euspen's 20th International Conference & Exhibition, Geneva, CH, June 2020
www.euspen.eu

A phase retrieval inspired approach for the determination of optical aberrations in microscopy

Jan Krüger, Rainer Köning, Bernd Bodermann

Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Brunswick, Germany

jan.krueger@ptb.de

Abstract

Accurate bidirectional measurements are performed at PTB using UV- microscopy. For this purpose, edge detection algorithms based on the rigorous calculation of the optical imaging problem are employed. Hence, all the parameters of the imaging system and the object must be considered due to their specific impact on the image formation. In order to further improve the model-based edge detection the small but inevitable optical aberrations of the imaging optics must be included into the simulations.

For the determination of the aberrations, microscopic images of state-of-the-art line gratings (shapes verified by AFM) are measured in the focus and several afocal planes of the microscope. This procedure is similar to a phase retrieval method with the only difference that usually idealized pinholes are measured there. A particle swarm optimisation (PSO) method is developed to determine the aberration of the used microscope in terms of Zernike polynomials. Therefore, the particles of the PSO are evenly spread over the parameter space that has been expanded by the Zernike polynomials. The optimisation problem consists of the minimization of the difference between the microscopic images in different focal planes and their respective simulated microscopic images. Because the illumination, imaging, and object parameters of the measured and the simulated microscopic images are identical, only a change of the Zernike polynomials is responsible for a minimization during an iteration of the PSO. First results show, that when convergence is achieved, the difference between the images is very small. The particle responsible for the minimum then holds the Zernike polynomials, which characterize the aberrations of the used microscope.

Keywords: microscopy, optical bidirectional measurements, particle swarm optimisation, rigorous simulations, physical edge detection

1. Introduction

In optical microscopy based dimensional metrology, the knowledge about the aberrations of the applied measurement system is crucial. While misalignments occurring over time are the obivious answer to why it is important to have an impression of the aberrant system, the consideration of the quantified optical aberrations in simulations is at least equally important. Especially, when closed housings prevent any further mechanical correction measures, an estimate of the unavoidable remaining aberrations is valueable.

For example, bidirectional measurements on micro- and nanostructures at PTB always involve supplementary simulations of the measurements to be able to obtain small measurement uncertainties [1]. In addition certain uncertainty contributions, like the uncertainty of the numerical aperture are determined using simulations. Hence, it is most crucial to be aware of the characteristics of the applied measuring system, since all the illumination, object and imaging parameters of the measurement need to be taken into account in the simulations [2]. Here, the optical aberrations are a part of the imaging parameters.

The optical aberrations of a measurement system can be derived experimentally or by phase retrieval techniques. Shack-Hartmann wavefront sensors and Tywmann-Green interferometers are also commonly applied methods for the measurements of optical aberrations [3]. However, they are usually used to investigate single optical components and have certain measurement demands concerning coherence or a plane wave incidence. Phase retrieval methods like the Gerchberg Saxton algorithm [4] only require a moveable camera along the optical axis to obtain the lateral intensity distributions for several planes. Through the application of a focus criterion, the the focal plane and the adjacent afocal planes are identified. The phase information of the light, and therefore the knowledge about the optical aberration, is embedded in the variation of the intensities of the neighboring focus planes. The derivation of the phase from the stack of intensity images is usually conducted by an iterative approach. Simplified, the algorithm compares the measured focus planes to numericaly calculated intensity distributions in corresponding focus planes. In each iteration, adjustments to the calculations are performed to achieve a better agreement with the measured intensities. Idealy, the simulated and measured profiles agree perfectly and yield the phase information after the execution of all iterations. Thereby, the optical aberrations are determined. Usually, very small and circular pinholes are positioned in the object plane during the measurements. This means that the acquired images in the respective focus planes are convolutions of the point spread function of the aberrant measuring system with the microscopical pinhole. A deconvolution for each measured image is necessary, since the algorithm requires the point spread function of the measurement system as an input value for its calculation. Therefore, the knowledge of the shape of the pinhole is most crucial for the success of the method [5].

Unfortunately, the fabrication of the desired microscopical pinholes in the regime of diameters below the diffraction limit is not satisfying. Occuring issues are that the pinholes are not perfectly circular, polluted during the fabrication or affected by unintentional light transmission in the proximity of the pinhole opening as a consequence of the limited absorption of the thin material layers due to limitations of the fabrication process.

