Correction on the effect of numerical aperture in optical scatterometry

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ABSTRACT

Optical scatterometry, also referred to as optical critical dimension (OCD) metrology, has been introduced for critical dimension (CD) monitoring and overlay metrology with great success in recent years. Forward modeling to calculate the optical signature from the measured diffractive structure is one of the most important issues in OCD metrology. To simplify the forward modeling approach, such as rigorous coupled-wave analysis (RCWA), the incidence and azimuthal angles are usually assumed to be constant. However, since some focusing elements, such as focusing lens or parabolic mirrors with finite numerical aperture (NA), are always used to gain a sufficient small spot size onto the sample, this assumption is not true in the whole exit pupil of the focusing elements, leading to a modeling error in forward modeling, and finally leading to a fitting error in OCD metrology. In this paper, we propose a correction method with consideration of the effect of NA to decrease the modeling error in the forward modeling. The correction method is an average integral method based on Gaussian quadrature in two dimensions inside a circle, and is performed on forward modeling with varied incidence and azimuthal angles over the exit pupil. Experiments performed on photoresist gratings with a Mueller matrix polarimeter have demonstrated that the proposed correction method achieves a higher accuracy in OCD metrology.

Keywords: optical scatterometry, optical critical dimension (OCD) metrology, rigorous coupled-wave analysis (RCWA), numerical aperture (NA).

1. INTRODUCTION

Process control in microelectronic manufacturing requires real-time monitoring techniques. Among the different techniques, optical scatterometry, sometimes also referred to as optical critical dimension (OCD) metrology, has achieved great success in the monitoring of CD and overlay in recent years [1-4]. There are two main procedures in OCD metrology [5]. The first one involves the calculation of the theoretical signature from a diffractive structure using reliable forward modeling techniques, such as the rigorous coupled-wave analysis (RCWA) [6-8], finite-difference time-domain (FDTD) method [9], or finite element method (FEM) [10, 11]. Here, the general term signature contains the scattered light information from the diffractive structure, which can be in the form of reflectance, ellipsometric angles, Stokes vector elements, or Mueller matrix elements. The second procedure involves the reconstruction of the structural profile from the measured signature, which is a typical inverse problem with the objective of finding a profile whose theoretical signature can best fit the measured one.

To simplify the forward modeling approach, such as RCWA in OCD metrology, the incidence and azimuthal angles are usually assumed to be constant [12, 13]. However, this assumption is not true in practical application, as some focusing elements, such as focusing lens or parabolic mirrors with finite NA, are always used to gain a sufficient small spot size onto the sample. This small spot size, down to several hundreds to even tens of microns, is critical to be suitable for the shrinking CDs in semiconductor manufacturing. Consequently, the incidence and azimuthal angles are actually not constant in the whole exit pupil of the focusing elements, thus leading to a modeling error and finally leading to a fitting error in OCD metrology. Recently, several works have been done to estimate the effect of NA. Munro et al established the theoretical basis of high-numerical-aperture Mueller matrix polarimetry (MMP) and gave a theoretical framework for

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analyzing high-NA MMP. They showed how confocal and conventional polarimeters may be considered as averaging the Jones and Mueller matrices of the samples respectively and proposed that high-NA MMPs would lead to nonzero depolarization factors even when the optical system and sample are nondepolarizing [14]. Germer et al consider the effects of NA in scatterometry measurements and proposed an integration method based upon Gaussian quadrature that account for the effect of NA. They performed this method to extract the effective numerical NA with a nominally 1000nm thick SiO2 thermal oxide film on a Si substrate and found that accounting for the effect is necessary to obtain satisfactory results in scatterometry [15]. However, previous works only studied the effect of NA without any considerations on the correction method to improve the accuracy in optical scatterometry. In this paper, we propose a method to correct this effect. To obtain an effective NA of the OCD system, we used a standard film as the sample and fit the measured data by integrating the varied incidence and azimuthal angles within the exit pupil. The obtained effective NA is then applied in actual OCD metrology by performing the same integration to fit the measured data. We performed experiments on the photoresist gratings with a dual-rotating compensator Mueller matrix ellipsometry, and expect to achieve higher measurement accuracy in the metrology.

