The beam is multimode for all waveguides @ 635nm. The ratio of width to height corresponds to the dimensions of the waveguides. The larger waveguides feature a beam with a much larger vertical extend, this indicates that the light is strongly scattered to cladding modes. There are two possible causes for this: either the grating or waveguide roughness scatters the light very strong outside the core to the cladding and/or the end-facets of the sample are very rough. The k-vector diagram for the case of 635nm light and $\Lambda = 1\mu m$ is drawn in Figure 3.6. From further tests, it appears that the cause of all troubles in the first sensor batch is due to the end-facets. By protecting the polymer layer with an extra glass plate on top prior to dicing, all measured optical parameters are greatly enhanced! This is explained in more detail in the next section where the measurements of the final design are discussed.
Figure 3.6: K-vector diagram of possible diffraction directions in the Bragg sensor for red light 635nm and 1µm period. The possible angles are calculated from this diagram: ±53°, 79°, 102°, 128°.

Figure 3.7: Beam profile measurements of light 635nm coupled into reference waveguides of sensor R1_1. Notice that in the larger waveguides (c,d,e) the vertical extent of the beam is far much larger than the expected 5µm which indicates that portion of the light is being scattered into cladding modes. 300 pixels of the image roughly correspond to 30µm.
### 3.2.3 Insertion loss

The insertion loss is measured with respect to the fibre-to-fibre coupling and expressed in dB:

\[
Loss = 10 \log_{10} \left( \frac{P_{\text{meas}}}{P_{\text{ref}}} \right)
\]

The total insertion loss @ 1554 nm was measured using the Newport 1930C power meter and Newport 918IR detector. The used source was a packaged infrared laser diode QDFBLD-1550-5. The fiber-to-fiber transmission is taken as the reference power. At 1554nm it is **3.75mW** for 9 µm single-mode fibre coupling to the 50µm mmf. For the insertion loss at 635nm the Newport 818-UV detector and Thorlabs QFLD-850-105 source were used with fiber-to-fiber reference power of **1011 µW**.

The expected intrinsic losses of EpoCore at the measured wavelengths of 635nm and 1550nm should be around 1dB/cm if one looks at results of other groups, for example [23] or in textbook references [24]. The measured transmission of the first batch of sensors appears to be very lossy, both at 1550 and 635 nm. Two different samples were measured (diced from the same substrate RIE1_1). Each diced sample contains 1x5 reference waveguides with different widths and 2x5 waveguides patterned on top of the grating. At 1554 nm, a total of 30 waveguides were measured. The measured losses were not significantly higher/lower for waveguides in grating regions compared to reference waveguides. For each waveguide dimension an average insertion loss was calculated in dB with respect to the fibre-to-fibre coupling. The results are presented graphically in Figure 3.8. The highest average transmission is only 80µW (-16.7dB) for the 5x20 waveguide of batch RIE1_1. The smaller waveguides are also more than 10dB more lossy than the larger ones. The mode-overlap of the input fibre decreases with smaller dimensions, but cannot explain these high losses. This could also not be caused by intrinsic losses. The losses appear to be on average higher for the longer sample, but this is inconclusive because the difference is very low for the 5x5 and 5x20 µm² waveguides.

To see if the losses are due to the mode-mismatch when coupling into the fibre, a tapered 1550nm fibre was used with 1.2mW fibre-to-fibre transmission. The lowest loss was then obtained of -20dB @ 1550nm for the largest waveguide 5x20 µm². This loss is even higher than when measured with the smf fibre (-16.5dB). At 635nm it was -24.2dB, compared to -14.8dB with a smf fibre. This rules out the option that the mode-mismatch is causing the severe losses.
3.2.4 OSA characterisation

The broadband Amplified Spontaneous Emission source *ASE FL-7002* produces a spectrum as shown in Figure 3.11 between 1.53 and 1.61 µm. The light is coupled to an optical circulator, designed for this wavelength range *Thorlabs 6015-3-APC*. Transmission losses for the circulator were also measured: port 1-2 = -0.87dB, port 2-3 = -0.52dB. The isolation for the opposite direction is around 60dB. *Agilent 86142B* Optical Spectrum Analyzer was used to measure the reflection and transmission spectra. No Bragg-reflection peaks or transmission dips were observed for the sensor batch *RIE1*. Because of the very high insertion losses it was not certain if the absence of the Bragg-peak is due to a problem of the waveguides, material loss at 1550nm or just a very bad grating transfer of the RIE.

3.3 Final design

In paper [23] a protective glass layer is glued on top of an epoxy waveguide structure. A similar approach was used for the final design. It is believed that by limiting the degrees of freedom of the top ‘soft’ epoxy layer less delamination and deformations will be formed in the waveguide during dicing. To achieve a higher grating depth and thus effective index modulation, the UV-illumination parameters for the phase mask have to be re-optimized because it appears that the optimal parameters for a thin layer of PMMA on glass are not the same as when PMMA is spincoated on EpoClad. This is due to the decreased intensity of back-reflections from the glass interface to the PMMA-layer as opposed to the case when there is only one layer.

By preparing several samples with the same parameters as in Figure 3.1 (a)-(b) the exposure and development time were optimized for maximum diffraction efficiency. Note that in this case, potential 500nm period grating will not be identified and will be discarded because there are no diffracted waves at the He-Ne laser 632.8nm wavelength. The potential 500nm grating
should still be visible to the naked eye though because of the wavelength dependent reflection for blueish light <500nm. The only way to optimize for the 500nm period uniquely would be to measure each sample with the AFM or at least with the SEM. However, in view of the inevitable variability between samples (same parameters yield different end-results) and non-uniformity of the gratings, a very large amount of samples would be needed. It was therefore chosen to optimize for the time being only for the 1 micron period using the relatively faster diffraction efficiency measurements.

First, a coarse sweep in exposure-time was performed: 5,10,15,20,25,30 min @ 70-80 mW/cm². Then the development was performed in steps of 10s until the PMMA was completely washed away. The developed grating was visually examined each time. It appears that there is a small window of parameters when the grating is visually strongest. 20 min exposure time was found to be the region of parameters where a finer sweep should be performed. The next sweep was 18,19,20,21,22 minutes. The 20-min sample produced the following diffraction efficiencies (total dose 84J/cm²):

<table>
<thead>
<tr>
<th>dev. time (s)</th>
<th>$T_{+1}$</th>
<th>$T_0$</th>
<th>$T_{-1}$</th>
<th>estimated depth RCWA (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.09</td>
<td>0.68</td>
<td>0.04</td>
<td>≈ 250</td>
</tr>
<tr>
<td>40</td>
<td>0.075</td>
<td>0.72</td>
<td>0.02</td>
<td>≈ 220</td>
</tr>
<tr>
<td>50</td>
<td>0.032</td>
<td>0.78</td>
<td>0.01</td>
<td>≈ 160</td>
</tr>
</tbody>
</table>

Table 3.1: Optimization of the UV-illumination parameters for PMMA on EpoClad samples. The optimal dose lies around 80J/cm².

