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Influence of Illumination Polarization and Target Structure on Measurement Sensitivity of **Through-Focus Scanning Optical Microscopy**

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Abstract: Unlike the optical information taken from a single in-focus image of general optical microscopy, through-focus scanning optical microscopy (TSOM) involves scanning a target through the focus and capturing of a series of images. These images can be used to conduct three-dimensional inspection and metrology with nanometer-scale lateral and vertical sensitivity. The sensitivity of TSOM strongly depends on many mechanical and optical factors. In this study, how illumination polarization and target structure affect the sensitivity of TSOM is analyzed. Firstly, the complete imaging procedure of the polarized light is investigated. Secondly, through-focus scanning results of different targets with two illumination polarizations are simulated using the finite-difference time-domain method. Thirdly, a few experiments are performed to verify the influence of illumination polarization and target structures on the sensitivity of TSOM. Both the results of the simulation and experiments illustrate an apparent influence of polarization on the sensitivity of inspecting the targets with center asymmetric structures. For enhanced sensitivity, illumination polarization should be perpendicular to the target texture. This conclusion is meaningful to adjust illumination polarization purposefully for different structure characteristics and improve the sensitivity of metrology.

Keywords: through-focus optical microscopy; illumination polarization; target structure; sensitivity

1. Introduction

With gradually increased applications of three-dimensional (3D) components in the fields of semiconductor industry and nanotechnology, obtaining 3D information of these targets is critical. However, conducting 3D topography optical metrology of nanoscale targets for general optical microscopy is becoming increasingly challenging due to severe diffraction.

Through-focus scanning optical microscopy (TSOM) is a novel and fast optical metrology. TSOM is not limited by the need to acquire an in-focus image in the conventional measurement. This method utilizes a TSOM image by scanning the target through the focus, and it extracts dimensional information of the targets by analyzing scattering intensity of the TSOM image and matching the TSOM image with the simulation results in the database [1]. Low resolution due to the diffractive limit in conventional optical metrology is consequently avoided. The lateral and vertical sensitivity of TSOM is quantified by the optical intensity range (OIR) of the TSOM image, which is defined as the absolute difference between the maximum and minimum intensity of the normalized TSOM image [2].

The sensitivity of TSOM strongly depends on many mechanical and optical factors [3–5]. The critical dimension of a target is usually smaller than 1/10 of wavelength of the illumination light;



thus, the interaction between incident light wave and target surface is complicated, and the spatial distribution of scattered light wave depends on illumination polarization and target structures [6]. TSOM images with different OIRs correspond to different spatial distributions of scattered light [7]. Consequently, the illumination polarization and structure characteristics of the target strongly affect the sensitivity of TSOM [8,9]. To address the lacking systematic analysis of these effects, many works attempt to optimize illumination polarization according to different targets through pre-tests [10,11]. The drawbacks are long preparation time and low inspection efficiency. To understand the light scattering around the target surface and conduct the inspection in the most optimized condition, the effects on TSOM sensitivity brought by illumination polarization and target structure are analyzed and summarized in this paper.

The reminder of this article is organized as follows: the complete image-forming procedure, from incidence of illumination to the imaging plane of the charge-coupled device (CCD), is analyzed in the second section. The simulation of the system is presented in the third section. A few experiments are performed in the fourth section to verify the simulation results. The simulation and experimental results are interpreted in the fifth section. A conclusion based on the analyses and results is proposed in the sixth section.

2. Principle Analysis

The principle analysis of TSOM is separated into three parts—illuminating, scattering, and imaging. Firstly, Köhler illumination in the TSOM system is explored. Secondly, the scattered electromagnetic field is analyzed after the illumination wave is reflected from a complex target. Thirdly, the image-scanning procedure along the optic-axis direction that collects an in-focus image and a series of defocused images of the target is investigated.

2.1. Köhler Illumination

A Köhler illumination system in reflective mode is widely used in TSOM. Under this condition, the illumination beam from each source point in the conjugate back focal plane of the objective lens converges to a few plane waves $E_{i,j}$ with different angular directions [12,13].