2. METHOD

2.1 Forward modeling with the consideration of NA

Forward modeling, which is the first main procedure in OCD metrology, involves the calculation of the theoretical signature from a diffractive structure, such as reflectance, ellipsometric angles, Stokes vector elements, or Mueller matrix elements. Mueller matrix, which contains much more information of the sample, has been widely used in optical scatterometry. The Mueller matrix can be calculated by forward modeling techniques, such as RCWA for periodic diffractive structures and optical film transfer-matrix method for multilayer films, with knowing structure parameters, wavelength, the incidence and azimuthal angles [6-8, 16]. In OCD metrology, as can be observed in Fig. 1, when we take the focusing elements, which with NA into consideration, the incidence angle will vary from θ_1 to θ_2 and azimuthal angle will vary from φ_1 to φ_2 within the whole exit pupil of the focusing elements. Therefore, when modeling the Mueller matrix of the measured sample, we should integrate the calculation within the whole exit pupil and obtain an average result:

$$\overline{M} = \frac{1}{\pi h^2}\int_{D_0} M(\theta,\varphi)dS\,, \tag{1}$$

where D_0 is the exit pupil; h is the radius of the exit pupil; θ and φ are the incidence angle and azimuthal angle, respectively; $M(\theta, \varphi)$ is calculated by the forward modeling techniques with certain incidence and azimuthal angles as mentioned above.

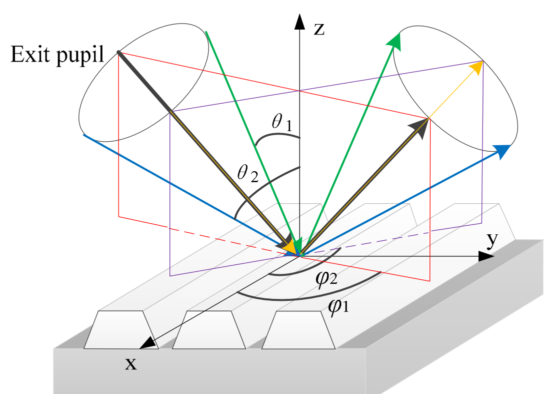


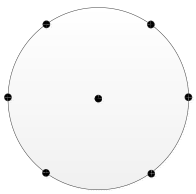
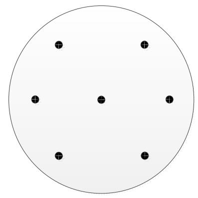
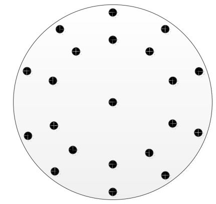
Figure 1. The variation of the incidence angle and azimuthal angle affected by NA.

The function $M(\theta, \varphi)$ is assumed to be relatively smooth, thus the Gaussian quadrature offers an extremely efficient and accurate approximation for the integral. Abramowit et al reported an appropriate numerical integration method for performing integrals on a circle [17]:

$$\frac{1}{\pi h^2}\iint_c f(x,y)dxdy = \sum_{i=1}^{n}\omega_i f(x_i,y_i) + R\,, \tag{2}$$

where ω_i is weight function and R is the residual term. Table 1 gives suitable values for ω_i , x_i and y_i in different order of R, which indicates the accuracy for the numerical integral.

Table 1. Parameters for numerical integral

$R=O(h^4)$		$R=O(h^6)$		$R=O(h^{10})$	
					
(x_i , y_i)	ω_i	(x_i , y_i)	ω_i	(x_i , y_i)	ω_i
(0, 0)	1/2	(0, 0)	1/4	(0, 0)	1/9
$(\pm h , 0)$	1/12	$\left(\pm\sqrt{\frac{2}{3}}h,0\right)$	1/8	$\left(\sqrt{\frac{6-\sqrt{6}}{10}}h\cos\frac{2\pi k}{10},\sqrt{\frac{6-\sqrt{6}}{10}}h\sin\frac{2\pi k}{10}\right)$, ($k$=1, ..., 10)	$\frac{16+\sqrt{6}}{360}$
$\left(\pm\frac{1}{2}h,\pm\frac{\sqrt{3}}{2}h\right)$	1/12	$\left(\pm\sqrt{\frac{1}{6}}h,\pm\frac{\sqrt{2}}{2}h\right)$	1/8	$\left(\sqrt{\frac{6+\sqrt{6}}{10}}h\cos\frac{2\pi k}{10},\sqrt{\frac{6+\sqrt{6}}{10}}h\sin\frac{2\pi k}{10}\right)$, ($k$=1, ..., 10)	$\frac{16-\sqrt{6}}{360}$