Where the depth is estimated using the Matlab RCWA simulations by comparing the values to the graphs in Figure 2.11. After 60s of development the grating was completely gone. The optimal parameters therefore lie in the neighbourhood of 20min exposure and 30s development. Each sample of the RIE3 sensor-batch was exposed 4 times: 19,20,21 and 22 min. The measured diffraction before and after the RIE are presented in the next tables:

<table>
<thead>
<tr>
<th>sample</th>
<th>UV@70mW/cm²(min)</th>
<th>dev. time (s)</th>
<th>$T_{+1}$</th>
<th>$T_0$</th>
<th>$T_{-1}$</th>
<th>depth RCWA (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RIE3, 1</td>
<td>22</td>
<td>30</td>
<td>0.014</td>
<td>0.883</td>
<td>0.007</td>
<td>≈ 80</td>
</tr>
<tr>
<td>RIE3, 1</td>
<td>21</td>
<td>30</td>
<td>0.003</td>
<td>0.856</td>
<td>0.002</td>
<td>≈ ?</td>
</tr>
<tr>
<td>RIE3, 1</td>
<td>20</td>
<td>30</td>
<td>0.043</td>
<td>0.767</td>
<td>0.021</td>
<td>≈ 190</td>
</tr>
<tr>
<td>RIE3, 1</td>
<td>19</td>
<td>30</td>
<td>no grating</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RIE3, 2</td>
<td>20 (nr 1)</td>
<td>35</td>
<td>0.028</td>
<td>0.805</td>
<td>0.013</td>
<td>≈ 150</td>
</tr>
<tr>
<td>RIE3, 2</td>
<td>20 (nr 2)</td>
<td>35</td>
<td>0.031</td>
<td>0.809</td>
<td>0.012</td>
<td>≈ 160</td>
</tr>
<tr>
<td>RIE3, 2</td>
<td>20 (nr 3)</td>
<td>35</td>
<td>0.065</td>
<td>0.750</td>
<td>0.032</td>
<td>≈ 240</td>
</tr>
<tr>
<td>RIE3, 2</td>
<td>20 (nr 4)</td>
<td>35</td>
<td>no grating</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RIE3, 3</td>
<td>20 (nr 1)</td>
<td>40</td>
<td>no grating</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RIE3, 3</td>
<td>20 (nr 2)</td>
<td>40</td>
<td>very weak</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RIE3, 3</td>
<td>20 (nr 3)</td>
<td>40</td>
<td>0.049</td>
<td>0.709</td>
<td>0.006</td>
<td>≈ 200</td>
</tr>
<tr>
<td>RIE3, 3</td>
<td>20 (nr 4)</td>
<td>40</td>
<td>no grating</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.2: Diffraction efficiency measurements before RIE for the final batch of sensors. Note the large variability among samples with the same parameters.

The large variability among samples is mainly due to non-conformal contact of the phase mask with the sample, as is clear from the results in Table 3.2.
The samples were dry-etched in the same mixture of CHF and O$_2$ gasses as the previous sample. The etching time was chosen to be 6 minutes. From previous samples, 5 minutes was close to the threshold where the etch front reaches the EpoClad sample. The remainder of the PMMA is solved in acetone. The best samples from the previous table are now measured again:

<table>
<thead>
<tr>
<th>sample</th>
<th>UV@70mW/cm$^2$(min)</th>
<th>dev. time (s)</th>
<th>$T_{+1}$</th>
<th>$T_0$</th>
<th>$T_{-1}$</th>
<th>depth RCWA (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RIE3_1</td>
<td>20</td>
<td>30</td>
<td>0.008</td>
<td>0.872</td>
<td>0.005</td>
<td>≈ 60</td>
</tr>
<tr>
<td>RIE3_1</td>
<td>22</td>
<td>30</td>
<td>0.005</td>
<td>0.889</td>
<td>0.005</td>
<td>≈ 50</td>
</tr>
<tr>
<td>RIE3_2</td>
<td>20 (nr 3)</td>
<td>35</td>
<td>0.010</td>
<td>0.839</td>
<td>0.014</td>
<td>≈ 75</td>
</tr>
<tr>
<td>RIE3_2</td>
<td>20 (nr 1)</td>
<td>35</td>
<td>0.007</td>
<td>0.862</td>
<td>0.008</td>
<td>≈ 60</td>
</tr>
</tbody>
</table>

Table 3.3: Diffraction efficiency measurements after RIE. For the estimated grating depth Matlab simulations are used from Figure 2.11.

The diffraction efficiency is clearly diminished. This is not what is expected for a perfect grating transfer, see Figure 2.11. The reason could be that the etching time was still too short than expected and only a portion of the sine was transferred to the cladding. Or that the RIE introduces a great deal of roughness to the grating, partially destroying the profile. Further processing steps of Figure 3.1 (f)-(h) are carried out on the two best samples: RIE3_1 and RIE3_2. It is believed that further optimization of the UV-illumination and RIE-transfer parameters would increase the diffraction-efficiency and thus the depth of the 1 $\mu$m period grating.

A final remark on dicing: after cutting the samples, droplets of water were sucked in between the glued glass layer on top and the polymers. On one of the samples the top glass layer detached by itself. The water droplets did not seem to affect the transmission properties.

### 3.3.1 Beam-profile measurements

The two samples eventually yield 4 sensors with diffraction efficiencies and estimated grating depths in table 3.3. They are further denoted as $S_{k \cdot l}$ with $k \in [1, 2, 3, 4]$ and $l \in [a, b, c, d]$. The letters denote the waveguide region on the sensor, a and b are all reference waveguides while c and d contain the waveguides with the grating beneath them. The numbers denote the sample: 1 and 2 are from RIE3_1, 3 and 4 are from RIE3_2. The light was coupled into the waveguides and it is directly visible that there is much less scattering present: compare the top and bottom photograph of Figure 3.5a. The light coupling out of the waveguide clearly does not scatter vertically as in the previous batch RIE1. This indicates that the facets are much more flat now. The beam is also less 'visible' when it is coupled to the waveguide. The good visibility of Figure 3.4b is due to the increased defects along the path of the waveguide. The outcoupling beam-profile was measured as well and results are presented in Figure 3.9. The beam is tightly confined to the waveguide region and practically no light is present in the cladding.

### 3.3.2 Insertion loss

The insertion losses were measured at 1554nm and 635nm, compared to fibre-to-fibre coupling. The average losses per waveguide dimension are compared graphically with the previous batch in Figure 3.8. The losses are now lowered by 10-25 dB as compared to the processing without
Figure 3.9: Beam profile measurements of light 635nm coupled into reference waveguides of sensor S4.1. Notice the clear confinement of the beam in the waveguide as compared to Figure 3.7. 300 pixels of the image roughly correspond to 30µm.

the protective glass layer on top. The lowest insertion loss is -5.7dB at 635 nm and -7.2dB at 1554 nm. The smallest waveguide now features only a slight increase of 1dB in insertion loss compared to the 5x20 waveguide due to the mode-mismatch. It is clear now that the main factor affecting the insertion is the dicing processing step. The degrees of freedom of the polymer layer are limited by sandwiching it between two glass plates. Without it, the softer polymer layer ‘reacts’ differently to the dicing blade than the harder glass plate and this introduces delamination and deformation of the polymer layers.

3.3.3 OSA characterisation

The reflection spectra of the samples were measured. A 28e smf fibre was used to couple light into the sensor. Note that tapered fibres would have a much lower acceptance angle for the light to couple back into the fibre. In the previous batch, no interference effects were observed in reflection. It appears that previously only the Fresnel facet reflection of the fibre were measured.

A typical Fabry-Perot interference is observed in the reflection spectrum. This was not the case in the previous batch R1, which is an extra indication that the end facets of the samples are much better now with this new dicing approach. The distance from the fiber-end to the sensor determines the spacing of the reflection dips in the observed reflection spectrum according to the known equation [15]

$$\Delta \lambda = \frac{\lambda^2}{2n_{eff}L}$$

(3.1)
Figure 3.10: Measured Fabry-Perot reflection spectrum, observed in the new batch RIE3. The red line indicates a measurement with the fibre at an unknown distance $X(<50\mu m)$ from the sensor facet. The FP-periodicity increases with distance to the sensor according to eq. 3.1. OSA parameters: sensitivity -71.6 dBm, resolution bandwidth 0.06nm, averaging 1 sweep

In Figure 3.10 the spacing $\Delta \lambda$ is calculated and equals 20.4nm from which one can approximate the distance to the sensor $X$ for that measurement: $X = \frac{1565^2}{2 \times 1.575 \times 20.4} \text{nm} = 38 \mu m$. The stage is then translated away from the sample by a fixed distance of $100 \mu m$ to check if the wavelength changes consistently with eq. 3.1:

$$\Delta \lambda = \frac{\lambda^2}{2n_{eff}L} = \frac{1.545^2}{2 \times 1.575 \times 138} = 5.7\text{nm}$$

which is quite close to the measured spacing of 6.9nm at 1545 nm wavelength. No reflection Bragg peak was observed.