These plane waves are similar with the definition of the angular spectrum. Thus, the Köhler illumination of the TSOM can be defined as a summation of these plane waves.

$$\boldsymbol{E}(\boldsymbol{r}) = \sum_{i,j} \boldsymbol{E}_{i,j} e^{-\hat{i}\boldsymbol{k}_{ij}\cdot\boldsymbol{r}} \ (i,j = integer), \tag{1}$$

where E(r) is the illuminating light wave near the object surface, \hat{i} is the imaginary unit here, k_{ij} is the corresponding wave vector of $E_{i,j}$, and r is the location vector.

2.2. Scattered Electromagnetic Field from the Target

The incident illumination light on the target surface is scattered and forms a superimposed field with the incident field and a scattered field. The superimposed field is defined as follows [14]:

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{(inc)}(\boldsymbol{r}) + \boldsymbol{E}^{(sca)}(\boldsymbol{r}), \tag{2}$$

$$H(\mathbf{r}) = H^{(inc)}(\mathbf{r}) + H^{(sca)}(\mathbf{r}),$$
(3)

where the superscript (*inc*) is the incident field, and the superscript (*sca*) denotes the scattered field. Combined with Maxwell equations, Equations (2) and (3) can be rewritten as follows:

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{(inc)}(\boldsymbol{r}) + \nabla \cdot \nabla \cdot \Pi_{e}(\boldsymbol{r}) + \hat{i}k \nabla \cdot \Pi_{m}(\boldsymbol{r}) - 4\pi \boldsymbol{P}(\boldsymbol{r}),$$
(4)

$$\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{H}^{(inc)}(\boldsymbol{r}) + \nabla \cdot \nabla \cdot \Pi_{m}(\boldsymbol{r}) - \hat{i}k \nabla \cdot \Pi_{e}(\boldsymbol{r}) - 4\pi \boldsymbol{M}(\boldsymbol{r}),$$
(5)

where P(r) and M(r) are the incident polarized intensity of the electric and magnetic vectors in the target, respectively.

$$P(\mathbf{r}) = \eta(\mathbf{r})E(\mathbf{r}),\tag{6}$$

$$M(\mathbf{r}) = \chi(\mathbf{r})H(\mathbf{r}),\tag{7}$$

where $\eta(\mathbf{r})$ and $\chi(\mathbf{r})$ are dielectric and magnetic susceptibilities, respectively. $\Pi_e(\mathbf{r})$ and $\Pi_m(\mathbf{r})$ are electric and magnetic Hertz potentials, respectively, as expressed in the following equations:

$$\Pi_{e}(\mathbf{r}) = \int_{V} \mathbf{P}(\mathbf{r}') \frac{e^{i\mathbf{k}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^{3}\mathbf{r}', \qquad (8)$$

$$\Pi_m(\mathbf{r}) = \int_V \mathbf{M}(\mathbf{r}') \frac{e^{i\mathbf{k}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r}', \qquad (9)$$

where *V* is the target's volume in space.

Equations (6), (7), (8), and (9) are substituted into Equations (4) and (5). The total field can be described by integral–differential equations in which each component of the electric and magnetic fields is coupled with others. The effect of coupling is negligible because the dimension of the target is much smaller than the wavelength. Therefore, this scattering should not be described with a simple scalar equation.

According to the relationship between $\eta(\mathbf{r})$ and relative permittivity $\varepsilon_r(\mathbf{r})$,

$$\varepsilon_r(\mathbf{r}) = 1 + \eta(\mathbf{r}),\tag{10}$$

the relationship between $\varepsilon_r(\mathbf{r})$ and refractive index $n(\mathbf{r})$,

$$\varepsilon_r(\mathbf{r})\cdot\varepsilon_0 = n^2(\mathbf{r}),$$
 (11)

and the equivalent transformation from the topographic structure to the refractive index around the surface, the effect of illumination polarization and target structure on the spatial distribution of the scattered light is provided as follows:

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{(inc)}(\boldsymbol{r}) + \nabla \cdot \nabla \cdot \int_{V} \boldsymbol{P}'(\boldsymbol{r}') d^{3}\boldsymbol{r}' + \hat{i}k \nabla \cdot \int_{V} \boldsymbol{M}'(\boldsymbol{r}') d^{3}\boldsymbol{r}' -4\pi \Big(\frac{n^{2}(\boldsymbol{r})}{\varepsilon_{0}} - 1\Big) \boldsymbol{E}(\boldsymbol{r}),$$
(12)

$$\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{H}^{(inc)}(\boldsymbol{r}) + \nabla \cdot \nabla \cdot \int_{V} \boldsymbol{M}'(\boldsymbol{r}') d^{3}\boldsymbol{r}' - \hat{i}k \nabla \cdot \boldsymbol{P}'(\boldsymbol{r}') d^{3}\boldsymbol{r}' - 4\pi \chi(\boldsymbol{r}) \boldsymbol{H}(\boldsymbol{r}),$$
(13)

where

$$\mathbf{P}'(\mathbf{r}') = \left(\frac{n^2(\mathbf{r}')}{\varepsilon_0} - 1\right) \mathbf{E}(\mathbf{r}') \frac{e^{\hat{i}\mathbf{k}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|},$$

and

$$M'(\mathbf{r}') = \chi(\mathbf{r}')H(\mathbf{r}')\frac{e^{\hat{i}\mathbf{k}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

For a target with given topographic features, calculating the specific marginal solution of Equations (12) and (13) provides the near-field scattered electromagnetic field theoretically. However, this procedure is complicated, in that obtaining analytic solutions is impossible. In this study, the finite-difference time-domain (FDTD) method is used to calculate the numerical solutions.

2.3. Imaging Procedure

The imaging system of the TSOM is the same as a bright-field microscopy. The complete imaging system includes an illuminating path and an imaging path. These two paths can be described by their corresponding optical transfer function (OTF). The OTF of the illuminating path is [6]

$$H_{ill}(k_{i,j}) = \exp\left[\hat{i}D\sqrt{\left(\frac{2\pi}{\lambda}\right)^2 - |k_{i,j}|^2}\right],\tag{14}$$

where *D* is the illumination spot defocus and a variable here. The OTF of the imaging path is

$$H_{ima}(k_{k,m}) = \begin{cases} 1 & |k_{k,m}| \le \frac{2\pi}{\lambda} NA\\ 0 & else \end{cases},$$
(15)

where *NA* is the numerical aperture of objective lens. The complete system–structure interaction is described by

$$\boldsymbol{E}_{k,m}^{out} = H_{ima}(k_{k,m}) \cdot \boldsymbol{S}_{i,j;k,m} \cdot H_{ill}(k_{i,j}) \cdot \boldsymbol{E}_{i,j'}^{in}$$
(16)

where $S_{i,j;k,m}$ is a four-dimensional scattering matrix, and the two pairs of indices *i*, *j* and *k*, *m* describe the in-plane components of the wavevectors for the illuminating plane waves $E_{i,j}^{in}$ and scattering plane waves $E_{k,m}^{out}$, respectively. Finally, as each illuminating plane wave component corresponds to a specific source point in Kohler illumination, and the light source is incoherent, the subsequent scattering plane waves are assumed as incoherent as well. Thus, each pixel of the image is generated from the incoherent sum of output plane waves scattered from a given location of the structure, as depicted in Equation (17).

$$I(\mathbf{r}) = \sum_{k,m} \left| E_{k,m}^{out} e^{\hat{i} \mathbf{k}_{k,m} \cdot \mathbf{r}} \right|^2, \tag{17}$$

where *r* denotes the location vector toward the CCD plane.

3. Simulation

3.1. Target Structure

A commercial optical simulation program (i.e., FDTD) was used to calculate the light wave scattered by the target and the simulation of imaging process. Table 1 lists the structure parameters of six different targets and three imaging parameters, namely the illumination numerical aperture (INA), the collection numerical aperture (CNA), and the wavelength. As Figure 1 depicts, a given INA determines a specific illumination cone, and the collection cone is constrained by CNA.