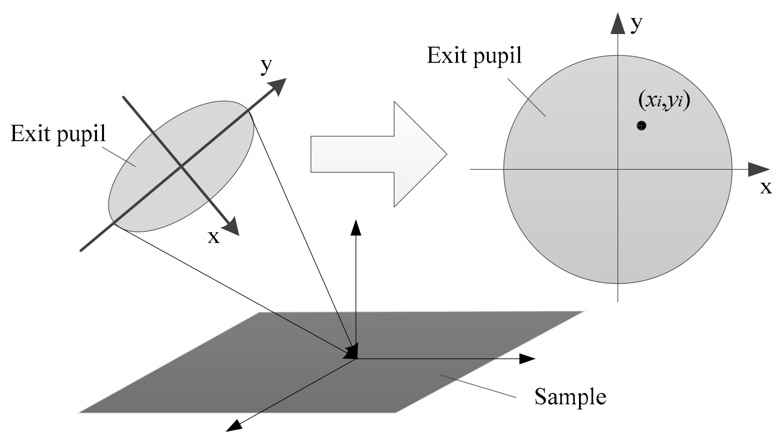


Figure 2. The corresponding incidence angle and azimuthal angle to the position in the exit pupil.

In optical scatterometry, as shown in Fig. 2, for any (x_i, y_i) in the exit pupil, the corresponding incidence angle and azimuthal angle (θ_i, φ_i) can be represented as:

$$\theta_i = \theta_0 + \arctan\frac{x_i}{f}, \tag{3.1}$$

$$\varphi_i = \varphi_0 + \arctan\frac{y_i}{f}, \tag{3.2}$$

where (θ_0, φ_0) are the original incidence angle and azimuthal angle when the effect of NA is ignored, and f is the focal length. Therefore, by employing the numerical integration method with Eq. 2, we can obtain the extremely accurate approximation modeling Mueller matrix as:

$$\overline{M} = \sum_{i=1}^{n}\omega_i M(\theta_i,\varphi_i) + R, \tag{4}$$

where M (θ_i, φ_i) is calculated by forward modeling techniques with any incidence and azimuthal angles (θ_i , φ_i) obtained from Eq. 3.

2.2 Parameter extraction with the corrected forward modeling

Figure 3 depicts the flowchart of parameter extraction with the corrected forward modeling to correct the effect of NA in OCD metrology. The extraction process is described in detail as follows.