**Improving the Signal-to-Noise Ratio**

It is thought that the reflected signal must be very weak. The diffraction efficiency measurements indicate that the grating is only around 60 nm deep. In this case, it is normal that the signal is not observed because the Fresnel background reflection signal is already of the order of 4% = -14dB. This reflectance can be estimated from the well-known Fresnel equations and is consistent with the OSA measurements in Figure 3.11.

$$R = \left(\frac{n_{fibre} - n_{air}}{n_{fibre} + n_{air}}\right)^2 \approx 0.04$$

Assuming that the reflected Bragg-signal and facet reflections do not add up coherently, the reflected power should consist of the linear sum of the two signals separately. On the log-scale this would result in a very tiny peak on top of the unwanted Fresnel signal. In order to counteract this and improve the Signal-to-Noise Ratio several steps were undertaken: the input fibre was angle-cleaved. This causes the light reflected at the fibre facet to be pushed into the evanescent cladding modes eliminating the Fresnel reflection. The comparison of the reflection signals for flat and angled fibre is given in Figure 3.11. The Fresnel-reflections are uniformly suppressed for all wavelengths by 15dB.
Now, a tiny peak is observed in the expected wavelength region of 1580 nm. Figure 3.12a. This peak is absent in reference waveguides, indicating that this might very well be the Bragg signal. To eliminate the Fresnel signal coming from the waveguide end-facet, an Index Matching Fluid was deposited between the fibre and sensor. The OrmoClad refractive index 1.51 lies halfway between the fibre index 1.465 and EpoCore 1.575 and should be ideal to eliminate the reflections even further.\footnote{In the future, the sensor should ideally be diced under an angle to eliminate the Fresnel reflections directly.} The transmission power of the waveguide was monitored during the dispension of OrmoClad, simultaneously measuring the reflection spectrum. The measurements were then performed with 'yellow'-lights so that OrmoClad does not polymerises and remains liquid. This way the fibre can be coupled to different waveguides. By coating each sensor-facet with the IMF, the noise floor was lowered by 10dB for the input facet and by another 7dB when the output sensor facet was covered as well. The Bragg peak now becomes clearly visible in the OSA measurements, Figure 3.12.
Figure 3.12: The effect an Index-Matching Fluid was investigated. The reflected signal of sensor S4_c: 5x5 $\mu m^2$ waveguide was measured for an angled single-mode fiber at the input side (a), then index-matched with OrmoClad at the input (b) and index-matched at both sides (c). Note that the vertical scale is different in all cases. OSA parameters: sensitivity -82dBm, resolution bandwidth 0.06nm, averaging 50 sweeps.

The reflected signal in dBm is converted to mW and then the signal is compared to the source signal coming towards the sensor. The source was measured with the exact same parameters as the Bragg-measurements. The ratio of the powers gives the reflectance of the Bragg sensor at each wavelength. These results, expressed in dB for the 5 different waveguides of sensor S4_c are plotted in Figure 3.13 and 3.14 and s4_d in Figure 3.15. The measured Bragg wavelengths and calculated Full Width at Half Maximum are given in table 3.4. Two peaks are observed for the single-mode waveguides 5x5 and 5x8 $\mu m^2$, this corresponds to the TE- and TM-modes excited in the waveguide. These two modes are closely spaced next to each other, which is consistent with the low birefringence associated with the polarization modes. The peak wavelengths are also compared to the expected Bragg wavelength, where the effective indices were simulated in Lumerical, $\lambda_b = 2n_{eff}\Lambda$. If one were to control the polarization of the input fibre, only one mode could be excited. The larger waveguides: 10, 15, 20 $\mu m$ width feature 4 Bragg peaks, corresponding to two possible modes, each with TE/TM polarization.

The maximum Bragg reflectance is only a modest -30.8dB or 0.083% at 1583.44 for the 5x8 $\mu m^2$ single-mode waveguide while commercial FBG’s feature reflectance values >99.9%. Similar results to the present work however, but with different materials and fabrication methods is found in [25] (-25dB in ZrO hybrids) or in PMMA [26] (-29dB). It is believed that by further optimizing the grating RIE transfer parameters it is possible to achieve much better reflectivities. The estimated grating depth of the measured Bragg spectra is around 60nm, but from the AFM results, depths > 200nm are certainly possible. Moreover it should be possible to lower the noise floor even further if the sensor samples are diced at an angle.
Figure 3.13: Bragg reflectance in dB of sample S4_c compared to the input ASE-broadband source measured with the same parameters. The inset shows the different dimensions of the measured waveguides. OSA parameters: sensitivity -82.34dBm, resolution bandwidth 0.06nm, averaging 20 sweeps.

Figure 3.14: Zoom on the largest Bragg reflection peak of Figure 3.13; S4_c: 5x8 µm². The highest reflectance is -30.8 dB = 0.083 % at 1583.44 nm.
<table>
<thead>
<tr>
<th>Waveguide</th>
<th>peak wavelength (nm)</th>
<th>expected peak wavelength (nm)</th>
<th>FWHM (pm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5x5 µm²</td>
<td>1582.03</td>
<td>1587.82</td>
<td>90</td>
</tr>
<tr>
<td></td>
<td>1581.46</td>
<td>1587.82</td>
<td>81</td>
</tr>
<tr>
<td>5x8 µm²</td>
<td>1583.44</td>
<td>1588.83</td>
<td>96</td>
</tr>
<tr>
<td></td>
<td>1582.85</td>
<td>1588.82</td>
<td>97</td>
</tr>
<tr>
<td>5x10 µm²</td>
<td>1583.94</td>
<td>1589.21</td>
<td>88</td>
</tr>
<tr>
<td></td>
<td>1583.35</td>
<td>1589.19</td>
<td>90</td>
</tr>
<tr>
<td></td>
<td>1580.15</td>
<td>1586.51</td>
<td>132</td>
</tr>
<tr>
<td></td>
<td>1580.04</td>
<td>1586.32</td>
<td>154</td>
</tr>
<tr>
<td>5x15 µm²</td>
<td>1583.82</td>
<td>1589.68</td>
<td>48*</td>
</tr>
<tr>
<td></td>
<td>1583.45</td>
<td>1589.66</td>
<td>46*</td>
</tr>
<tr>
<td></td>
<td>1581.76</td>
<td>1588.03</td>
<td>48*</td>
</tr>
<tr>
<td></td>
<td>1581.38</td>
<td>1588.03</td>
<td>38*</td>
</tr>
<tr>
<td>5x20 µm²</td>
<td>1584.78</td>
<td>1589.89</td>
<td>80*</td>
</tr>
<tr>
<td></td>
<td>1584.17</td>
<td>1589.88</td>
<td>68*</td>
</tr>
<tr>
<td></td>
<td>1581.30</td>
<td>1588.84</td>
<td>110</td>
</tr>
<tr>
<td></td>
<td>1580.65</td>
<td>1588.83</td>
<td>108</td>
</tr>
</tbody>
</table>

Table 3.4: Bragg wavelength and Full Width at Half Maximum for the different modes and waveguides of sensor S4_c. Note that the resolution bandwidth of the OSA is 60pm. Calculated FWHM* lower or close to 60 pm are therefore not accurate.