Figure 1. Schematic of (**a**) illumination numerical aperture (INA; red) and (**b**) collection numerical aperture (can; blue).

Target	Structure Parameter		Imaging Parameter		
			Illumination Numerical Aperture	Collection Numerical Aperture	Wavelength (nm)
Nano-pit	Radius	100 nm	0.4	0.8	546
Nano-dot	Length Width Height	121 nm 121 nm 71 nm	0.4	0.8	546
Nano-bump	Radius	100 nm	0.4	0.8	546
Double silicon lines	Width Height Pitch Sidewall angle	30 nm 50 nm 20 nm 90°	0.4	0.8	546
Dense line arry	Width Height Pitch Sidewall angle	30 nm 50 nm 60 nm 90°	0.4	0.8	546
Infinite line grating	Width Height Pitch Sidewall angle	30 nm 50 nm 600 nm 90°	0.4	0.8	546

Table 1. Structure and imaging parameters used in the simulation.

The materials of the four targets were all silicon, and the target structures are demonstrated in Figure 2, where different colors are used to highlight their structural features. Each model was illuminated by two kinds of light waves with the electric vector perpendicular or parallel to the incident plane. The structure of the first three targets was centrosymmetric, that is, the structures were consistent along *X*- and *Y*-axes, whereas the structure of the last target was center asymmetric. For convenience, the lines of the silicon line array were oriented perpendicular to the incident plane, so the porization of illumination light could be described as either perpendicular (0° polarization) or parallel (90° polarization) to the silicon lines.



Figure 2. Computer-aided design (CAD) models for (**a**) nano-pit, (**b**) nano-dot, (**c**) nano-bump, (**d**) double silicon lines, (**e**) dense line array, and (**f**) infinite line grating.

3.2. Simulation Procedure

The complete simulation was separated into three parts. In the first part, the interaction between the light wave and target was calculated with the FDTD method. In this part, the scattering matrix $S_{i,j;k,m}$ depicted in Equation (16) is expected to be derived. The scattering matrix is dependent only on the simulated structure and wavelength of light, and it describes the complete interaction with two illumination polarizations. In the second part, an in-focus image and a set of defocused images were

simulated by changing the value of *D* in Equation (14). In the last part, a TSOM image was obtained using a particular method.

Attota et al. proposed the details of obtaining both the simulated and experimental TSOM images [10], and the procedure is restated below for convenience.

- Obtain an in-focus image and a series of defocused images of the target and a smooth background surface, respectively, as they are scanned along the axis direction.
- Normalize each through-focus image of the target and background as follows:

Normalized Image =
$$\frac{Unnormalized Image}{Mean Value} - 1.$$
 (18)

- For the in-focus or each defocused position, directly subtract the normalized background image from the normalized target image.
- Select the inspection region with a strip window on the subtracted normalized image at each focus height, and extract the intensity profile by averaging the image intensity along the width of the window.
- Stack the averaged intensity profile of each subtracted normalized through-focus image according to its corresponding focus height to construct a raw TSOM image, which contains three-dimensional information. *X* (horizontal), *Y* (vertical), and *Z*-axes represent the spatial position across the target, the focus position, and the optical intensity, respectively.
- Interpolate and smooth the raw TSOM image and add pseudo color. The result is the final TSOM image needed.

3.3. Simulation Results

The simulated TSOM images of the six targets in the illumination polarizations of 90° and 0° are illustrated in Figure 3. The relative difference of OIR (OIR_{*rd*}) is calculated in Equation (19).





Figure 3. Simulated through-focus scanning optical microscopy (TSOM) images of the six targets with different structural features with illumination polarizations of 90° (the first column) and 0° (the second column); OIR—optical intensity range; INA = 0.4.

Table 2 provides the results.

Table 2. Relative difference between optical intensity ranges (OIRs) with two illumination polarizations.TSOM—through-focus scanning optical microscopy.