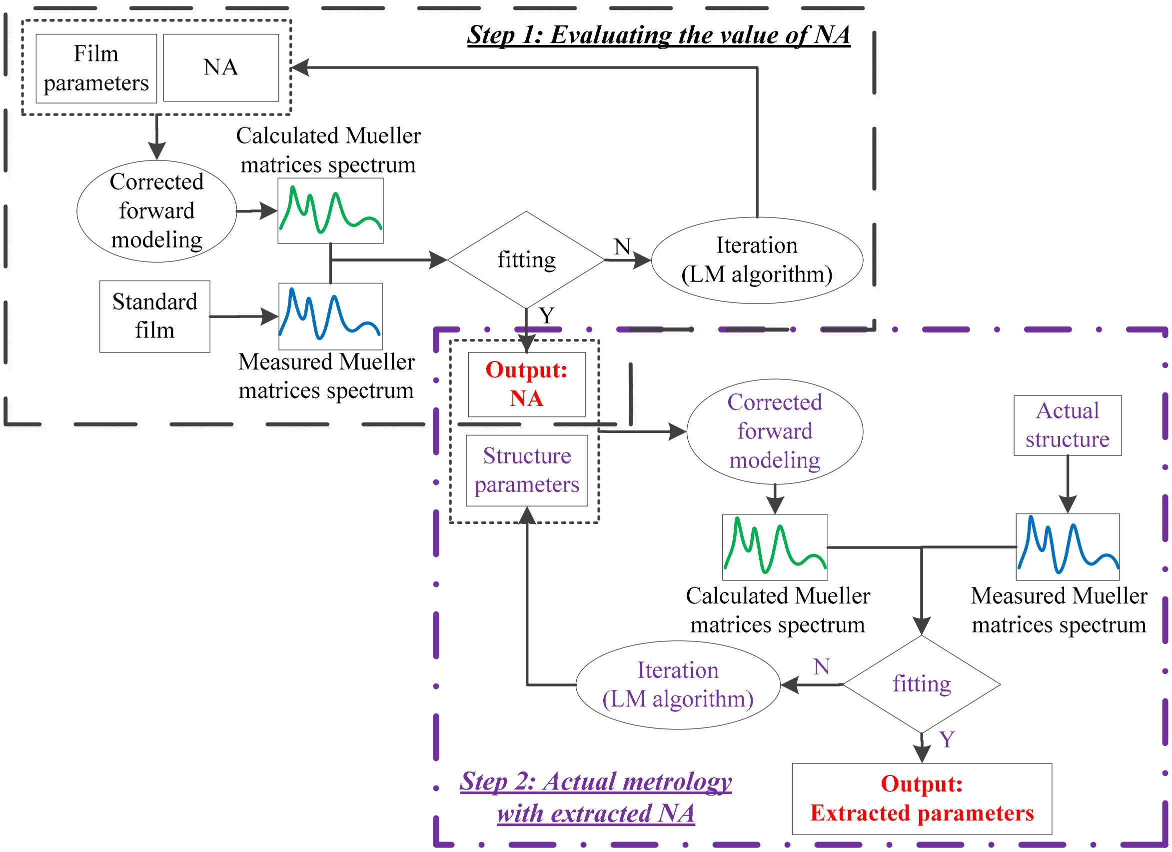


Figure 3. Flowchart of parameter extraction with corrected forward modeling.

The first step is to evaluate the effective value of NA. There are two main approaches to obtain the effective NA. The brief one is to calculate NA by the given radius of the light beam h and focus length of the focusing element f, with the function: $NA = h/f$. The other one is to perform a measurement with the focus elements on a standard film as the sample. The theoretical Mueller matrices is calculated by the optical film transfer- matrix method based corrected forward modeling [16]. To extract the value of NA, the Levenberg-Marquardt (LM) algorithm [18] is employed here by minimizing the χ^2 function, which represents the fitting errors between the measured and calculated Mueller matrix elements defined as:

$$\chi^2 = \sum_{\lambda=1}^{N}\left[\sum_{i,j}\frac{(m_{ij}^{m})_\lambda - (m_{ij}^{c})_\lambda}{\sigma(m_{ij})_\lambda}\right]^2, \tag{5}$$

where λ denotes the spectral point from the total number N. $(m_{ij}^{m})_\lambda$ is a measured data of the Mueller matrix element with the λth wavelength, and $(m_{ij}^{c})_\lambda$ is the corresponding calculation value. Indices i and j show all the Mueller matrix elements except m_{11}. $\sigma(m_{ij})_\lambda$ is the standard deviation associated with $(m_{ij}^{m})_\lambda$. In this case, the values of NA as also as film parameters, which are set as fitting parameters, will be extracted when fitting the measured data with the corrected forward modeling.

The second step is to apply the evaluated effective NA in actual OCD metrology. After the Mueller matrices spectrum of actual structures is measured by the optical scatterometer, the same LM algorithm is used to extract the structure parameters. The theoretical Mueller matrices of actual structures can be usually calculated by the RCWA based corrected forward modeling. By fixing the effective NA to the extracted value from step one, the structure parameters, set as fitting parameters, will be extracted when fitting the measured data with the corrected forward modeling. In addition, the NA will be only fixed to the extracted value from step one until changing the setup of the OCD metrology instrument.

3. EXPERIMENTS

All our experiments in this paper were performed on a dual-rotating compensator MMP and in-house forward modeling software based on RCWA [6-8]. As shown in Figure 4, this dual-rotating compensator MMP is with a system configuration of PCr_1SCr_2A, where P and A stand for the fixed polarizer and analyzer, Cr_1 and Cr_2 refer to the 1st and 2nd frequency-coupled rotating compensators, and S stands for the sample. In this dual-rotating compensator configuration, we can obtain the full Mueller matrix elements of the sample. More details for data reduction can be referred to references [19, 20].