Figure 3.15: Bragg reflectance in dB of sample S4_d compared to the incoming ASE-broadband source measured with the same parameters. The inset shows the different dimensions of the measured waveguides. OSA parameters: sensitivity -82.34dBm, resolution bandwidth 0.06nm, averaging 20 sweeps.
3.3.4 Strain measurements and embedding of the sensor

The previous results proof that this fabrication method leads to the desired single-mode sensor characteristics, albeit with small reflectance values. Further tests reveal that with 18 min UV-illumination \( @ 70 \text{mW/cm}^2 \) and 40s development in IPA:\( H_2O \) produces the following diffraction efficiency values:

<table>
<thead>
<tr>
<th>sample</th>
<th>UV@70mW/cm(^2)(min)</th>
<th>dev. time (s)</th>
<th>( T_{+1} )</th>
<th>( T_0 )</th>
<th>( T_{-1} )</th>
<th>depth ( RCWA ) (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AD4</td>
<td>18 (nr 1)</td>
<td>40</td>
<td>0.055</td>
<td>0.664</td>
<td>0.010</td>
<td>( \approx 200 )</td>
</tr>
<tr>
<td>AD4</td>
<td>18 (nr 2)</td>
<td>40</td>
<td>0.175</td>
<td>0.461</td>
<td>0.018</td>
<td>( \approx 350 )</td>
</tr>
<tr>
<td>AD4</td>
<td>20 (nr 1)</td>
<td>40</td>
<td>0.014</td>
<td>0.888</td>
<td>0.004</td>
<td>( \approx 100 )</td>
</tr>
</tbody>
</table>

Table 3.5: Diffraction efficiency measurements of a new PMMA on EpoClad sample.

The major limitation of the production method is that it is very hard to reproducibly fabricate samples. For the exact same parameters, two very different gratings were produces, AD4, 18min, 40s. It is possible however, when the contact with the phase mask is very good to achieve grating depths > 300nm. This last sample was sent to the AFM in TU/e for inspection, results are still pending.

The next steps would be to release the glass-plates by focussing the KrF excimer laser on the interface between cladding and epoxy and scanning over the whole surface. The released polymer sensor structure can then be embedded on a stretchable substrate in order to measure the strain relationship of the Bragg wavelength peaks. By stretching the structure, the period of the grating should increase, shifting the Bragg wavelength to longer wavelengths. Simultaneously, the temperature can be controlled to eliminate or monitor the temperature dependent shifts. Unfortunately, there was not enough time to perform these experiments.
Chapter 4

Conclusion

Two major techniques to fabricate polymer planar Bragg grating sensors were investigated.

The first one is the imprinting method where the profile of a Si master stamp with a predefined period is transferred to a silicone such as PDMS. The stamp is pressed on the liquid silicone and subsequently cured together. Various brands were investigated such as Sylgard 186/184 PDMS, Nusil Lightspan LS-6257 and LS-6943. The master stamp is mechanically released and the resulting silicone stamp is used for stamping the pattern into an uncured cladding or core material such as EpoClad or OrmoClad and subsequently polymerized and released. The resulting grating pattern features the required period but this method has several issues:

- Scanning Electron Microscope characterisation shows that the transfer of the master stamp to silicone stamp is not conformal, the formed grating is very shallow with a large amount of defects present. These effects are further amplified after the second transfer from silicone to cladding.
- The silicone stamp soaks up the solvent of the cladding/core materials. This introduces unwanted ridge structures which would greatly affect the optical path of the waveguide.

The second method uses a phase mask where a sine grating pattern is formed by interference of the transmitted orders of a UV-source through the phase mask. Surface dielectric gratings with a period of 1.01μm were formed in an epoxy-based material EpoCore and also in PolyMethylMethAcrylate (PMMA). Volume gratings by refractive index modification were produced in Norland optical methacrylate-based adhesives (NOA) and in PMMA.

The best results were obtained by developing exposed PMMA to produce a surface dielectric grating. This grating was then successfully transferred by Reactive Ion Etching to the epoxy optical material system EpoClad/Core for which it is possible to produce smooth single-mode 5x5 μm² waveguides with an accurate direct laser inscription method.

The sensors were then sandwiched between two glass plates and diced together. This step was proven to be crucial to achieve optically flat end-facets. The minimum achieved insertion loss of the Bragg sensor is -5.7dB @ 635 nm and -7.2dB @ 1554nm. Bragg reflection signals were observed for different waveguides in the wavelength region of 1580-1584nm. The highest Bragg reflectivity that was achieved is -30.8dB @ 1583.44nm with a FWHM of 90pm for a single-mode 5x8μm² waveguide.

Further optimization of the RIE parameters should result in higher reflectance values. The
major limitation of this method of grating fabrication is the requirement of conformal contact between substrate and phase mask due to the limited coherence length of the UV-source. This leads to poor reproducibility of gratings even when the same parameters are used.

In parallel, Rigorous Coupled-Wave Theory of plane wave diffraction was implemented in Matlab and extended to multiple stacked layers in order to link diffraction efficiency measurements to the formed sine grating amplitude. The results are in agreement with AFM measurements. The best PMMA grating amplitude depth that was measured with the AFM is 210nm. FDTD Lumerical was investigated as a tool to simulate Bragg reflection sensors using the input from diffraction efficiency measurements. This software is very inefficient for large z-invariant millimetre-size structures. Other approaches should be investigated, such as the transfer matrix method and MODE-solution software.
Appendices
Appendix A

Rigorous Coupled-Wave Analysis
Matlab GUI

%%%%---GUI:Diffraction Analysis dielectric lossless surface gratings---%%% 

% Anton Vasiliev version 21/05/14 
% incident TE plane wave is assumed 
% TE = Linearly polarized field perpendicular to the plane of incidence. 

function varargout = DE Gui(varargin) 
% Begin initialization code -- DO NOT EDIT 
  gui_Singleton = 1; 
  gui_State = struct('gui_Name', mfilename, ... 
                    'gui_Singleton', gui_Singleton, ... 
                    'gui_OpeningFcn', @DE Gui_OpeningFcn, ... 
                    'gui_OutputFcn', @DE Gui_OutputFcn, ... 
                    'gui_LayoutFcn', [], ... 
                    'gui_Callback', []); 
  if nargin && ischar(varargin{1}) 
    gui_State.gui_Callback = str2func(varargin{1}); 
  end 
  if nargout 
    [varargout{1:nargout}] = gui_mainfcn(gui_State, varargin{:}); 
  else 
    gui_mainfcn(gui_State, varargin{:}); 
  end 

function DE Gui_OpeningFcn(hObject, eventdata, handles, varargin) 
  guidata(hObject, handles); 

function varargout = DE Gui_OutputFcn(hObject, eventdata, handles) 
  varargout{1} = handles.output; 

% ---- Executes on button press in pushbutton1. 
function pushbutton1_Callback(hObject, eventdata, handles, varargin) 
  warning('off','MATLAB:nearlySingularMatrix');
if get(handles.checkbox4,'Value') == 1.0
cla
end
lambda = str2double(get(handles.edit2,'String'));
% um free space wavelength
eps_1 = str2double(get(handles.n_region1,'String'))^2;
%dielectric constant region I
eps_3 = str2double(get(handles.n_region2,'String'))^2;
%dielectric constant region III —> n3=1.57 ...
Lambda = str2double(get(handles.edit1,'String'));
%grating period
theta_in=str2double(get(handles.edit9,'String'))*pi/180;
% incidence angle in radians
sweep = eval(get(handles.edit10,'String'));
$sweep in d$
Dparam = (1:size(sweep));
Dcount=0;
K= 2*pi/Lambda; %Crystal K-vector
m=2*Lambda*sqrt(eps_1)*sin(theta_in)/lambda;%scaled input spatial frequency
k1= 2*pi*sqrt(eps_1)/lambda; %length k-vector region I
k1i=k1; %length k-vector region I = length reflected k-vector region I
k3=2*pi*sqrt(eps_3)/lambda; %length k-vector region III
x_res=5e-9; %1nm x-resolution of numerical computations
Nx=ceil(Lambda/x_res); %number of discrete x-cells
N=str2double(get(handles.edit3,'String'));
%number of slabs to approximate grating
s=str2double(get(handles.edit4,'String'));
%number of space-harmonics i=-1,0,+1, only odd numbers allowed
ExportM2={'d'};
Angles2={'order'};
for x=1:s
    ExportM2=vertcat(ExportM2,strcat('T',num2str(x-(s+1)*0.5)));
    Angles2=vertcat(Angles2,strcat('T',num2str(x-(s+1)*0.5)));
end
for x=1:s
    ExportM2=vertcat(ExportM2,strcat('R',num2str(x-(s+1)*0.5)));
    Angles2=vertcat(Angles2,strcat('R',num2str(x-(s+1)*0.5)));
end
for d=sweep
    Dcount=Dcount+1;
    disp({'progress: ',num2str(Dcount),'/',num2str(length(sweep))})
end

