Proceedings of the 2011 6th IEEE International
Conference on Nano/Micro Engineered and Molecular Systems
February 20-23, 2011, Kaohsiung, Taiwan

Zernike Representation of Angle-Resolved Mueller Matrix for Dimensional Analysis of Nanoscale Structures

Xiuguo Chen
Wuhan National Laboratory for Optoelectronics,
Huazhong University of Science and Technoloy,
Wuhan, China

Shiyuan Liu*, Chuanwei Zhang, Yuan Ma
State Key Lab of Digital Manufacturing Equipment & Technology,
Huazhong University of Science and Technology,
Wuhan, China

Abstract – **The angle-resolved Mueller matrix polarimetry has been recently introduced for dimensional metrology of nanoscale structures. Due to the redundant information contained in the measured Mueller matrix, it is difficult to find the implicit relationship between the geometrical parameters of the structure and the elements of the Mueller matrix. In this paper, a novel method based on Zernike representation is proposed to simplify the analysis of the angle-resolved Mueller matrix. The simulation results have demonstrated that the Zernike coefficients can be applied as useful metrics for dimensional analysis of nanoscale structures.**

Keywords - Mueller matrix polarimetry; angle-resolved; Zernike polynomial; nanometrolgy; nanomanufacturing

I. BACKGROUND

With the development of optical lithography process and resolution enhancement technology, the traditional very large scale integrated circuit (VLSI) has broken through from micron magnitude to nanometer scale, and it is hoped that the critical dimension (CD) will continue to advance towards 22 nm and below. The metrology challenges for the next technology nodes will not only focus on CD and overlay, but also include line edge roughness (LER), line width roughness (LWR), and even three-dimensional profile metrology. Compared with the conventional optical scatterometry which usually obtains two parameters (the amplitude ratio and the phase shift difference) under a certain measurement configuration, the Mueller matrix polarimetry can obtain up to 16 parameters of a 4×4 Mueller matrix during each measurement. Consequently, the Mueller matrix polarimetry can provide much more useful information than the conventional optical scatterometry, and thus has drawn more and more attention.

Recently the angle-resolved Mueller matrix polarimetry has been successfully introduced for dimensional metrology of nanoscale structures [1]. The Mueller matrix in this configuration is measured over a range of polar angles α and over all azimuthal angles ψ (0 – 360°), and each element of the Mueller matrix is similar to a circular pupil with each point (ρ, θ) in the polar coordinate corresponding to (sinα, ψ). However, due to the redundant information contained in the measured Mueller matrix, it is complicated and difficult to find the intrinsic relationship between the structural and optical parameters of the sample under measurement and the elements of the Mueller matrix. Therefore, it is highly desirable to develop a simple model that can be used to simplify the representation of the Mueller matrix and thus can be applied in nanoscale dimensional analysis.

The Zernike polynomials introduced by F. Zernike have been widely used in optical design as well as in optical testing for a long time [2]. Noticing that each element of the angle-resolved Mueller matrix is similar to an optical pupil, in this paper, we intend to represent each element by the Zernike coefficients related to their corresponding Zernike polynomials. In order to achieve such a representation, we try to select an appropriate series of Zernike polynomials firstly and then fit the angle-resolved Mueller matrix. Consequently, all the structural and optical information about the measured sample is condensed into several Zernike coefficients. We may only focus on the Zernike coefficients to extract optical and structural parameters of the sample. Accordingly, the calculation and analysis of the angle-resolved Mueller matrix will be greatly simplified.

II. THEORY

The configuration of the angle-resolved Mueller polarimeter is outlined in Fig. 1(a) [1]. The polarization state generator (PSG) and polarization state analyzer (PSA) are each composed of a linear polarizer and two nematic liquid crystal devices. The sample stage rotates over all azimuthal angles ψ (0–360°). A microscopic objective with a high numerical aperture is illuminated with a parallel beam and provides a range of incident angles α on the sample. Due to the limitation of the numerical aperture of the objective, the maximum value of the incident angle α is less than 90°. The Mueller matrices measured in this configuration can be organized in polar coordinates where each point (ρ, θ) stands for a (α, ψ) combination. The radial coordinate ρ corresponds to the sine of the incident angle α and the angular coordinate θ corresponds to the azimuthal angle ψ, i. e., $\rho \propto \sin\alpha$ and θ=ψ. As an example, one element of the Mueller matrix measured in this configuration is depicted in Fig. 1(b).