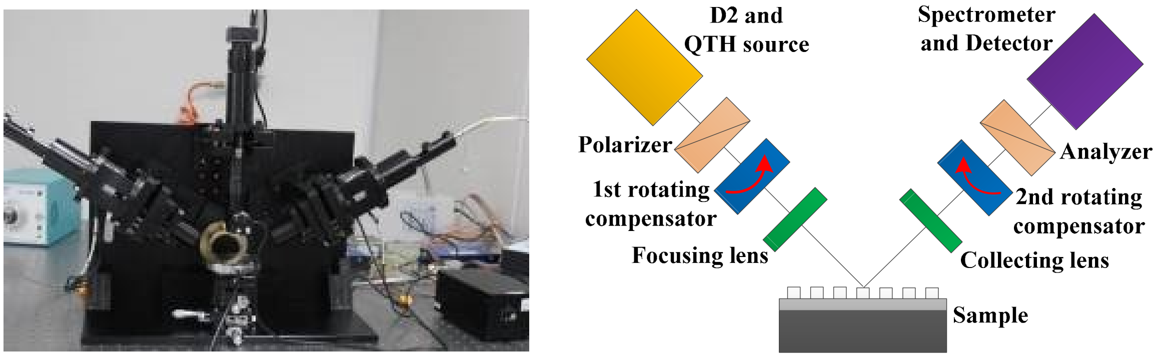


Figure 4. System setup and basic scheme of the dual-rotating compensator Mueller matrix ellipsometer.

To obtain the effective NA of the ellipsometer, with a said NA as 0.06, we performed a measurement on a nominally 1000nm thick SiO_2 thermal oxide film on a Si substrate with loading the focus optical elements. The incidence angle is set to 65° and the spectral range is between 200~800nm with a step of 5nm in the experiment. The order of remainder R is chosen as 10, $R= O(h^{10})$. The model we used is consisted of a SiO_2 thermal oxide film with thickness t_{oxide} as the first layer, an interface SiO_2 layer with thickness fixed to 1nm and the Si substrate. The optical properties of each layer are taken from the literature [21]. When we fit the data, letting the thickness t_{oxide}, the original incidence angle θ_0 and the value of NA float, we obtain the result as NA=0.065, which is quite close to the nominal value 0.06.

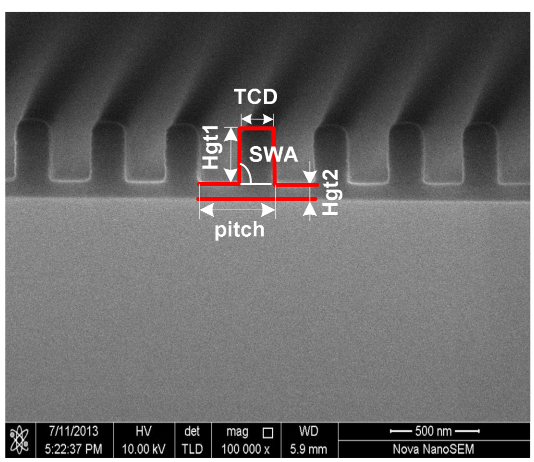


Figure 5. SEM cross-section image of the investigated photoresist grating.

The obtained effective NA was then applied in an actual OCD metrology on a one-dimensional (1D) photoresist grating structure on a Si substrate, the scanning electron microscope (SEM) cross-section image of which is shown in Fig. 5. The optical properties of photoresist were calculated by the Tauc-Lorentz model for the grating layer and the Forouhi-Bloomer model for the bottom anti-reflective coating (BARC) layer. As depicted in Fig. 5, the cross section of the photoresist grating is characterized by a symmetrical trapezoidal model on the BARC layer with top critical dimension *TCD*, line height of the grating *Hgt*1, side wall angle *SWA*, line height of the BARC layer *Hgt*2, and period pitch. The nominal value the structural parameters obtained from Fig. 5 are *TCD* = 0.2μm, *Hgt*1 = 0.312μm, *SWA* = 90°, and *Hgt*2 = 0.117μm, respectively. In the following experiment, the parameters to be extracted include the *TCD*, *Hgt*1, *SWA* and *Hgt*2, while the grating period is fixed at its nominal dimension, i.e., *pitch* = 0.4μm.