K= 2*pi/Lambda; %Crystal K-vector
m=2*Lambda*sqrt(eps_1)*sin(theta_in)/lambda;%scaled input spatial frequency
k1= 2*pi*sqrt(eps_1)/lambda; %length k-vector region I
k1i=k1; %length k-vector region I = length reflected k-vector region I
k3=2*pi*sqrt(eps_3)/lambda; %length k-vector region III
x_res=5e-9; %1nm x-resolution of numerical computations
Nx=ceil(Lambda/x_res); %number of discrete x-cells
N=str2double(get(handles.edit3,'String'));
%number of slabs to approximate grating
s=str2double(get(handles.edit4,'String'));
%number of space-harmonics i=-1,0,+1, only odd numbers allowed
ExportM2={'d'};
Angles2={'order'};
for x=1:s
    ExportM2=vertcat(ExportM2,strcat('T',num2str(x-(s+1)*0.5)));
    Angles2=vertcat(Angles2,strcat('T',num2str(x-(s+1)*0.5)));
end
for x=1:s
    ExportM2=vertcat(ExportM2,strcat('R',num2str(x-(s+1)*0.5)));
    Angles2=vertcat(Angles2,strcat('R',num2str(x-(s+1)*0.5)));
end
for d=sweep
    Dcount=Dcount+1;
    disp({'progress: ',num2str(Dcount),'/',num2str(length(sweep))})
end

% d=(50e-9)+parameter*(50e-9);% 200nm depth
% Dparam(parameter)=d/Lambda;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%--Calculate fixed quantities:--%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
for p=1:s
    orders(p)=-p*(s+1)*0.5; %orders = [-s, -s+1, ... , -1, 0, 1,..., +s]
end

for p = orders %calculation of the z-components of the k-vectors
    number=k1^2-(k1*sin(theta_in)-p*K)^2;
    if number<0

46
k1_iz(floor(p+(s+1)*0.5))=li*abs(sqrt(number));
% exp decay into region I
else
    k1_iz(floor(p+(s+1)*0.5))=sqrt(number);% abs value of k1_iz
end

number=k3^2-(k1*sin(theta_in)-p*K)^2;
if number<0
    k3_iz(floor(p+(s+1)*0.5))=-li*abs(sqrt(number));
    % exp decay into region III
else
    k3_iz(floor(p+(s+1)*0.5))=sqrt(number);% abs value of k3_iz
end
k1_iz(floor(p+(s+1)*0.5))=k1*sin(theta_in)-p*K;

%%%%%%%%%----Fourier series expansion of periodic slab function----%%%%%
grating=zeros(Nx,N); % grating f(x,n) zero when in region I, 1 in region III
profile= get(handles.listbox,'Value');
switch profile
    case 1 % square
        DC=str2double(get(handles.DutyCycle,'String'));
        for i=1:(Nx)
            X(i)=(i-1.0+0.5)*x_res;
            if X(i) > (Lambda*(1-DC/100))
                for n=1:N
                    grating(i,n)=1;
                % this defines the regions of 1's for a sine
                end
            end
        end
    case 2 % sine
        for i=1:(Nx)
            X(i)=(i-1.0+0.5)*x_res;
            for n=1:N
                y=(n-1.0+0.5)*d/N;
                number = 0.5*d*(1.0+sin(K*X(i)));
                if y > number
                    grating(i,n)=1;
                    % this defines the regions of 1's for a sine
                end
            end
        end
    case 3 % blazed grating
        alpha= str2double(get(handles.edit14,'String'))*pi/180;
        a = d*cot(alpha);
        if a < Lambda
            beta = atan(d/(Lambda-a));
            set(handles.beta_angle,'String',num2str(beta*180/pi,3));
            for i=1:(Nx)
                X(i)=(i-1.0+0.5)*x_res;
                if X(i)<a
                    for n=1:N
                        y=(n-1.0+0.5)*d/N;
                        number = -tan(alpha)*X(i)+d;
                        if y > number
                            grating(i,n)=1;
                            % this defines the regions of 1's for a sine
                        end
                    end
                end
            end
        end
else
  for n=1:N
    y=(n-1.0+0.5)*d/N;
    number = tan(beta)*(X(i)-a);
    if y > number
      grating(i,n)=1;
      %this defines the regions of 1's for a sine
    end
  end
end
else
  set(handles.edit14,'String','angle too small !');
end

for n=1:N
  %fraction=0.5;
  fraction=nnz(grating(:,n))/length(grating(:,n));
  %fraction of non-zero elements of the grating function
  eps_2(n)=eps_3*fraction+eps_1*(1.0-fraction);
  %average permittivity in slab n
  k2(n)=2*pi*sqrt(eps_2(n))/lambda;
  number= k2(n)^2-(k1*sin(theta_in))^2;
  if number < 0
    k2_z(n)=-1i*abs(sqrt(number)); %exp decay in region II
  else
    k2_z(n)=sqrt(number);
  end
  for h=1:s
    eps_F3(h,n)=(1.0/Lambda)*x_res*trapz(grating(:,n).*exp(-1i*K*h.*X(:)));
  end
  eps_F2(:,n)=(x_res/Lambda).*fft(grating(:,n)); %fast fourier transform, gives almost same results as eps_F3
end

%%%%%%%%%%%%%%%%%%eigenvectors and eigenvalues of the spaceharmonics Si---%%%%%%%%%%%%%%%%
A=zeros(s,s);
D=zeros(s,s);
B=zeros(s,s);
S=zeros(2*s,2*s,N); %the state-space matrix for each slab n
for n=1:N
  for x=1:s
    for y=1:s
      if x==y
        p=x-((s+1)*0.5);
        C(x,y)=-(K^2)*p*(m-p);
        D(x,y)=2*1i*k2_z(n);
        B(x,y)=1.0;
      else

    end
if y > x
    C(x,y) = -(2*pi/lambda)^2 * (eps_3 - eps_1) * ...
    conj(eps_F3(y-x,n));
else
    C(x,y) = -(2*pi/lambda)^2 * (eps_3 - eps_1) * ...
    (eps_F3(x-y,n));
end
end
end

S1=[A,B];
S2=[C,D];
S(:,:,n)=[S1;S2];
end

% sum_flags=0;
for n=1:N
    % [Vectoren2,EigMatrix2, flag] = eigs(S(:,:,n),2*s);
    % there are different eigenvalue solvers in matlab
    [Vectoren,EigMatrix] = eig(full(S(:,:,n)));
    % sum_flags=sum_flags+sum(flags);
    for x=1:2*s
        eigenwaarden(x,n)=EigMatrix(x,x); % eigenvalues
        eigenwaarden2(x,n)=EigMatrix2(x,x);
        for y=1:2*s
            eigenvectoren(x,y,n)=Vectoren(x,y); % eigenvectors
            % eigenvectoren2(x,y,n)=Vectoren2(x,y);
        end
    end
end

