

## Development of a Small-scale Spectrometer for Visible Light

<sup>1,\*</sup> Matthias HAUPT, <sup>1</sup> Sebastian SMARZYK, <sup>1</sup> Katharina STRATHMANN

<sup>1</sup>Jade University of applied sciences, Friedrich-Paffrath-Straße 101,  
26389 Wilhelmshaven, Germany

<sup>1</sup>Tel.: +49 4421 – 985 2625

\*E-mail: [matthias.haupt@jade-hs.de](mailto:matthias.haupt@jade-hs.de)

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**Abstract:** This paper details the development of a polymer-based miniaturized spectrometer as part of the "Minispectral" project at Jade University of Applied Sciences. The spectrometer's design leverages advanced injection molding techniques to create a polymer dome, which forms the core structure of the device. A concave diffraction grating is incorporated on the dome's surface to disperse incoming light into its constituent wavelengths. The dome and grating are designed with a generalized Rowland circle radius ratio in three-dimensional space, producing a lens effect for focused detection and analysis. Zemax ray tracing simulations are used to model the optical setup, while wave optics simulations, utilizing Rigorous Coupled-Wave Analysis (RCWA) implemented through Dynamic Link Libraries (DLLs) in Zemax, simulate critical parameters such as dome alignment, blazing, and the line density of the concave diffractive optical element (DOE). These simulations are vital for optimizing the spectrometer's performance. This paper presents the basic design, simulations, and the first test grating masters.

**Keywords:** Spectrometer, Polymer-based, Miniaturized, Injection molding, Diffraction grating, Optical simulations.

### 1. Introduction

Analyzing the optical spectrum of matter provides valuable insights into its chemical and molecular composition. In various applications, such as examining food, blood, or medications, miniaturized mobile spectrometers can serve as a time-saving alternative or valuable supplement to traditional stationary spectrometers typically used in laboratory settings. The primary objective of this project is to develop a polymer-based optic through a single manufacturing step. This is achieved by leveraging advanced injection molding technology and specially developed innovative tools. This paper not only focuses on the fundamental functions of the miniaturized spectrometer but also delves into its current development status. Chapter two and three present the concept of the spectrometer as showcased

at the OPAL Conference '24 through a presentation and proceedings [1].

Starting from Chapter 3.1, the focus shifts to new findings, with particular emphasis on the initial fabrication of optical gratings.

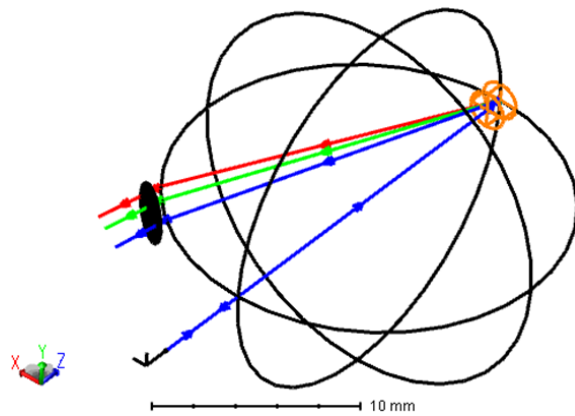
### 2. Design of the Spectrometer

#### 2.1. Basic Concept

The spectrometer utilized in this study is built upon the fundamental concept of a Rowland circle [2]. The three-dimensional dome shape of the optics enables efficient light guiding, thereby improving the signal-to-noise ratio (S/N) [3]. The specific geometry of the dome, coupled with a concave diffraction

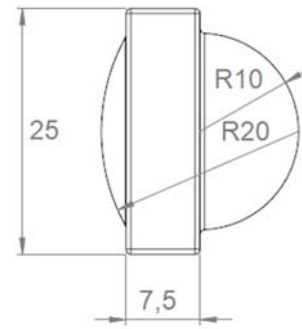
grating, allows all functions of a spectrometer to be fulfilled, eliminating the need for previously required individual components such as elaborate lens systems.