This project was funded by National Natural Science Foundation of China (Grant No. 91023032, 51005091, 50775090), Fundamental Research Funds for the Central Universities of China (Grant No. 2010ZD004), and Postdoctoral Science Foundation of China (Grant No. 20100470052).

*Contact author: Shiyuan Liu; phone: +86-27-87792409; fax: +86-27-87792413; email: shyliu@mail.hust.edu.cn.

978-1-61284-777-1/11/$26.00 ©2011 IEEE

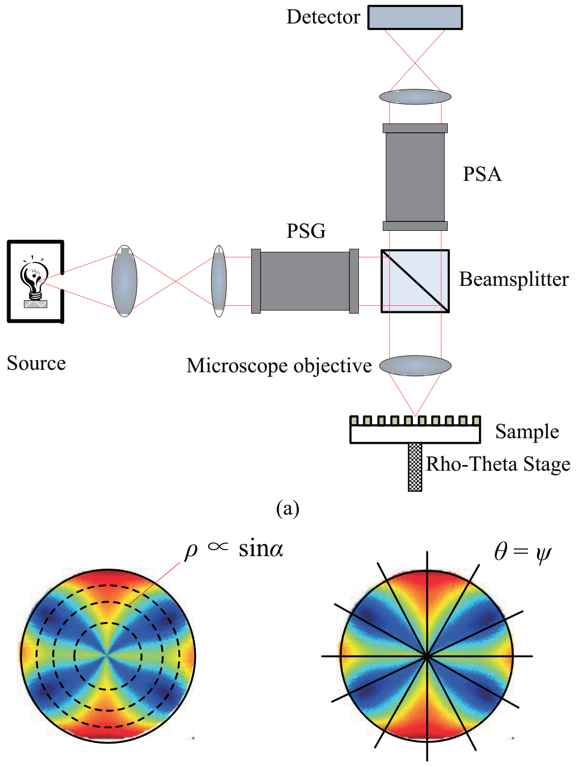

Figure 1. (a) Configuration of the angle-resolved Mueller polarimeter; (b) One element of the measured Mueller matrix in this configuration

In the angle-resolved Mueller matrix polarimeter, an appropriate model based on the electromagnetic theory which properly accounts for the physical essence of the scattering process is indispensable to determine the feature of the sample under measurement. As for samples with periodic properties, the rigorous coupled-wave analysis (RCWA) is always one of the best choices for the optical modeling [3]. The implementation of the standard RCWA is extended by using factorization of permittivity tensor based on the inverse rules to improve the convergence of the method [4]. In addition, boundary conditions on each interface are treated by the scattering matrix (S-matrix) algorithm to improve the numerical stability and efficiency of this method [5]. Nowadays the RCWA with these two extensions is the standard approach used for the modeling of different kinds of periodic structures.

A calculated angle-resolved Mueller matrix of a two-dimensional grating with arrays of square holes using the RCWA algorithm is shown in Fig. 2, from which it is noted that each element of the Mueller matrix is similar to an optical pupil. Therefore, we can try to represent the angle-resolved Mueller matrix using the Zernike polynomials by taking each element of the Mueller matrix as a pseudo optical pupil. In this way, the optical and structural properties of the sample are condensed into several Zernike coefficients, and hence we can only focus on these Zernike coefficients to analyze the properties of the sample. With this motivation, it is highly expected that the calculation and analysis of the angle-resolved Mueller matrix may be greatly simplified.