%%%%%%%%%%%%%%%%%%%%%%%%---Boundary condition equations for E_tan, H_tan---%%%%%%%%%%%%%%%%%%%%%%%%
% M=zeros(2*s*(N+1),2*s*(N+1)); % the equation to be solved is M*X=Bx
M_start=zeros(2*s,2*(N+1)*s); % equations between I and first slab
M_end=zeros(2*s,2*(N+1)*s); % equations between last slab and III
M_n=zeros(2*s*(N-1),2*s*(N+1)); % equations between n and n+1
Bx=zeros(2*s*(N+1),1);
for x=1:s
    for y=1:2*s
        M_start(x,y)=eigenvectoren(x,y,1); % E field tang
        M_start(x+s,y)=eigenvectoren(x,y,1)*(eigenwaarden(y,1)-1i*k2*z(1));
    end
    M_end(x,x+2*s*N)-=-1.0; % the components for Ri
    M_end(x+s,x+2*s*N)-=1i*k3i*z(x); % the components for Ti
end

for x=1:s
    for y=1:2*s
        M_end(x,y+2*s*(N-1))=-1.0; % the components for Ri
        M_start(x+s,x+2*s*N)-=-1i*k1i*z(x); % the components for Ri
    end
end

for x=1:s
    for y=1:2*s
        M_end(x,y+2*s*(N-1))=eigenvectoren(x,y,N)*...
        exp((eigenwaarden(y,N)-1i*k2*z(N))*d); % E field tang
        M_end(x+s,y+2*s*(N-1))=eigenvectoren(x,y,N)*...
        (eigenwaarden(y,N)-1i*k2*z(N))*...
        exp((eigenwaarden(y,N)-1i*k2*z(N))*d); % H field tangential
    end
end

M_end(x,x+2*s*N+s)-=-1.0; % the components for Ti
M_end(x+s,x+2*s*N+s)=1i*k3i*z(x); % the components for Ti

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end

for n=1:N
  for x=1:s
    for y=1:2*s
      M_n(x+2*s*(n-1),y+2*s*(n-1))=eigenvectoren(x,y,n)*... 
        (eigenwaarden(y,n)-1i*k2_z(n))*n*d/N; \ E slab n
      M_n(x+2*s*(n-1),y+2*s*n)==eigenvectoren(x,y,n+1)*... 
        (eigenwaarden(y,n)-1i*k2_z(n))*n*d/N; \ E n+1
      M_n(x+s+2*s*(n-1),y+2*s*(n-1))=eigenvectoren(x,y,n)*... 
        (eigenwaarden(y,n)-1i*k2_z(n))*... 
        exp((eigenwaarden(y,n)-1i*k2_z(n))*n*d/N); \ H n
      M_n(x+s+2*s*(n-1),y+2*s*n)==eigenvectoren(x,y,n+1)*... 
        (eigenwaarden(y,n)-1i*k2_z(n))*... 
        exp((eigenwaarden(y,n)-1i*k2_z(n))*n*d/N); \ H n+1
    end
  end
end
M=vertcat(M_start,M_n,M_end); \put the 3 matrices together

%the right hand side of the equation
Bx((s+1)*0.5)=1.0;
Bx(((s+1)*0.5)+s)==-1i*k1_z(((s+1)*0.5));

X_result=M\Bx; \Gaussian elimination solver
for x=1:s
  Ri(x)==X_result(x+2*N*s); \amplitude reflection coefficient
  Ti(x)==X_result(x+2*N*s+s); \amplitude transmission coefficient
  DE_1i(x)==real(k1i_z(x)/k1i_z((s+1)*0.5))*abs(Ri(x))^2; \power reflectance coefficient region I
  DE_3i(x)==real(k3i_z(x)/k1i_z((s+1)*0.5))*abs(Ti(x))^2; \power transmittance coefficient region III
end
DE_3i_1(Dcount)==DE_3i((s+1)*0.5+1);
DE_3i_0(Dcount)==DE_3i((s+1)*0.5);
DE_3i_min1(Dcount)==DE_3i((s+1)*0.5-1);
DE_1i_1(Dcount)==DE_1i((s+1)*0.5+1);
DE_1i_0(Dcount)==DE_1i((s+1)*0.5);
DE_1i_min1(Dcount)==DE_1i((s+1)*0.5-1);
convergence(Dcount)==abs(1-sum(DE_1i(:)))-sum(DE_3i(:))); \% 1.0 - sum (DE's) , the smaller the better
Combine1=horzcat(d,DE_3i,DE_1i);
Combine1=transpose(Combine1);
Combine1=num2cell(Combine1);
ExportM2=horzcat(ExportM2,Combine1);
end
ExportM=vertcat(sweep,DE_3i_1,DE_3i_0,DE_3i_min1,DE_1i_1,DE_1i_0,DE_1i_min1);
ExportM=num2cell(ExportM);
ExportM=horzcat (['d';'T+1';'T+0';'T-1';'R+1';'R+0';'R-1'],ExportM);

Angles(1,1)==atan(k1i_x((s+1)*0.5+1)/k3i_z((s+1)*0.5+1))*180/pi;
Angles(2,1)==atan(k1i_x((s+1)*0.5)/k3i_z((s+1)*0.5))*180/pi;
Angles(3,1)==atan(k1i_x((s+1)*0.5-1)/k3i_z((s+1)*0.5-1))*180/pi;
Angles(4,1)==atan(k1i_x((s+1)*0.5+1)/k1i_z((s+1)*0.5+1))*180/pi;
Angles(5,1)==atan(k1i_x((s+1)*0.5)/k1i_z((s+1)*0.5))*180/pi;
Angles(6,1)==atan(k1i_x((s+1)*0.5-1)/k1i_z((s+1)*0.5-1))*180/pi;
Angles=num2cell(Angles);
Angles=horzcat({'T+1';'T+0';'T−1';'R+1';'R+0';'R−1'},Angles);
Angles=vertcat({'order','angle [deg]'},Angles);

Combine2={'angle [deg]'};
for x=1:s
    Combine2=vertcat(Combine2,num2cell(atan(k1i_x(x)/k3i_z(x))*180/pi));
end
for x=1:s
    Combine2=vertcat(Combine2,num2cell(atan(k1i_x(x)/k1i_z(x))*180/pi));
end
Angles2=horzcat(Angles2,Combine2);

hold on
plot(handles.axes1,sweep.*1e9,DE3i1(:),'-r','LineWidth',2)
plot(handles.axes1,sweep.*1e9,DE3i0(:),'-r','LineWidth',2)
plot(handles.axes1,sweep.*1e9,DE3i_min1(:),'-g','LineWidth',2)
plot(handles.axes1,sweep.*1e9,DE1i1(:),'-g','LineWidth',2)
plot(handles.axes1,sweep.*1e9,DE1i0(:),'-b','LineWidth',2)
plot(handles.axes1,sweep.*1e9,DE1i_min1(:),'-b','LineWidth',2)

hold off
figure
set(gcf,'Visible','off');
hold on
plot(sweep.*1e9,DE3i1(:),'-r','LineWidth',2)
plot(sweep.*1e9,DE3i0(:),'-r','LineWidth',2)
plot(sweep.*1e9,DE3i_min1(:),'-g','LineWidth',2)
plot(sweep.*1e9,DE1i1(:),'-g','LineWidth',2)
plot(sweep.*1e9,DE1i0(:),'-b','LineWidth',2)
plot(sweep.*1e9,DE1i_min1(:),'-b','LineWidth',2)

hold off
name = get(handles.edit11,'String');
if get(handles.checkbox1,'Value') == 1.0
    saveas(gcf, name, 'pdf')
end
if get(handles.checkbox2,'Value') == 1.0
    xlswrite(name,ExportM2)
end
if get(handles.checkbox3,'Value') == 1.0
    saveas(gcf, name, 'eps')
end
foregroundColor = [1 1 1];
set(handles.uitable2, 'ForegroundColor', foregroundColor);
backgroundColor = [.4 .1 .1; .1 .4 .4];
set(handles.uitable2, 'BackgroundColor', backgroundColor);
set(handles.uitable2,'Data',ExportM2);
set(handles.uitable3, 'ForegroundColor', foregroundColor);
set(handles.uitable3, 'BackgroundColor', backgroundColor);
set(handles.uitable3,'Data',Angles2);

