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Overlay metrological system for overlaid linear gratings by an interferoscatterometer

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Interferoscatterometry is an optical measurement technology based on the analysis of light scattered and interfered from a periodic structure. In this work, first we build up a model for this system by the rigorous coupled wave analysis. With the model we calculate the diffractive efficiency of overlaid linear gratings with a mirror located in the incident region. Then, from the analyses of the overlaid linear gratings we obtain the best structure which has the highest sensitivity in the interferoscatterometry. Finally, we measure a sample and get experimental signatures. In order to get the overlay between the upper and lower grating, we compare the experimental signatures with theoretical signatures which are built in a library. The application of the interference technique on the scatterometry shows a higher sensitivity and a longer measurement range. © 2005 American Institute of Physics. [DOI: 10.1063/1.1994920]

I. INTRODUCTION

The development of the semiconductor industry has created the need for reliable overlay metrology. According to a developmental report of the semiconductor technology by ITRS 2004 (International Technology Roadmap for Semiconductor), the pitch of 70 nm needs overlay control (accuracy) below 25 nm and overlay metrology precision below 2.5 nm. In the future, the pitch below 50 nm will need a metrological tool which has higher overlay control and precision to the overlay metrology. It is difficult to achieve by the conventional bright-field microscope because of the diffractive limit and optical aberrations.\textsuperscript{1,2}

Takahiro et al.\textsuperscript{3–5} proposed a heterodyne interference method instead of the bright-field microscope method. In their system, the upper and lower marks of the target were linear gratings which were overlaid each other and had the same pitches. The overlaid linear gratings are used as the alignment key. A $p$-polarization ray and an $s$-polarization ray were projected on the overlaid linear gratings and modulated at the same time. The diffractive beams from the overlaid linear gratings were subjected to frequency modulation. The frequency-modulated diffracted light beams were subjected to the heterodyne interference, and photoelectric conversion generated electrical signals so that the overlay between the upper and lower grating could be detected from phases of the two electrical signals. Another method\textsuperscript{6,7} was proposed to measure the overlaid linear gratings with a scatterometry-based metrology. In this method the reflectance of the zero diffraction order from the overlaid linear gratings was measured by scanning the incident angle. Scatterometry has the advantages of being noncontact and nondestructive.

In order to obtain higher accuracy for the scatterometry-based overlay metrology, we must shrink the pitches of the upper and lower linear gratings.\textsuperscript{8} Since the overlaid linear gratings have the reflection symmetry along the pitch direction when the overlay is zero, it will shorten the range of overlay measurement to half the pitch only. Huang\textsuperscript{9} et al. used asymmetric overlay gratings to extend the range of overlay measurement from the half pitch to the whole pitch. But it also reduces the accuracy of the scatterometry-based overlay metrology.

In this article, we propose a method, interferoscatterometry, in which an interference of the zero order beam with a retroreflected $+1$ order beam is measured, as shown in Fig. 1. In this scheme we can get a higher accuracy and much longer measurement range than those in the scatterometry-based overlay metrology. Moreover, this system arrangement, named the interferoscatterometer, is simpler than that of an angular scatterometer, where the incident angle needs to scan.

II. RIGOROUS COUPLED WAVE ANALYSIS FOR THIS SYSTEM

Electromagnetic wave scattering from the periodic structure can be calculated by rigorous coupled wave analysis (RCWA).\textsuperscript{10–13} In our simulation, the RCWA is modified for the mirror which is located in the incident region.

We follow Chateau’s algorithm to describe the system in the matrix form...
where $f_F$, $b_F$, and $f_L$ are the complex amplitude of the incident beam, reflective beam, and transmissive beam, respectively, and $b_L$ is the complex amplitude of the reflective beam from the transmissive region. Generally, $b_L$ is set to be zero. $[C(z_0)]$ and $[C(z_m)]$ are the interface matrices in the incident region and transmissive region. $[G_i]$ is the characteristic matrix of the $l$th layer in the grating region, and is defined by

$$
\left[ \begin{array}{c}
    f_F^{(i-1)} \\
    \vdots \\
    b_F^{(i-1)} \\
    \vdots \\
    f_L^{(i-1)} \\
    \vdots \\
    b_L^{(i-1)} \\
\end{array} \right] = [C(z_0)]^{-1} \prod_{j=0}^{m-1} [G_j] \left[ \begin{array}{c}
    f_F^{(i-1)} \\
    \vdots \\
    b_F^{(i-1)} \\
    \vdots \\
    f_L^{(i-1)} \\
    \vdots \\
    b_L^{(i-1)} \\
\end{array} \right], \quad (1)
$$