Targets	Relative Difference (TSOM)
Nano-pit	0.74%
Nano-dot	2.3%
Nano-bump	0.25%
Double silicon lines	31.9%
Dense line array	447%
Infinite line grating	145%

The first three targets were centrosymmetric. Under this condition, their TSOM images appear to be qualitatively similar. The corresponding OIRs in the two illumination polarizations were not strongly different, which illustrates a weak influence of polarization on the sensitivity of TSOM with regards to the targets of centrosymmetric features.

The others were center asymmetric, that is, the silicon lines were oriented parallel to the *Y*-axis, but periodic along the *X*-axis. Under this condition, an apparent influence of illumination polarization on the sensitivity of TSOM can be observed as the two TSOM images and corresponding OIRs were strongly different.

The effect brought about by illumination numerical aperture (INA) was also studied by simulating the TSOM of the double silicon line upon setting INA = 0.8 and keeping other parameters in line with those in the previous simulation. Figure 4 presents the simulation results.

By comparing the results of Figures 3 and 4, it is demonstrated that the OIR of the TSOM image with the illumination numerical aperture of 0.8 is smaller than that with the illumination numerical aperture of 0.4. However, the two corresponding OIRs in both illumination polarizations are still different. It is concluded that the effect brought about by the illumination polarization and the

target structural feature exists as long as the metrology is performed in the same illuminating and imaging conditions.



Figure 4. Simulated TSOM images of double silicon lines with illumination polarizations of 90° (the first column) and 0° (the second column); INA = 0.8.

To analyze this phenomenon further, the line height of the double silicon line and dense line array were increased by 10 nm, but the other parameters are kept constant. This dimensional change produced a new TSOM image. The dimensional change was highlighted by a simple subtraction of the new and previous TSOM images and illustrated in a differential TSOM (DTSOM) image. The inspection of the vertical sensitivity of the dimensional change was directly quantified by the OIR of the DTSOM image. The DTSOM images in the two illumination polarizations are shown in Figure 5. The relative difference of OIR is provided in Table 3.



Figure 5. Simulated differential TSOM (DTSOM) images for silicon line array with illumination polarizations of 90° (the first column) and 0° (the second column). The line height was increased by 10 nm, but the line width and pitch were kept constant.

Table 3. Relative difference between OIRs with two illumination polarizations.DTSOM—differential TSOM.

Target	Relative Difference (DTSOM)	
Double silicon lines	62.9%	
Dense line array	203%	

4. Experiment

4.1. Experimental Set-Up

The optical scheme of the experiment is shown in Figure 6. A Zeiss Axio Imager M2 was used as the inspection device. The illumination numerical aperture (INA) and collection numerical aperture

(CNA) were both 0.8, and the magnification of the objective was $100 \times$. The wavelength of illumination light was 555 nm. The optical path of illumination was designed as a Köhler illumination with a polarizer to produce the two kinds of linear polarizations mentioned above. A motor stage in closed-loop control was located beneath the microscope. The in-focus image and defocused images were collected by moving the motor stage vertically.



Figure 6. Schematic of the TSOM nanoscale metrology device, where the red ray is the illumination ray and the green ray is the imaging ray. The INA of the illuminating system is defined by the iris and the CNA of imaging system is defined by the objective. The motor stage and charge-coupled device (CCD) were controlled by a computer so that the CCD took one picture as soon as the motor stage moved a certain distance.

4.2. Experimental Sample

Two Au line arrays deposited on smooth silicon substrates were inspected. The line heights of the array were 50 nm and 70 nm, and the width of each Au line was approximately 20 nm. Each array was separated into 10 groups, and the nominal pitch of each group decreased from 1000 nm to 50 nm. The SEM of one Au line array is presented in Figure 7.

4.3. Experimental Results

To verify our analysis and prove the effects of illumination polarization and structural features, the Au line array with the pitch of 1000 nm was inspected using TSOM with two illumination polarizations.