Since a 1D grating has rotating symmetry, its Mueller matrices remain unchanged after 180° rotation in the azimuthal angle [22]. In addition, the 1D grating also has reflection symmetry relative to the plane that is perpendicular to the direction of grating period. In other words, replacing φ with $-\varphi$ has no effect on the measured Mueller matrices. Therefore, we could limit the range of azimuthal angles to 0~90°. The incidence angle is fixed to 65° and the spectral range is between 200~800nm with a step of 5nm in the experiment. When applying RCWA to calculate the Mueller matrices, the number of the retained orders in the truncated Fourier series is 12, and the photoresist grating as shown in Fig. 5 is sliced into 15 layers along the vertical direction. When fitting the measured data with the RCWA calculated data, the order of the remainder R is chosen as 10, i.e., $R = O(h^{10})$, and the value of NA is fixed at 0.065.

A comparison of the fitting results from the same measured data by MMP at different azimuthal angles with and without applying the correction method is shown in Fig. 6. It is clear that the CD exacted from the same measured data is much closer to the SEM result with correction than that without any consideration of NA over the whole azimuthal angle. As shown in Fig. 7, the root mean squared error (RMSE), which represents the goodness of the fitting, is dramatically reduced after applying the correction method. This observation means that the Mueller matrices calculated by the corrected modeling method show a better agreement with the measured data. Therefore, we can conclude that the correction method by considering the effect of NA dramatically decreases the fitting error and thus gives access to a higher accuracy in the actual OCD metrology. Figure 8 depicts an example of the measured and the calculated Mueller matrices for the investigated photoresist grating at the azimuthal angle of 60° and incidence angle of 65°.

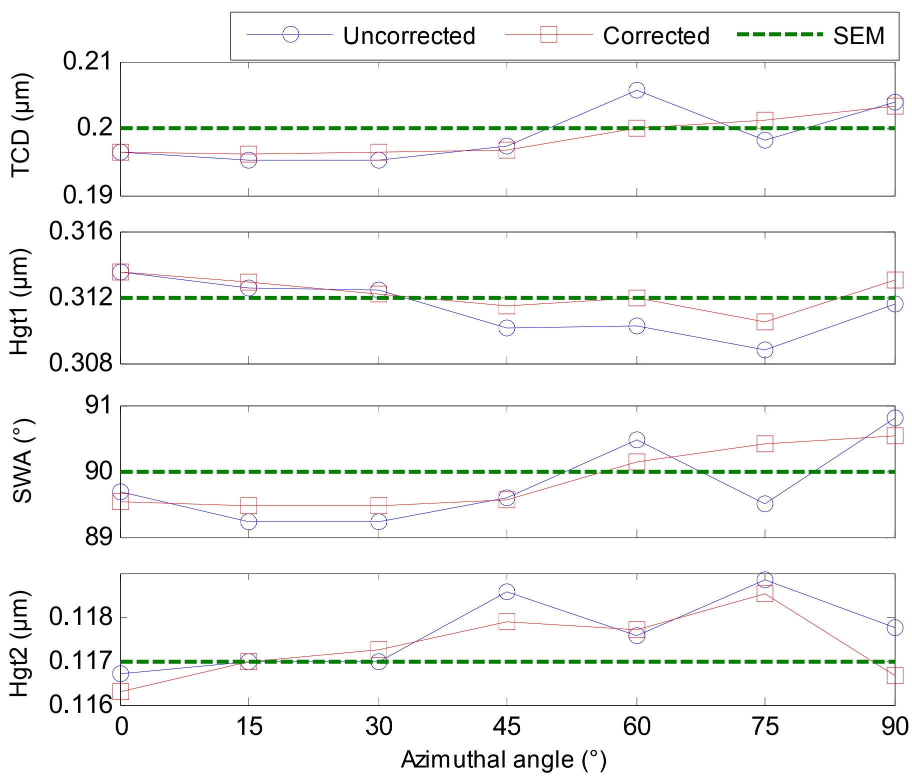


Figure 6. Comparison between the CDs measured by SEM and exacted from the same measured data by MMP at different azimuthal angle with and without the correction.