In this contribution, we propose a new approach based on very well studied binary line gratings and supplementing rigorous calculations in a particle swarm optimization (PSO). The geometry of the chrome on glas grating, and thereby the fabrication process, is verified by measuring techniques like atomic force microscopy (AFM). This enables an accurate consideration of the object in the numerical calculations which in theory leads to a more resilient result. In section 2 the PSO approach is presented and first results are shown in section 3. The paper is then concluded in section 4.

2. Principle of the PSO approach

In PSO, the particles represent individual solutions to a cost function based on their respective position in a common parameter space. The particles also have the information about their own personal best solution for the optimization problem and the global best solution of all the particles. Depending on these information, the particles move inside the parameter space to obtain a better solution for the optimization problem during the next iteration [6].

The cost function at hand compares the previously performed measurements to rigorously calculated image profiles. Here, the images are calculated by the rigorous coupled wave analysis (RCWA) which takes the illumination and imaging parameters of the microscope as well as the geometrical and optical properties of the grating into account and solves the Maxwell equations exact for the specific diffraction problem [7]. The parameter space for the particles is here extended by the coefficients of the first 36 Zernike polynomials. The polynomials are a set of orthogonal polynomials above circular pupils which are widely used to describe the aberrations of optical systems [8]. It is assumed that all the other parameters are very well known and maintained over the course of the PSO. In the cost function, the simulated intensity profiles are fitted to the measured profiles by a least-squared algorithm for each of the particles. It is the goal of the PSO to minimize the result of the least squared algorithm since then the difference between the simulated and the measured profiles is minimized, too. Then, the particle with the global best solution holds the Zernike polynomials which describe the optical aberrations of the measuring system.

3. Optimization results

In figure 1, the course of the optimization is indicated for 50 particles and 150 iterations. Here, convergence for the result of the PSO is achieved after roughly 140 iterations. The overlap between the measured and the simulated profiles at the point of convergence is shown in figure 2. The difference between the two profiles for the 10 µm period of the investigated grating is visualized as well and it showcases the good agreement. A

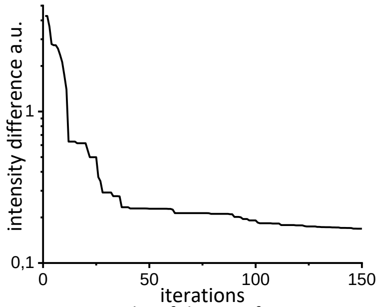

Figure 1. Optimization results of the PSO for 150 iterations

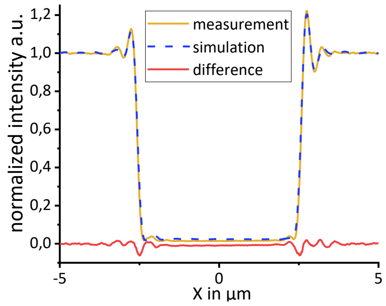

Figure 2. Comparison between the measured and simulated images

maximum deviation of 6 % is observed between the profiles. A linewidth determination of the grating at hand differs by a few nanometers (6 nm) depending on the inclusion or the neglect of the aberration. The measurement is performed by a transmission UV- microscope with an objective NA of 0.9 and in Köhler illumination. Figure 3 illustrates the Zernike polynomials which are determined for the aberrations of the optical system. Here, the assignment of the single polynomials corresponds to [8]. The 18th Zernike polynomial which represents the fourfold astigmatism is according to the PSO approach the most prominent aberration with a coefficient of 0.4270.

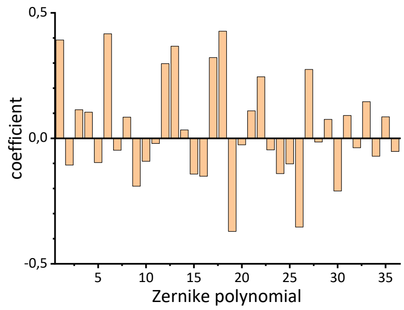

Figure 3. Optical aberration results in terms of Zernike polynomials

4. Conclusion

The presented approach yields the aberration of an optical system through a PSO and previously performed measurements on well manufactured gratings. The advantages of this approach are that like in common phase retrival methods, it only requires measurements along the optical axis while it avoids the difficulties of not perfectly manufactured pinholes by relying on gratings, too. At this point, the PSO only considers the image in the focal plane but it is planed to consider afocal planes in the future since the effects of the aberration are more prominent there. However, this requires a very good knowledge of the distances in between the images to ensure a comparison with the correct simulated image. Furthermore, comparisons with other techniques for the determination of optical aberrations should be pursuit.

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