The operation of the spectrometer is illustrated in Fig. 1. Light enters through an input fiber into the polymer-based dome with a radius of  $r$ . At the end of the dome lies a mirrored, concave dispersion grating with a radius of  $2r$ . This grating disperses the light into its individual wavelengths and reflects it back into the polymer dome. Due to the Rowland circle radius ratio of 2 to 1, the rays focus on the surface of the dome. A detector array is placed on the surface of the dome to detect the light decomposed into individual wavelengths and to utilize it for further analysis [4].



**Fig. 1.** Simulation created with Ansys Zemax to illustrate the concept of the spectrometer: The optics of the spectrometer are based on a polymer-based dome with a radius of  $r$ . A mirrored grating is applied to this dome, which has a curvature radius of  $2r$ .

To better understand the system, Fig. 2 depicts a detailed drawing of the planned layout of the entire optics of the spectrometer. The dimensions are provided in millimeters, with the grating sphere having a radius of 20 mm and the input sphere having a radius of 10 mm. The drawing clearly illustrates the various components of the optical system. The grating sphere is shown as a circular structure, but it is important to note that only a small portion of it will be covered with the actual grating, where the light will interact. This grating will be precisely applied to this specific area to disperse the incoming light into its spectral components effectively. Similarly, the input sphere is prominently displayed, with a radius of 10 mm. This sphere serves as the entry point for light into the system. It is important to mention that the light into the input sphere will be coupled using an optical polymer fiber (POF), enhancing the precision of light transmission and alignment for accurate analysis. Additionally, the drawing features a rectangular thickening in the center, serving as a mounting bracket for the integration of the optical system into a larger framework. This strategic design facilitates the handling and installation of the spectrometer across various application scenarios.



**Fig. 2.** Drawing depicting a planned layout of the entire optics of the spectrometer, showcasing dimensions in millimeters. It highlights the different radii, with the grating sphere at a radius of 20 mm and the input sphere at a radius of 10 mm. The rectangular thickening in the center may serve as a future mounting bracket for integration into a system.

## 2.2. Challenges of Curved Gratings Compared to Flat Gratings in Polymer-based DOEs

Curved gratings in polymer-based diffractive optical elements (DOEs) present unique challenges compared to their flat counterparts but also offer distinct advantages, including the exploitation of focal effects. Unlike flat gratings, curved gratings can be designed to focus light at specific points or along specific paths, enabling enhanced light manipulation and control. This focal effect can be harnessed for various applications, including beam shaping, spectral focusing, and aberration correction. In spectroscopy, curved gratings hold immense potential for improving the resolution and sensitivity of optical systems. Precisely controlling the curvature and geometry of the grating allows for tailoring the dispersion characteristics to achieve optimal spectral resolution and efficiency.

The production of curved gratings in polymer-based diffractive optical elements (DOEs) presents a unique set of challenges compared to their flat counterparts, primarily concerning fabrication methods and associated difficulties. Unlike flat gratings, which can be relatively straightforward to manufacture using techniques such as photolithography or electron beam lithography on planar substrates, the fabrication of curved structures requires more intricate processes. One significant hurdle lies in achieving precise and uniform curvature profiles across the polymer substrate. Traditional lithographic techniques may struggle to pattern curved surfaces accurately, leading to deviations from the desired geometry and potentially compromising optical performance.

Traditional lithographic techniques struggle with accurate pattern replication on curved substrates, prompting the development of advanced manufacturing methods such as nanoimprint lithography, hot embossing, and ultraprecision machining (UPM). Nanoimprint lithography and hot

embossing enable the replication of complex curvature profiles with high precision, while UPM offers direct machining of curved surfaces with submicron accuracy. These methods address the need for precise curvature profiles and feature replication, though challenges such as material compatibility and scalability persist.

### **2.3. Optical Simulation**

Raytracing simulations through Zemax software are utilized to ascertain the optimal dimensions of both the diffraction grating radius and dome radius, particularly when dealing with a large numerical aperture (NA), as observed in optical polymer fibers (POF). The polymer dome's diameter is targeted to be no more than 10 mm. Unfortunately, ray tracing is insufficient for accurately modeling diffractive optical elements due to its inherent limitation in accurately representing diffraction phenomena. Diffractive optical elements manipulate light through interference patterns rather than simple ray propagation, so more sophisticated computational methods are needed.