function edit1
    Callback(hObject, eventdata, handles)
    function edit1_CreateFcn(hObject, eventdata, handles)
        if ispc && isequal(get(hObject,'BackgroundColor'),
            get(0,'defaultUicontrolBackgroundColor'))
            set(hObject,'BackgroundColor','white');
        end
    end
    function edit9
        Callback(hObject, eventdata, handles)
        function edit9_CreateFcn(hObject, eventdata, handles)
            if ispc && isequal(get(hObject,'BackgroundColor'),
                get(0,'defaultUicontrolBackgroundColor'))
                set(hObject,'BackgroundColor','white');
            end
        end
        function edit11
            Callback(hObject, eventdata, handles)
            function edit11_CreateFcn(hObject, eventdata, handles)
                if ispc && isequal(get(hObject,'BackgroundColor'),
                    get(0,'defaultUicontrolBackgroundColor'))
                    set(hObject,'BackgroundColor','white');
                end
            end
function checkbox1_Callback(hObject, eventdata, handles)
function checkbox2_Callback(hObject, eventdata, handles)
function checkbox3_Callback(hObject, eventdata, handles)
function checkbox4_Callback(hObject, eventdata, handles)
function listbox_Callback(hObject, eventdata, handles)
function listbox_CreateFcn(hObject, eventdata, handles)
if ispc && isequal(get(hObject,'BackgroundColor'), ...
    get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end
set(hObject,'String',
    {'1: Square';'2: Sine';'3: General Blazed'});
function edit14_Callback(hObject, eventdata, handles)
function edit14_CreateFcn(hObject, eventdata, handles)
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end
function DutyCycle_Callback(hObject, eventdata, handles)
function DutyCycle_CreateFcn(hObject, eventdata, handles)
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end
function n_region1_Callback(hObject, eventdata, handles)
function n_region1_CreateFcn(hObject, eventdata, handles)
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end
function n_region2_Callback(hObject, eventdata, handles)
function n_region2_CreateFcn(hObject, eventdata, handles)
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end
function uitable2_CellSelectionCallback(hObject, eventdata, handles)
Appendix B

RCWA algorithm in Matlab extended to layered structures

close all
clear all

for parameter3=1:1
Nlay= 3; % number of layers under grating
lambda = 632.8e-9; %1 um free space wavelength
eps_1 = 1.0; %dielectric constant region I
eps_3 = 2.2201; %PMMA : layer 1 dielectric constant region III
d3 = 1e-6; % 1 micron pmma
eps_4 = 2.16031204; %EpoClad : layer 2 dielectric constant region IV
d4=20e-6; %20 micron epoclad
eps_5 = 2.16031204; %Borofloat glass : layer 3 dielectric constant region V
d5= 700e-6; %700um glass
eps_6 = 1.0; %air dielectric constant region VI
Lambda = 1010e-9; %grating period
theta_in=0; % incidence angle in radians

K= 2*pi/Lambda; %Crystal K-vector

k1= 2*pi*sqrt(eps_1)/lambda; %length k-vector region I
k1i=k1; %length k-vector region I = length reflected k-vector region I
k3=2*pi*sqrt(eps_3)/lambda; %length k-vector region III
k4=2*pi*sqrt(eps_4)/lambda; %length k-vector region 4
k5=2*pi*sqrt(eps_5)/lambda; %length k-vector region 5
k6=2*pi*sqrt(eps_6)/lambda; %length k-vector region 6

x_res=1e-10; %1nm x-resolution of numerical computations
Nx=ceil(Lambda/x_res); %number of discrete x-cells
sweep=(10:10:400);
%this was used for a sweep in depth d to compare with paper results
 parameter1=0;
for parameter2=1:1
tic
 for d=sweep.*1e-9
   tic

N=70; %number of slabs to approximate grating
s=51; %number of Bloch modes i=-1,0,+1, only odd numbers allowed

% Calculate fixed quantities:

for p=1:s
    orders(p)=p-(s+1)*0.5; % orders = [−s, −s+1, ... , −1, 0, +1,..., +s]
end

for p = orders % calculation of the z-components of the k-vectors
    number=k1^2-(k1*sin(theta_in)-p*K)^2;
    if number<0
        k1z(floor(p+(s+1)*0.5))=1i*abs(sqrt(number));% exp decay into region I
    else
        k1z(floor(p+(s+1)*0.5))=sqrt(number);%abs value of k1z
    end
    number=k3^2-(k1*sin(theta_in)-p*K)^2;
    if number<0
        k3z(floor(p+(s+1)*0.5))=-1i*abs(sqrt(number));% exp decay into region III
    else
        k3z(floor(p+(s+1)*0.5))=sqrt(number);%abs value of k3z
    end
    number=k4^2-(k1*sin(theta_in)-p*K)^2;
    if number<0
        k4z(floor(p+(s+1)*0.5))=-1i*abs(sqrt(number));% exp decay into region 4
    else
        k4z(floor(p+(s+1)*0.5))=sqrt(number);%abs value of k4z
    end
    number=k5^2-(k1*sin(theta_in)-p*K)^2;
    if number<0
        k5z(floor(p+(s+1)*0.5))=-1i*abs(sqrt(number));% exp decay into region 5
    else
        k5z(floor(p+(s+1)*0.5))=sqrt(number);%abs value of k5z
    end
    number=k6^2-(k1*sin(theta_in)-p*K)^2;
    if number<0
        k6z(floor(p+(s+1)*0.5))=-1i*abs(sqrt(number));% exp decay into region 6
    else
        k6z(floor(p+(s+1)*0.5))=sqrt(number);%abs value of k3z
    end
end

grating=zeros(Nx,N); % grating f(x,n) zero when in region I, 1 in region III
% remove the comments to switch between sine and rectangular
% example: square profile.
for i=1:(Nx+1)
    X(i)=(i−1)*x_res;
end
for n=1:N
    grating(i,n)=heaviside(i−Nx/2); %this defines the symmetrical 50% duty cycle square grating for all slabs N
end

--example: sine profile.--
for i=1:(Nx+1)
    X(i)=(i−1.0+0.5)*x_res;
    for n=1:N
        y=(n−1.0+0.5)*d/N;
        number = 0.5*d*(1.0+sin(K*X(i)));
        if y > number
            grating(i,n)=1; %this defines the regions of 1's for a sine
        end
    end
end

for n=1:N
    fraction=0.5;
    fraction=nnz(grating(:,n))/length(grating(:,n)); %fraction of non-zero elements of the grating function
    eps_2(n)=eps_3*fraction+eps_1*(1.0−fraction); %average permittivity in slab n
    k2(n)=2*pi*sqrt(eps_2(n))/lambda;
    number= k2(n)^2−(k1*sin(theta_In))^2;
    if number < 0
        k2_z(n)=-1i*abs(sqrt(number)); %exp decay in region II
    else
        k2_z(n)=sqrt(number);
    end
    for h=1:s
        eps_F3(h,n)=(1.0/Lambda)*x_res*trapz(grating(:,n).*exp(−1i*K*h.*X(:))); %direct numerical evaluation of the integral
    end
    eps_F2(:,n)=(x_res/Lambda).*fft(grating(:,n)); %fast fourier transform, gives almost same results as eps_F
end

% eigenvectors and eigenvalues of the spaceharmonics Si
A=zeros(s,s);
D=zeros(s,s);
B=zeros(s,s);
S=zeros(2*s,2*s,N); %the state-space matrix for each slab n
for n=1:N
    for x=1:s
        for y=1:s
            if x==y
                p=x−((s+1)*0.5);
                C(x,y)=−(K^2)*p*(m−p);
                D(x,y)=2+1i*k2_z(n);
                B(x,y)=1.0;
            end
        end
    end
end