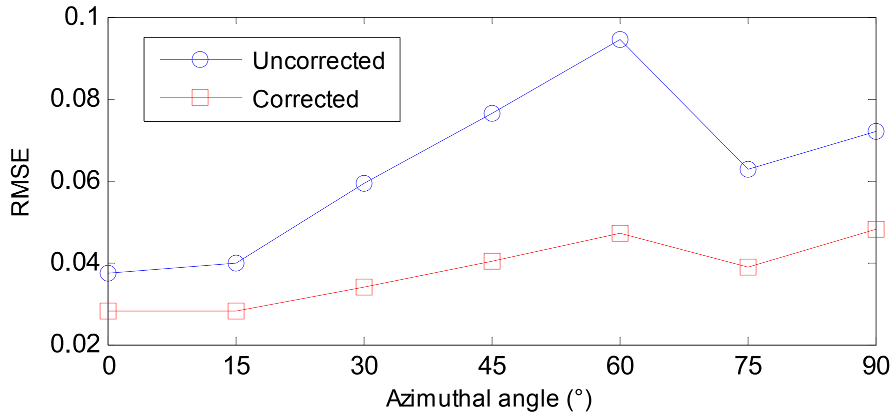


Figure 7. The RMSE difference in fitting the same measured data at different azimuthal angle with and without the correction.

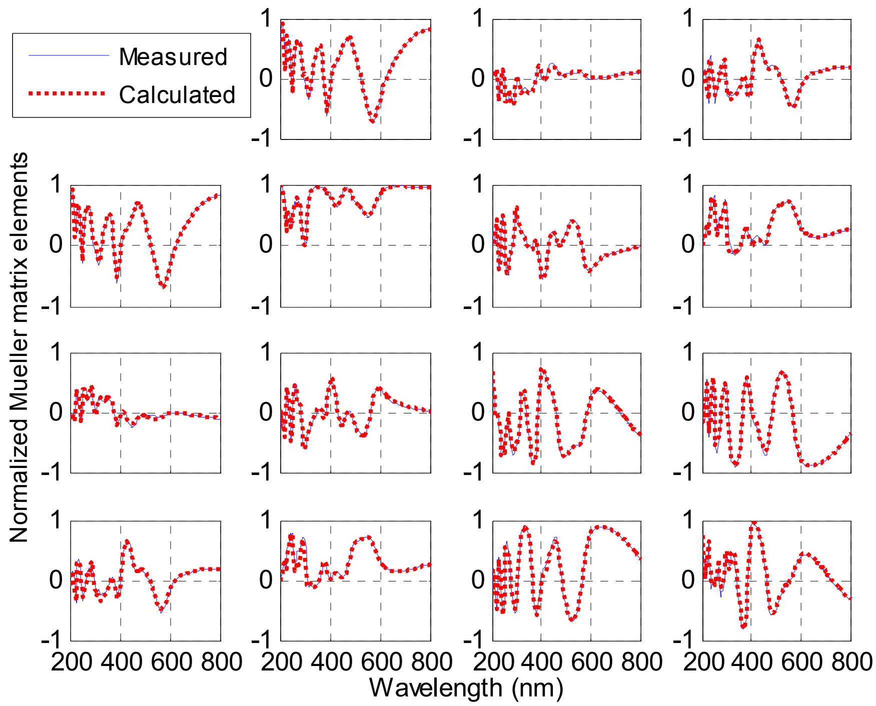


Figure 8. Example of the measured (red dash lines) and calculated (blue solid lines) spectra of normalized Mueller matrices for the investigated photoresist grating at the azimuthal angle of 60° and incidence angle of 65° by performing the correction method.

4. CONCLUSIONS

The NA in optical scatterometry, which is the main cause of variations of the incidence and azimuthal angles, will induce modeling errors by the RCWA calculation and thus affect the measurement accuracy in OCD metrology. We have investigated the effect of the finite NA on the accuracy of OCD metrology, and then proposed a method to correct this effect. The correction method is an average integral method based on Gaussian quadrature in two dimensions inside a circle, since the NA affect the incidence and azimuthal angles over the whole exit pupil. To correct the effect of NA, two steps have been performed based on the proposed correction method. The first step is to evaluate the effective value of NA by performing a measurement on a standard film as the sample. The second one is to apply the evaluated effective NA in actual OCD metrology by modeling the RCWA calculation with the evaluated effective NA. And then, the modeling error is decreased by employing the correction method over the NA and thus we achieve much higher measurement accuracy in OCD metrology. Experiments performed on a photoresist grating with a dual-rotating compensator Mueller matrix polarimeter have demonstrated the validity of the proposed correction method.

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