Various mathematical models can be considered for simulating curved optical gratings, including Finite Difference Time Domain (FDTD) and Finite Element Method (FEM). However, among these options, Rigorous Coupled-Wave Analysis (RCWA) emerges as a promising choice. RCWA offers precise solutions to Maxwell's equations while maintaining computational efficiency and adaptability to different geometries and materials. Compared to methods such as FDTD and FEM, RCWA excels in accuracy, computational speed, and ease of parameter exploration. These features make RCWA an attractive option to effectively model curved grating systems.

Within Zemax, the diffraction grating is simulated using Dynamic Link Libraries (DLLs) and employing RCWA. This allows dynamic adjustment and simulation of key parameters such as the curvature radius and blazing of the grating. The grating is anticipated to have a line density of up to 1000 lines/mm, with the objective of achieving a resolution of less than 1 nm.

The optical path depicted in Fig. 1 was simulated using the simulation software Ansys Zemax OpticStudio for various combinations of wavelengths and radii. As illustrated in Fig. 1, three wavelengths (400 nm, 550 nm, 650 nm) and a Rowland circle radius of 10 mm were considered. The grating has a line density of 1000 lines/mm. Aluminum emerges as a promising material for mirroring the grid, as it enhances reflectivity in the visible spectrum [5]. Therefore, it was assumed for this purpose in the simulation. In this case, the entrance aperture of the spectrometer has a diameter of 1 mm, corresponding to the diameter of a standard SI polymer optical fiber (POF) [6]. To optimize the performance further, extensive parametric studies were conducted within Zemax, exploring a wider range of parameters such as

different grating materials, variations in dome diameter, and line densities. These simulations were crucial in refining the design parameters to achieve superior optical performance, especially in terms of resolution and spectral efficiency. Furthermore, the simulations allowed for the identification of potential challenges and trade-offs, enabling informed decision-making during the design process. Overall, the comprehensive simulation approach facilitated the development of a robust and efficient spectrometer system tailored to the specific requirements of optical polymer fibers.

### **2.4. Challenges in Optical Injection Molding with Aluminum Coating**

Injection molding optical components poses inherent challenges such as achieving smooth surfaces, managing thermal stresses, and ensuring precise mold design. Despite these hurdles, we've opted to utilize PMMA for our initial demonstrator due to its favorable optical properties. Optical injection molding with subsequent aluminum coating application presents several challenges, encompassing both technological intricacies and process-related considerations. Initially, the injection molding process must ensure precise replication of complex geometries or thin-walled structures on the substrate material. Once the molding is complete, the application of the aluminum coating poses additional challenges. Achieving uniform distribution and proper adhesion of the aluminum onto the molded part becomes crucial, considering the specialized properties of aluminum coatings. Thermal stresses generated during the coating process could potentially compromise the optical characteristics or integrity of the coating, necessitating careful temperature control. When exploring methods for applying the aluminum coating, sputtering emerges as a promising option due to its ability to achieve uniform thickness and excellent adhesion onto substrates. While other techniques such as physical vapor deposition (PVD), chemical vapor deposition (CVD), and thermal spraying offer alternatives, sputtering appears particularly well-suited for this application. However, the selection of the most suitable method depends on factors such as substrate material, coating thickness requirements, and production volume. Thorough consideration of these factors is essential to determine the optimal coating method, ensuring the production of high-quality optical injection molded parts with aluminum coating.