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else
    if y > x
        C(x, y) = -(2*pi/lambda)^2 * (eps_3 - eps_1) * conj(eps_F3(y-x,n));
    else
        C(x, y) = -(2*pi/lambda)^2 * (eps_3 - eps_1) * eps_F3(x-y,n);
    end
end

S(:,:,n) = [S1, S2];

% sum_flags = 0;
for n = 1:N
    % [Vectoren2, EigMatrix2, flag] = eigs(S(:,:,n), 2 * s);
    % there are different eigenvalue solvers in Matlab
    [Vectoren, EigMatrix] = eig(full(S(:,:,n)));
    % sum_flags = sum_flags + sum_flags;
    for x = 1:2 * s
        eigenwaarden(x, n) = EigMatrix(x, x); % eigenvalues(i,n)
        % eigenwaarden2(x, n) = EigMatrix2(x, x);
        for y = 1:2 * s
            eigenvectoren(x, y, n) = Vectoren(x, y); % eigenvectors(i,n)
            % eigenvectoren2(x, y, n) = Vectoren2(x, y);
        end
    end
end

% sum_flags

%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%) Boundary condition equations for E_tan, H_tan
%%%%%%%%%%%%%%%%%%%%%%%%%%%%

M = zeros(2 * s * (N + 1 + Nlay), 2 * s * (N + 1 + Nlay)); % the equation to be solved is M * X = Bx
M_start = zeros(2 * s, 2 * (N + 1 + Nlay) * s); % equations between I and first slab
M_end = zeros(2 * s, 2 * (N + 1 + Nlay) * s); % equations between last slab and III
M_n = zeros(2 * s * (N - 1), 2 * s * (N + 1 + Nlay)); % equations between n and n+1
M_lay_end = zeros(2 * s, 2 * s * (N + 1 + Nlay)); % equations between homogenous layers
Bx = zeros(2 * s * (N + 1 + Nlay), 1);
for x = 1:s
    for y = 1:2 * s
        M_start(x, y) = eigenvectoren(x, y, 1); % E field tang
        M_start(x+s, y) = eigenvectoren(x, y, 1)*...
            (eigenwaarden(y, 1) - li * k2_z(1)); % H field tangential
    end
    M_start(x, x+2 * s * N) = -1.0; % the components for R01
    M_start(x+s, x+2 * s * N) = -li * k1i_z(x); % the components for R01
end

for x = 1:s
    for y = 1:2 * s
        M_end(x, y+2 * s * (N-1)) = eigenvectoren(x, y, N)*...
            exp((eigenwaarden(y, N) - li * k2_z(N)) * d); % E field tang
M_end(x+s,y+2*s*(N-1)) = eigenvectoren(x,y,N) * ...
  (eigenwaarden(y,N)-li*k2_z(N)) * ...
  exp((eigenwaarden(y,N)-li*k2_z(N))*d); % H field tangential
end
M_end(x,x+2*s*N+s) = -1.0; % the components for T3i
M_end(x,x+2*s*N+2*s) = exp(-li*k3i_z(x)*d3); % the components for T3i
M_end(x,x+2*s*N+2*s) = -li*k3i_z(x) * exp(-li*k3i_z(x)*d3); % the components for T3i

for n=1:N-1
  for x=1:s
    M_{n}(x+2*s*(n-1),y+2*s*(n-1)) = eigenvectoren(x,y,n) * ...
    exp((eigenwaarden(y,n)-li*k2_z(n))*n*d/N); % E field tangential slab n
    M_{n}(x+2*s*(n-1),y+2*s*n) = eigenvectoren(x,y,n+1) * ...
    exp((eigenwaarden(y,n+1)-li*k2_z(n+1))*n*d/N); % E field tangential slab n+1
    (eigenwaarden(y,n+1)-li*k2_z(n+1)) * ...
    exp((eigenwaarden(y,n)-li*k2_z(n))*n*d/N); % H field tangential slab n
    (eigenwaarden(y,n+1)-...)
    li*k2_z(n+1) * exp((eigenwaarden(y,n+1))-...
    li*k2_z(n+1))*n*d/N); % H field tangential slab n+1
  end
end

for x=1:s
  M_{lay}(x,x+2*s*N+s) = exp(-li*k3i_z(x)*d3); %
  M_{lay}(x,x+2*s*N+s+2) = 1.0; %
  M_{lay}(x,x+2*s*N+s+3) = -1.0; %
  M_{lay}(x,x+2*s*N+s+4) = exp(-li*k4i_z(x)*d4);
  M_{lay}(x,x+2*s*N+s+5) = k3i_z(x) * exp(-li*k3i_z(x)*d3); %
  M_{lay}(x,x+2*s*N+s+6) = -k3i_z(x); %
  M_{lay}(x,x+2*s*N+s+7) = -k4i_z(x); %
  M_{lay}(x,x+2*s*N+s+8) = k4i_z(x) * exp(-li*k4i_z(x)*d4);
  M_{lay}(x,x+2*s*N+s+9) = -k4i_z(x); %
  M_{lay}(x,x+2*s*N+s+10) = -k5i_z(x); %
  M_{lay}(x,x+2*s*N+s+11) = k5i_z(x) * exp(-li*k5i_z(x)*d5); %
end

for x=1:s
  M_{lay_end}(x,x+2*s*N+5*s) = exp(-li*k5i_z(x)*d5); %
  M_{lay_end}(x,x+2*s*N+6*s) = 1.0; %
  M_{lay_end}(x,x+2*s*N+7*s) = -1.0; %
  M_{lay_end}(x,x+2*s*N+8*s) = k5i_z(x) * exp(-li*k5i_z(x)*d5); %
end

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M\_lay\_end(x+s,x+2*s*N+6*s)=−k5i\_z(x);%
M\_lay\_end(x+s,x+2*s*N+7*s)=−k6i\_z(x);%
end

M=vertcat(M\_start,M\_n,M\_end,M\_lay\_n,M\_lay\_end); %put the 3 matrices together

%the right hand side of the equation
Bx(((s+1)*0.5)+s)=−1i*k1i\_z(((s+1)*0.5));

X\_result=M\_lay\_end; %Gaussian elimination solver
for x=1:s
    Ri(x)=X\_result(x+2*N*s); %amplitude reflection coefficient
    Ti(x)=X\_result(x+2*s*(N+N\_lay+1)-s); %amplitude transmission coefficient
    DE\_1i(x)=real(k1i\_z(x)/k1i\_z(((s+1)*0.5)))*...%power reflectance coefficient region I
        abs(Ri(x))^2;
    DE\_3i(x)=real(k6i\_z(x)/k1i\_z(((s+1)*0.5)))*...%power transmittance coefficient region III
        abs(Ti(x))^2;
end

DE\_3i\_min1(parameter1)=DE\_3i((s+1)*0.5+1);
DE\_3i\_0(parameter1)=DE\_3i((s+1)*0.5);
DE\_3i\_min1(parameter1)=DE\_3i((s+1)*0.5-1);
DE\_1i\_1(parameter1)=DE\_1i((s+1)*0.5+1);
DE\_1i\_0(parameter1)=DE\_1i((s+1)*0.5);
DE\_1i\_min1(parameter1)=DE\_1i((s+1)*0.5-1);
convergence(parameter1)=...%1.0 − sum (DE's) , the smaller the better
abs(1−sum(DE\_1i(:))−sum(DE\_3i(:)));
toc

end

Dparam=sweep;
figure
hold on
plot(Dparam,DE\_3i\_1,':r','LineWidth',2)
plot(Dparam,DE\_3i\_0,':r','LineWidth',2)
plot(Dparam,DE\_3i\_min,':g','LineWidth',2)
plot(Dparam,DE\_1i\_1,':g','LineWidth',2)
plot(Dparam,DE\_1i\_0,':b','LineWidth',2)
plot(Dparam,DE\_1i\_min,':b','LineWidth',2)
hold off
end
Bibliography