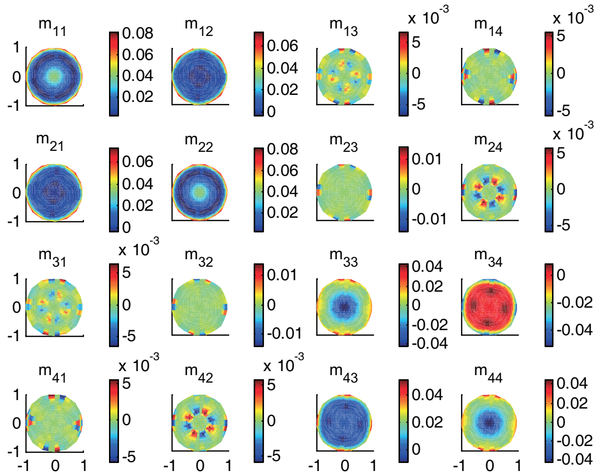

Figure 2. The calculated angle-resolved Mueller matrix of a two-dimensional grating with arrays of square holes

The Zernike polynomials are one of an infinite number of complete sets of functions in two variables, ρ ($0 \le \rho \le 1$) and θ ($0 \le \theta \le 2\pi$), that are orthogonal in a continuous form over a circle of unit radius and are convenient for serving as a set of basis functions. This makes them suitable for accurately describing wave aberration as well as data fitting in the circular domain. The Zernike polynomials are defined as follows [6]:

$$f_l(\rho,\theta) = Z_n^m(\rho,\theta) = \begin{cases} N_n^m R_n^{|m|}(\rho)\cos(m\theta) & m \ge 0 \\ -N_n^m R_n^{|m|}(\rho)\sin(m\theta) & m < 0 \end{cases}, \quad (1)$$

where the natural number n is the radial degree or the order of the radial polynomial since it represents the highest power of ρ in the polynomial, the integer m is the azimuthal or angular frequency of the sinusoidal component (note that $n-|m| \ge 0$), the index l is used to indicate the mode number of the corresponding Zernike polynomial, $N_n^m = \sqrt{2(n+1)/(1+\delta_{m0})}$ is the normalization factor, and δ_{m0} denotes the Kronecker delta function (i.e., $\delta_{m0}=1$ for m=0 and $\delta_{m0}=0$ for $m \ne 0$); $R_n^{|m|}(\rho)$ is the radial polynomial and is defined by:

$$R_n^{|m|}(\rho) = \sum_{s=0}^{(n-|m|)/2} \frac{(-1)^s (n-s)!}{s!\left(\dfrac{n+|m|}{2}-s\right)!\left(\dfrac{n-|m|}{2}-s\right)!}\rho^{n-2s}. \quad (2)$$

We can obtain a series of Zernike polynomials by substituting different indices (n, m) into Eqs. (1) and (2). Here, assuming that there is a series of fixed Zernike polynomials $\{f_1(\rho,\theta), f_2(\rho,\theta), \ldots, f_L(\rho,\theta)\}$ that can be used to fit the angle-resolved Mueller matrix with L being the maximum mode number, we can represent each element of the angle-resolved Mueller matrix by the above Zernike polynomials as follows:

$$m_{ij}(\rho_k,\theta_k) = \sum_{l=1}^{L} f_l(\rho_k,\theta_k) Z_{l,ij} + \varepsilon_{k,ij}, \left(1 \le i,j \le 4; k = 1,2,\cdots,K\right), \quad (3)$$

where $m_{ij}(\rho_k, \theta_k)$ is the value of the (i, j) element of the Mueller matrix at sampling point (ρ_k, θ_k), and K is the number of sampling points ($K \geq L$); $Z_{l,ij}$ denotes the Zernike coefficient corresponding to the lth Zernike polynomial $f_l(\rho, \theta)$ and the element $m_{ij}(\rho, \theta)$; $\varepsilon_{k,ij}$ denotes the fitting error corresponding to the element $m_{ij}(\rho, \theta)$. In matrix notation, Eq. (3) can be written as:

$$\widetilde{\mathbf{M}} = \mathbf{FZ} + \mathbf{E}, \tag{4}$$

where

$$\widetilde{\mathbf{M}} = \begin{bmatrix} m_{11}(\rho_1,\theta_1) & m_{12}(\rho_1,\theta_1) & \cdots & m_{44}(\rho_1,\theta_1) \\ m_{11}(\rho_2,\theta_2) & m_{12}(\rho_2,\theta_2) & \cdots & m_{44}(\rho_2,\theta_2) \\ \vdots & \vdots & & \vdots \\ m_{11}(\rho_K,\theta_K) & m_{12}(\rho_K,\theta_K) & \cdots & m_{44}(\rho_K,\theta_K) \end{bmatrix}, \ \mathbf{Z} = \begin{bmatrix} Z_{1,11} & Z_{1,12} & \cdots & Z_{1,44} \\ Z_{2,11} & Z_{2,12} & \cdots & Z_{2,44} \\ \vdots & \vdots & & \vdots \\ Z_{L,11} & Z_{L,12} & \cdots & Z_{L,44} \end{bmatrix},$$