## **3. Manufacturing and Characterization**

Following the simulations and laboratory pre-tests, the production of initial demonstrators ensues. Here, the dome will be manufactured using state-of-the-art

injection molding technology in a single process step. The fabrication of the grating on the surface of the polymer dome is proposed to be executed through Ultra-Precision Machining (UPM). This involves a manufacturing technique where very small layers of the material's surface are removed using diamond tools. UPM enables the creation of highly precise structures with sub-micrometer tolerance deviations, making it suitable for producing spherical and aspherical surfaces with high optical quality [7]. The initial demonstrators thus produced will undergo thorough examination and characterization in the laboratory. To ensure the accuracy of the grating structures, an Atomic Force Microscope (AFM) will be employed. AFM provides high-resolution imaging and precise measurements at the nanometer scale, allowing for detailed analysis of surface features. This step is crucial as it ensures that the manufactured gratings match the intended specifications with minimal deviation. Subsequently, the findings will be compared with the simulation results. Leveraging these insights, the optics parameters and production workflows will be optimized to enhance the subsequent generation of spectrometers. This achievement sets the stage for the near-future launch of the first fully functional, miniaturized spectrometer, utilizing polymer-based materials. Expanding upon this process, once the initial demonstrators are successfully produced, a comprehensive evaluation will be conducted to validate their performance under various conditions and operational scenarios. This evaluation will involve a meticulous analysis of the spectral data obtained from the spectrometer, assessing its accuracy, resolution, and sensitivity. Building upon the insights gained from both experimental evaluations and computational simulations, iterative refinements will be made to the optics parameters and production workflows. This iterative process will aim to enhance the overall performance, reliability, and manufacturability of the miniaturized spectrometer.

Additionally, advancements in material science and manufacturing technologies will be explored to further push the boundaries of performance and miniaturization.

### **3.1. Fabrication of Initial Gratings in Nickel Phosphorus**

Nickel phosphorus offers several advantages for the fabrication of optical gratings, particularly with lattice constants around  $1\ \mu\text{m}$ , due to its unique properties, primarily its non-crystalline structure. Unlike crystalline materials, nickel phosphorus is amorphous, lacking defined crystal grains or axes. This characteristic reduces scattering and interference effects in optical applications, allowing for the production of high-resolution and precise optical gratings with minimal side effects. The amorphous nature of nickel phosphorus also ensures a uniform

refractive index distribution across the grating surface, essential for accurate dispersion of light into different wavelengths and the mitigation of optical aberrations. Despite its non-crystalline structure, nickel phosphorus maintains high mechanical stability, crucial for long-term performance and reliability of grating structures in optical devices. Furthermore, nickel phosphorus exhibits excellent chemical resistance, enhancing the durability of gratings in diverse environmental conditions [8]. Its chemical composition and amorphous structure facilitate the precise fabrication of fine gratings with lattice constants as small as  $1\ \mu\text{m}$ , meeting the stringent requirements of high-resolution optical applications. In summary, the combination of amorphous properties, precise manufacturability, good optical characteristics, mechanical stability, and chemical resistance makes nickel phosphorus an ideal material for producing optical gratings with small lattice constants in the micron range.

### **3.2. Investigating Nickel Phosphorus Gratings**

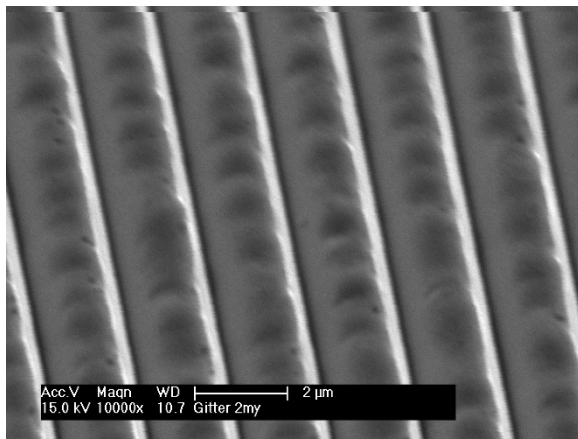
Gratings fabricated in nickel phosphorus using a monocrystalline diamond tip were thoroughly investigated in this study. Three distinct grating designs with lattice constants of  $1\ \mu\text{m}$ ,  $1.5\ \mu\text{m}$ , and  $2\ \mu\text{m}$ , each featuring a  $60^\circ$  blazing angle, were subjected to detailed examination using both Atomic Force Microscopy (AFM) and scanning electron microscopy (SEM). AFM provided precise measurements of surface topography, including grating pitch and depth, offering insights into the structural dimensions critical for optical performance.