Figure 8 presents the simulation results of the Au line array with 50-nm height. The TSOM images were simulated with a 0.8 INA, 0.8 CNA, and 555-nm illumination wavelength, which was identical to the experimental conditions. Figure 9 shows the experimental results of the Au line arrays with 50-nm and 70-nm height.

The microscope system noise is dependent on the stray light, blurs on the wafer, aberration of the microscope, and imprecision of the motion and location component of the stage [2,15]. The TSOM images of the system noise with two illumination polarizations were obtained by subtracting two background TSOM images corresponding to line heights of 70 nm and 50 nm. The TSOM images are demonstrated in Figure 10.



Figure 7. SEM of Au line array. In this figure, the width of the Au line is 23.6 nm, and the pitch of this group is approximately 1000 nm.



Figure 8. Simulated TSOM images of Au line arrays with illumination polarizations of 90° (a) and 0° (b).



Figure 9. Experimental TSOM images for the Au line arrays with illumination polarizations of 90° (the first column) and 0° (the second column). The line heights were 50 nm and 70 nm.



Figure 10. Experimental TSOM images of the system noise with 90° polarization (**a**) and 0° polarization (**b**).

Clearly, the intensity of signal and system noise are quantified by the OIR of the TSOM images of the target and noise, respectively. By dividing the OIR of the TSOM image of the target by that of the TSOM image of the noise, the signal-to-noise ratio (SNR) of TSOM is retained. The SNRs in the two illumination polarizations are presented in Table 4. According to the result, for the given target, the sensitivity and SNR apparently increase when the polarization is perpendicular to the Au lines.

Table 4. Signal-to-noise ratio (SNR) of each Au line array with different illumination polarizations.

Line Height	90° Polarization	0° Polarization
50 nm	SNR = 2.47	SNR = 8.45
70 nm	SNR = 6.47	SNR = 9.62

5. Analysis and Discussion

When light is scattered from the targets, its amplitude is changed. These changes depend on the sample material and shape, as well as the illumination polarization. As mentioned in Section 3.1, the structural features of nano-pit, nano-dot, and nano-bump were centrosymmetric. According to the analysis in Section 2, the function of their effective refractive index is also centrosymmetric, that is, in the polar coordinate

$$\mathbf{n}(\rho, \theta) = \mathbf{n}(\rho).$$

Therefore, the effective refractive indices of these three targets are constant with respect to the two illumination polarizations. For the silicon or Au lines, the function of the equivalent refractive index along the horizontal (*X*) axis is inconsistent but periodic. From the simulation and experimental results, the TSOM image and its OIR of the centrosymmetric targets is similar regardless of the different illumination polarizations, but an apparent difference can be observed for center asymmetric targets, which supports our hypothesis.

From the data of the last three rows of Table 2 and the data of Table 3 (double silicon lines and dense line array), the relative differences between OIRs of TSOM and DTSOM increase as the number of lines increases or the pitch of the array decreases. This phenomenon can be explained through the effect of form birefringence, which leads to two effective refractive indices for two orthogonal polarizations. The form birefringence strongly depends on the sample structure even if the sample material is non-birefringent. As the number of lines increases or the pitch of the array decreases, the scattered light intensity of the perpendicular polarization varies more significantly across the line and space than that of the parallel polarization, which is eventually illustrated through the relative difference between OIRs with the two illumination polarizations.

6. Conclusions

In this study, the complete image-forming procedure of TSOM was modeled, and it included Köhler illumination in the TSOM, the scattered electromagnetic field reflected from a complex target,

and the image-scanning procedure. The FDTD method was performed to simulate the TSOM images of four targets with representative structural features, and the OIRs with two illumination polarizations were analyzed. The simulation and experimental results demonstrate that, for centrosymmetric targets, neither of the polarizations is effective for improving inspection sensitivity and SNR. On the contrary, for the asymmetric targets such as silicon and Au line arrays, the sensitivity and SNR apparently improved when the illumination polarization light was perpendicular to the lines. This result is valuable in TSOM applications for micro- and nano-inspection by saving time and improving measuring efficiency and precision.

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