$$\mathbf{F} = \begin{bmatrix} f_1(\rho_1,\theta_1) & f_2(\rho_1,\theta_1) & \cdots & f_L(\rho_1,\theta_1) \\ f_1(\rho_2,\theta_2) & f_2(\rho_2,\theta_2) & \cdots & f_L(\rho_2,\theta_2) \\ \vdots & \vdots & & \vdots \\ f_1(\rho_K,\theta_K) & f_2(\rho_K,\theta_K) & \cdots & f_L(\rho_K,\theta_K) \end{bmatrix}, \ \mathbf{E} = \begin{bmatrix} \varepsilon_{1,11} & \varepsilon_{1,12} & \cdots & \varepsilon_{1,44} \\ \varepsilon_{2,11} & \varepsilon_{2,12} & \cdots & \varepsilon_{2,44} \\ \vdots & \vdots & & \vdots \\ \varepsilon_{K,11} & \varepsilon_{K,12} & \cdots & \varepsilon_{K,44} \end{bmatrix}$$

denote the $K \times 16$ combined and rearranged Mueller matrix, the $L \times 16$ Zernike coefficient matrix, the $K \times L$ Zernike polynomial matrix, and the $K \times 16$ error matrix, respectively. In the absence of depolarization, the Mueller matrix **M** can be obtained from the RCWA algorithm, which provides the complex Jones matrix **J** of zero diffraction order of the grating:

$$\mathbf{J} = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix}. \tag{5}$$

The corresponding Mueller matrix **M** can be calculated from the above Jones matrix **J** as follows:

$$\mathbf{M} = (m_{ij}) = \mathbf{A}(\mathbf{J} \otimes \mathbf{J}^*)\mathbf{A}^{-1}, \tag{6}$$

where $\otimes$ denotes the Kronecker product, and the matrix **A** is given by:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & i & -i & 0 \end{bmatrix}. \tag{7}$$

Then we can obtain the Zernike coefficient matrix **Z** from Eq. (4) by the least square method:

$$\mathbf{Z} = \mathbf{F}^{+}\mathbf{M}, \tag{8}$$

where the matrix $\mathbf{F}^{+}$ denotes the Moore-Penrose pseudo-inverse of the Zernike polynomial matrix **F**, i. e., $\mathbf{F}^{+} = (\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}$.

It is noted that an appropriate scheme used to obtain the discrete sampling points (ρ_k, θ_k) is of great importance when fitting the angle-resolved Mueller matrix. In general, we can define an error propagation matrix (EPM) **E** to scale the propagation errors in the Zernike coefficients:

$$\mathbf{E} = \mathbf{F}^{+}(\mathbf{F}^{+})^{\mathrm{T}}. \tag{9}$$

In addition, the condition number of matrix **F** is also used in the calculation to obtain a relatively stable result, which is defined by:

$$cond(\mathbf{F}) = \|\mathbf{F}\| \cdot \|\mathbf{F}^{-1}\|, \tag{10}$$

where $\|\mathbf{F}\|$ denotes the 2-norm of the matrix **F**. By continuously minimizing the error propagation matrix **E** and the condition number *cond*(**F**), we can eventually obtain a relatively optimal sampling scheme.

III. SIMULATION

We simulated the angle-resolved Mueller matrix polarimetry and fitted the Mueller matrices of different samples by using a series of fixed Zernike polynomials. A two-dimensional grating structure used in the simulation is shown in Fig. 3, which contains arrays of square holes in 500nm thick layers of crystalline silicon. The grating period is 800nm in both directions, the dimension of the holes are 400×400nm, and the incident wavelength is 850nm. The calculated angle-resolved Mueller matrix is shown in Fig. 2. We used up to 49th-mode (L=49) Zernike polynomials to fit the calculated Mueller matrix. To obtain the Zernike coefficients, we chose 72 sampling points in the pseudo pupil plane.