SEM analysis, on the other hand, delved into the internal structure and composition of the gratings, examining crystalline quality and potential defects. In addition to microscopy, diffraction efficiency measurements were conducted across various wavelengths to assess optical performance.

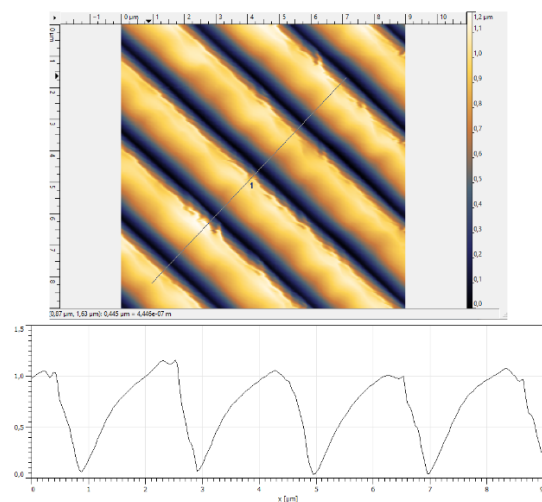
SEM analysis, on the other hand, delved into the internal structure and composition of the gratings, examining crystalline quality and potential defects. In addition to microscopy, diffraction efficiency measurements were conducted across various wavelengths to assess optical performance.

Figs. 3 to 8 depict scanning electron microscopy (SEM) and atomic force microscopy (AFM) images of the investigated grids. These images provide detailed insights into the structural characteristics and surface morphology of the grids under study. Through meticulous analysis, the lattice constants have been precisely determined to be  $1\ \mu\text{m}$ ,  $1.5\ \mu\text{m}$ , and  $2\ \mu\text{m}$ , indicating the varied periodicity across different samples. Notably, the fabrication process has demonstrated the capability to produce homogeneous grids over extensive areas, suggesting robust manufacturing techniques. However, upon closer examination, a minor undulation is noticeable at the apex of the grooves, which could potentially influence

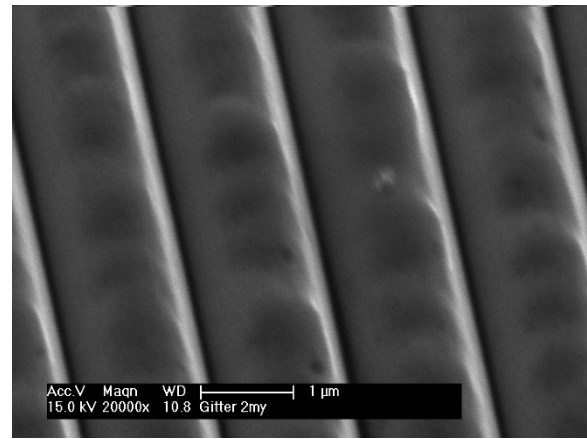
the functional properties of the grids. The depth of the grid structures measures approximately  $0.5 \mu\text{m}$ , underscoring their substantial structural integrity and depth profile. Nonetheless, further investigations are required to verify the blazing angle, a critical parameter influencing the optical performance of the grids. This ongoing verification process aims to ensure accurate and consistent measurement of this angle across all samples. In summary, the SEM and AFM images provide valuable data confirming the uniformity and structural characteristics of the grids, while also highlighting areas for potential refinement and optimization in future manufacturing processes. This version expands on the details of the SEM and AFM images, discusses the precision of lattice constants, mentions surface characteristics, and emphasizes the need for further verification of the blazing angle, providing a comprehensive overview of the findings.



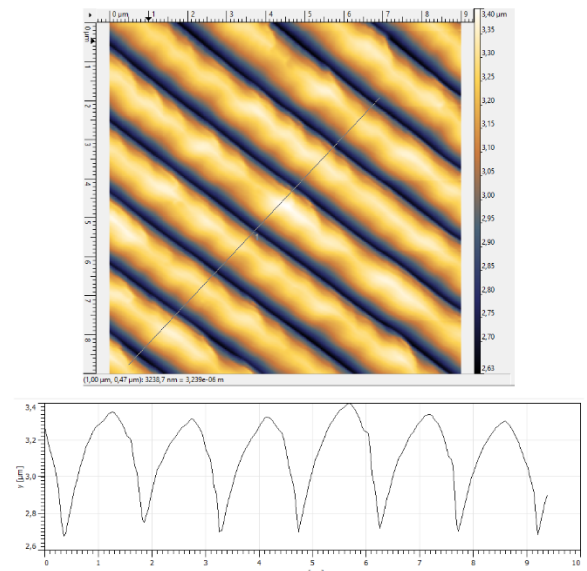
**Fig. 3.** SEM image of an investigated grid at 10,000× magnification. The image clearly shows the regular grid structures with a lattice constant of  $2 \mu\text{m}$ . Minor irregularities are visible at the tips of the grooves.



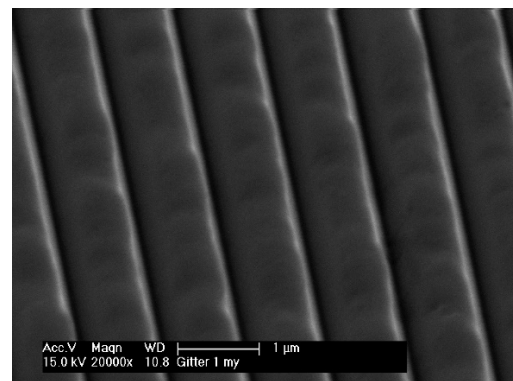
**Fig. 4.** AFM image of the same grid as shown in Fig. 3. The image displays the three-dimensional topography of the grid structures with a lattice constant of  $2 \mu\text{m}$ . Surface fluctuations along the grid grooves are evident.



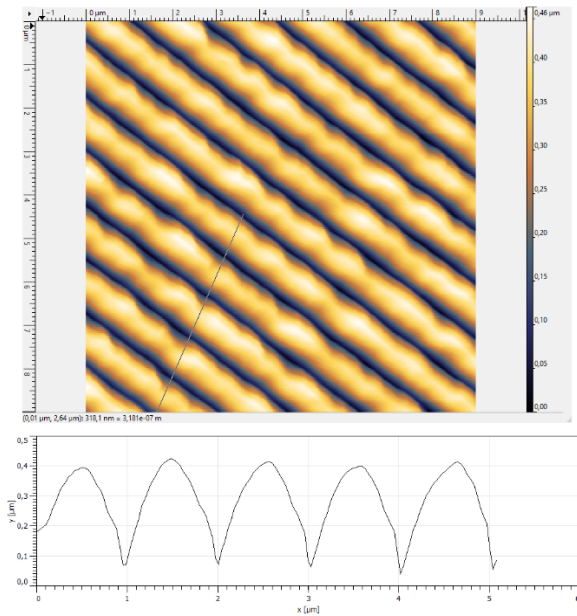
**Fig. 5.** SEM image of an investigated grid at 20,000× magnification. The image clearly shows the regular grid structures with a lattice constant of  $1.5 \mu\text{m}$ . Minor irregularities are visible at the tips of the grooves.



**Fig. 6.** AFM image of the same grid as shown in Fig. 5. The image displays the three-dimensional topography of the grid structures with a lattice constant of  $1.5 \mu\text{m}$ . Surface fluctuations along the grid grooves are evident.

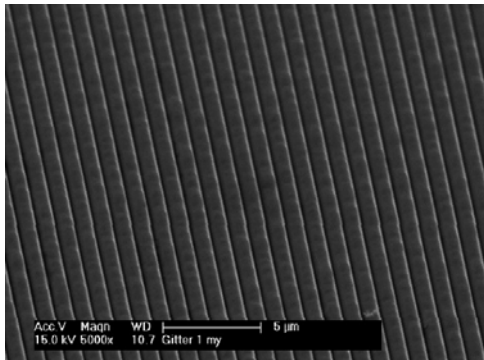


**Fig. 7.** SEM image of an investigated grid at 20,000× magnification. The image clearly shows the regular grid structures with a lattice constant of  $1 \mu\text{m}$ . Minor irregularities are visible at the tips of the grooves.