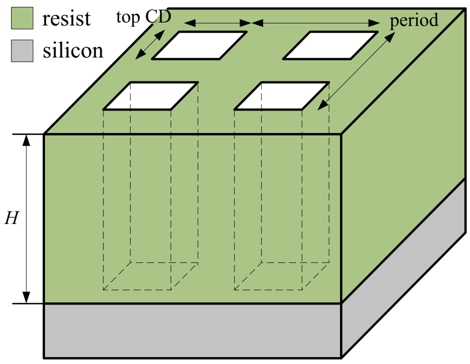

Figure 3. Two-dimensional grating structure used in the simulation

The fitting Mueller matrix of the two-dimensional grating sample is depicted in Fig. 4(a), and the residual error of each Mueller element during the fitting process is shown in Fig. 4(b). In the simulation, it is found that different types of Zernike polynomials play different roles when fitting the Mueller matrix, and only even terms (i.e. m is even number) of the Zernike polynomials are sensitive to the Mueller matrix of samples with rotational symmetry. As a matter of fact, the fitting Mueller matrix shown in Fig. 4(a) is the result by only using even terms of up to the 49th Zernike polynomials, and the Zernike coefficients corresponding to the odd terms of the Zernike polynomials are nearly equal to zero.

From Fig. 4(b), it is observed that the fitting result is not so perfect since the errors of some Mueller matrix elements have the same order of the magnitude compared with the corresponding calculated Mueller matrix elements. Furthermore, when we chose small incident wavelength or small structural parameters, we found that the calculated Mueller matrix contained so many "high-frequency" components that the 49 Zernike polynomials were not enough to fit it. Therefore, higher order Zernike polynomials are necessary when fitting the

Mueller matrix to decrease the residual error.

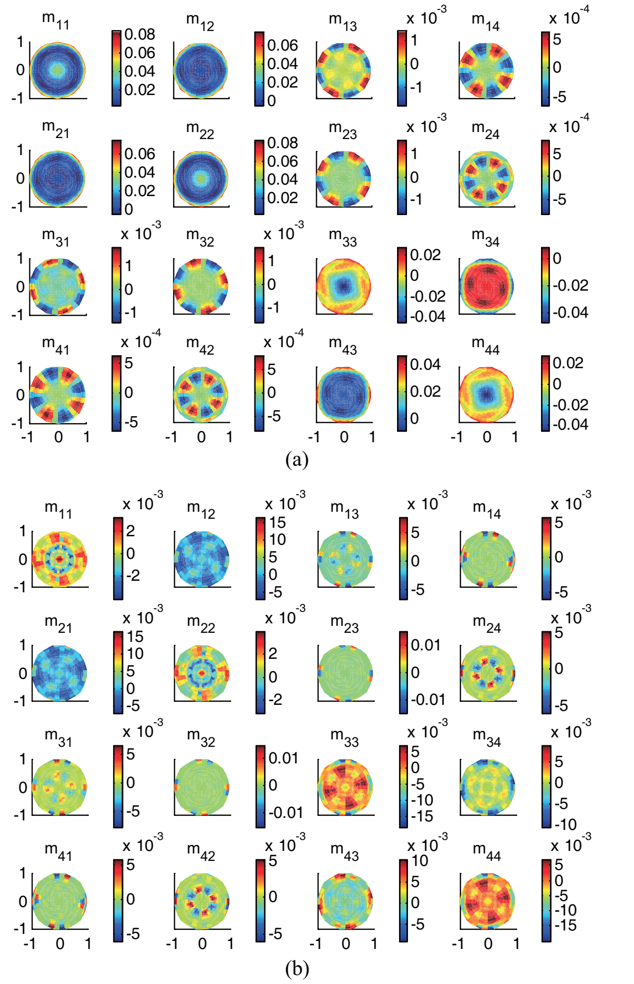

Figure 4. (a) The fitting Mueller matrix of the two-dimensional grating sample by only using the even terms of 49th-mode Zernike polynomials; (b) The residual error of each Mueller element during the fitting process

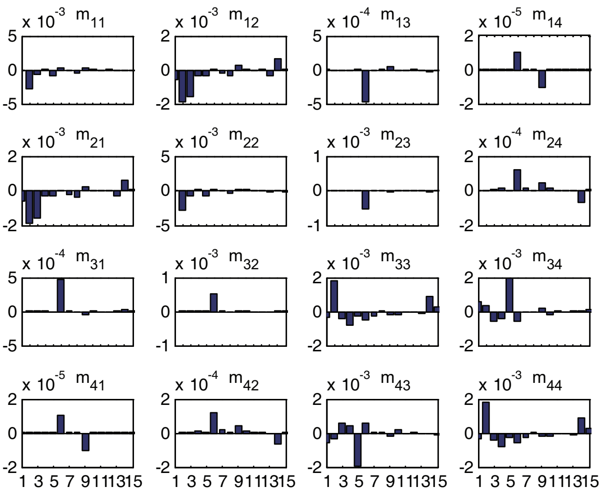

Figure 5. Sensitivity of Zernike coefficients when the dimensions of the samples holes as shown in Fig. 3 vary in ten nanometers (390×390nm).

In addition, the number of Zernike polynomials depends on the fitting accuracy of the Mueller matrix as well as on the sensitivity of the Zernike coefficients to the structural variation of the sample. We also simulated the sensitivity of the Zernike coefficients to the structural parameters, as shown in Fig. 5. It is noted that the values of the Zernike coefficients in Fig. 5 are too small to be used for dimensional analysis of nanoscale structures. We believe that this is due to the large incident wavelength. If we choose smaller incident wavelength, the values of the calculated Zernike coefficients will become larger. However, as mentioned above, the calculated Mueller matrix under the condition of small incident wavelength will contain so many "high-frequency" components that more Zernike polynomials are necessary to sufficiently fit it. The more the number of the Zernike polynomials is used, the more complication of the Zernike coefficients becomes to analyze the properties of the sample. Therefore, we need to make a compromise between the fitting results and the complexity of the final analysis.

IV. Summary and Discussion

In this paper, the Zernike representation of the angle-resolved Muller matrix is proposed for the dimensional analysis of nanoscale structures. The theory about how to use the Zernike polynomials to fit the angle-resolved Mueller matrix is presented firstly, and then the corresponding simulation is performed. Finally, some conclusions were presented in the simulation part. Although perfectly fitting results are not obtained, we believe that the Zernike polynomials can fully represent the angle-resolved Mueller matrix if we choose an appropriate series of Zernike polynomials. Of course, it still remains as a challenge to apply the Zernike polynomials and the corresponding Zernike coefficients to analyze the properties of the sample under measurement. Two of the most critical issues that need to figure out in future are: (1) the choice of an appropriate series of Zernike polynomials to fit the angle-resolved Mueller matrix with minimized fitting errors; and (2) the analysis of the relationship between the Zernike coefficients and the optical and structural properties of the sample to simplify the modeling and data analyzing processes.

Acknowledgment

Xiuguo Chen would like to thank Mr. Wei Liu for his helpful discussions and suggestions in preparing this paper.

References

[1] S. Ben Hatit, M. Foldyna, A. De Martino, and B. Drévillon, "Angle-resolved Mueller polarimeter using a microscope objective," Phys. Stat. Sol. (a), vol. 205, pp. 743-747, 2008.

[2] F. Zernike, "Beugungstheorie des Schneidenverfahrens und seiner verbesserten form, der Phasenkontrastmethode," Physica, vol. 1, pp. 689-704, 1934.

[3] M. G. Moharam, E. B, Grann, and D. A. Pommet, "Formulation of stable and efficient implementation of the rigorous coupled-wave analysis of binary gratings," J. Opt. Soc. Am. A, vol. 12, pp. 1068-1076, 1995.

[4] L. Li, "Use of Fourier series in the analysis of discontinuous periodic structures," J. Opt. Soc. Am. A, vol. 13, pp. 1870-1876, 1996.

[5] L. Li, "Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings," J. Opt. Soc. Am. A, vol. 13, pp. 1024-1035, 1996.

[6] M. Born and E. Wolf, Principles of Optics, 7th ed. Pergamon, 1999, chap. 9