**Fig. 8.** AFM image of the same grid as shown in Fig. 7. The image displays the three-dimensional topography of the grid structures with a lattice constant of  $1\ \mu\text{m}$ . Surface fluctuations along the grid grooves are evident.

SEM image at  $5000\times$  magnification displaying a grid structure with a consistent lattice constant of  $1\ \mu\text{m}$ . The image vividly illustrates the uniformity of the grid pattern across a substantial area. This high degree of consistency underscores the precision and reliability of the manufacturing process in producing intricate microscale features. This observation is particularly evident in Fig. 9.



**Fig. 9.** SEM image at  $5000\times$  magnification showcasing a grid structure with a precise lattice constant of  $1\ \mu\text{m}$ . The image reveals the remarkable homogeneity of the grid pattern across an extensive area. This level of uniformity underscores the effectiveness of the fabrication process in achieving consistent microscale features.

### 3.2. From Nickel Phosphorus to Reflective Optics: Molding and Characterization Process

The next phase involves transferring the fabricated grids made from nickel phosphorus into silicone

molds. This transfer process is crucial as it ensures the replication of intricate grid patterns with high fidelity. The grids are meticulously embedded into silicone, leveraging its moldability to capture the precise details of the nickel phosphorus structure. Once molded, these grids undergo thorough optical inspection to analyze their diffraction properties as transmissive gratings. This examination aims to verify the accuracy of the silicone replication process in preserving the intended diffraction orders and spatial characteristics of the original grids. Following the transmissive analysis, the grids undergo a crucial enhancement step by being coated with a layer of silver. This silver coating serves multiple purposes: it enhances the reflectivity of the grids and provides durability against environmental factors, ensuring long-term optical performance. After silver coating, the grids are subjected to further scrutiny using advanced microscopy techniques such as Scanning Electron Microscopy (SEM). This examination verifies the exactness of the silicone molding process and ensures that the silver coating adheres uniformly across the grid surfaces, maintaining the precision required for their optical functionality. Once the structural integrity and coating uniformity are confirmed, the grids are reassessed for their optical characteristics, this time as reflective gratings. The reflective properties are meticulously evaluated to assess factors such as reflectance efficiency, spectral response, and overall optical quality. This evaluation phase is critical as it validates the grids' performance as reflective optical elements suitable for various applications in optics and photonics. In summary, the transformation of nickel phosphorus grids into silicone molds, followed by optical inspection, silver coating, and final reflective evaluation, underscores a meticulous process aimed at ensuring the grids' functionality and reliability as high-performance optical components.

## 4. Outlook

This chapter introduces a forward-looking perspective split into two essential areas: simulation and manufacturing. We explore how virtual simulations and actual production processes interact and evolve, reshaping efficiency and precision.

### 4.1. Simulation

Continuing from our previous chapters where simulations were conducted and physical optical grids were fabricated and measured, this section marks a critical advancement: integrating these measured grids into a digital simulation environment. Our goal now is to accurately translate real-world measurements into a virtual context. This includes capturing detailed dimensions, angles, and spatial relationships with precision, ensuring that our digital simulation faithfully represents the physical grids created earlier.

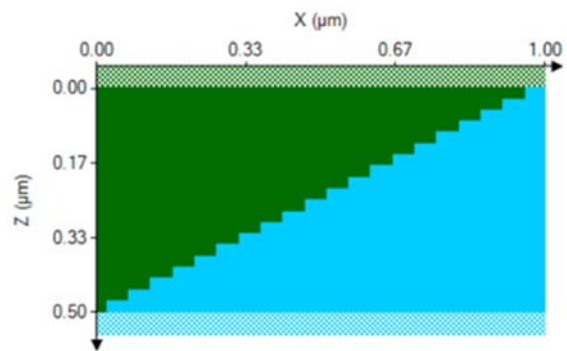
Optical simulations are instrumental in this process, facilitated through advanced software such as Zemax. Utilizing sophisticated computational algorithms and modeling techniques inherent in Zemax, our aim is to faithfully replicate the optical properties of the measured grids. By inputting these measured data points into Zemax, we create virtual models that simulate how light interacts with these optical structures. This process not only validates our simulations but also enables us to predict and optimize optical performance across different scenarios.

In Fig. 10, we present a visualization of the grid simulation implemented in Zemax using an RCWA DLL (Rigorous Coupled Wave Analysis Dynamic Link Library). This implementation allows the grid to be replicated layer by layer within the software environment. Our objective is to systematically recreate the measured structures, refining the simulation iteratively to achieve accurate representation.

## 4.2. Manufacturing

In the manufacturing process, there are several critical considerations to keep in mind for the next step. One of the foremost tasks is the creation of a stamp. This stamp must be designed in such a way that its microstructures can be accurately replicated not only in silicone but also in other polymers, such as polymethyl methacrylate (PMMA). This requirement demands a precise understanding of the material properties and the behavior of these polymers during the replication process. The stamp's microstructures must maintain their integrity and detail across different materials to ensure the fidelity of the replicated patterns. Additionally, there is the challenge of shaping a curved grating surface. Unlike planar surfaces, curved surfaces introduce complexities in both the design and manufacturing stages. These complexities arise from the need to ensure that the grating's microstructures are uniformly transferred onto a non-flat surface. Achieving this requires advanced techniques and tools capable of handling the intricacies involved in curving the grating while preserving the desired optical properties. The gratings presented in section three are currently planar, which simplifies the manufacturing process to a certain extent. Planar gratings are easier to produce and replicate because they do not involve the added complexity of working with curved surfaces. However, the transition to curved gratings is a necessary step to meet the evolving requirements of various applications. Curved gratings can offer enhanced performance and new functionalities that planar gratings cannot provide. To successfully move from planar to curved grating surfaces, it is essential to develop a thorough understanding of how to control the replication process on a curved geometry. This includes investigating the optimal conditions for transferring microstructures onto curved surfaces and

ensuring that the mechanical and optical properties of the gratings are not compromised. Furthermore, the manufacturing techniques must be adapted or even redesigned to accommodate the new geometrical challenges posed by curved surfaces. In summary, the next step in the manufacturing process involves careful consideration of two main aspects: the creation of versatile stamps capable of replicating microstructures in various polymers, and the development of methods to shape and replicate curved grating surfaces.



**Fig. 10.** Visual representation of the optical grid simulation in Zemax utilizing Rigorous Coupled Wave Analysis Dynamic Link Library (RCWA DLL). The grid structure is modeled layer by layer, exemplifying parameters such as a lattice constant of  $1 \mu\text{m}$ , a blaze angle of  $63^\circ$ , and a grid depth of  $0.5 \mu\text{m}$ . The simulation calculation includes 20 uniformly decreasing layers, aiming to systematically replicate and validate measured optical structures.

## 5. Conclusions

In summary, our research highlights the progress made in developing a miniaturized spectrometer based on polymer optics. By integrating modern injection molding technology with innovative design principles, we've achieved a compact yet efficient analytical tool suitable for diverse applications such as food analysis, medical diagnostics, and pharmaceutical quality control. In this context, we have also elucidated the fundamental concept of the spectrometer. Additionally, we have presented the first grids made from nickel-phosphorus and examined their structures using Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The successful simulation and manufacturing of initial prototypes signify a significant step forward in spectroscopic instrumentation. Further refinement through laboratory characterization and optimization of production workflows will enhance the performance and scalability of this technology, facilitating its integration into various industrial and scientific settings. This advancement holds the promise of revolutionizing spectral analysis, offering a practical and accessible solution for rapid chemical and molecular composition determination.


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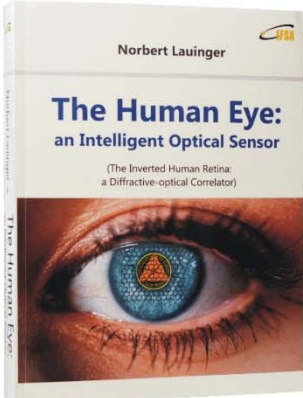
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### Norbert Lauinger



# The Human Eye: an Intelligent Optical Sensor

(The Inverted Human Retina: a Diffractive-optical Correlator)





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