where $f_F$, $b_F$, and $f_L$ are the complex amplitude of the incident beam, reflective beam, and transmissive beam, respectively, and $b_L$ is the complex amplitude of the reflective beam from the transmissive region. Generally, $b_L$ is set to be zero. $[C(z_0)]$ and $[C(z_m)]$ are the interface matrices in the incident region and transmissive region. $[G_i]$ is the characteristic matrix of the $l$th layer in the grating region, and is defined by

$$
[G_i] = [P_i(z_i)] \exp[-(z_{i+1} - z_i)] [D_i] \times [P_i(z_i)]^{-1}, \quad (2)
$$

where $[P_i]$ and $[D_i]$ are the eigenvectors and the diagonal matrix of the eigenvalues, respectively, in the $l$th layer of the grating region.

We define the matrix of incident beams as

$$
\begin{bmatrix}
    f_F^{(-2)} \\
    f_F^{(-1)} \\
    f_F^{(0)} \\
    f_F^{(+1)} \\
    f_F^{(+2)} \\
    \vdots \\
\end{bmatrix} =
\begin{bmatrix}
    \vdots \\
    0 \\
    0 \\
    1 \\
    A_{+1} \exp(i \theta_{f,+1}) \\
    0 \\
    \vdots \\
\end{bmatrix}, \quad (3)
$$

where $f_F^{(0)} = 1$ is the normal incident beam and $f_F^{(+1)} = A_{+1} \exp(i \theta_{f,+1})$ is from the feedback of the output diffractive beam at the $+1$ order. $A_{+1}$ and $\theta_{f,+1}$ are the amplitude and phase of the retroreflected beam, respectively. Furthermore, the matrix of reflective beams can be defined as

$$
\begin{bmatrix}
    b_F^{(-1)} \\
    b_F^{(0)} \\
    b_F^{(+1)} \\
    \vdots \\
\end{bmatrix} =
\begin{bmatrix}
    \vdots \\
    B_{-1} \exp(i \theta_{h,-1}) \\
    B_0 \exp(i \theta_{h,0}) \\
    B_{+1} \exp(i \theta_{h,+1}) \\
    \vdots \\
\end{bmatrix}, \quad (4)
$$

where $B_n$ and $\theta_{h,n}$ are the amplitude and phase of reflective beams at the $n_{th}$ order, respectively. From Eqs. (3) and (4), $A_{+1}$ and $\theta_{f,+1}$ are defined by

$$
A_{+1}^2 = \eta_m \times B_{+1}^2.
$$
Here $\eta_m$ is the reflectivity of the mirror, $d_{m0}$ is the initial distance from the mirror to grating surface [see Fig. 1(a)], and $\Delta \theta_m$ is the phase shift due to the mirror moving. Using the iterative method, we can get the accurate amplitude and phase $\theta_{b,+1}$ of the feedback beam. Figure 2 shows the calculation flowchart. After the reflective beam $b_F^{(0)}$ with the amplitude $B_0$ and phase $\theta_{b,0}$ is determined, the reflection diffraction efficiency of the zero order $\eta_B^{(0)}$ is obtained by

$$\eta_B^{(0)} = |b_F^{(0)}|^2.$$  \hspace{1cm} (6)

III. EXPERIMENTAL ARRANGEMENT AND SIMULATION

The experimental arrangement is illustrated in Fig. 1. A He–Ne laser is used as the light source. A polarizer is used to control the polarizations of the input beam. In this experiment, we only consider the s polarization [transverse electric (TE) mode]. The input beam is normally incident on the overlaid linear grating surface, and the +1 order diffractive beam is retroreflected to the overlaid linear gratings by a mirror. Interference happens between a reference beam and a modulation beam, where the reference beam is referred to the zero order diffractive beam and the modulation beam is referred to the +1 order diffractive beam reflected by the mirror. Finally, the interference intensity is measured by a charge coupled device (CCD) camera.

The interferoscopy as a metrology technique is used to determine the geometric parameters and the overlay between the upper and the lower linear gratings by the efficiency measurements of the light diffracted by the overlaid linear gratings. A schematic diagram of the sample used in this experiment is shown in Fig. 3. On a silicon substrate, two layers with linear grating structure are overlaid and in-between a thin film layer is deposited. An offset bias between the upper and the lower linear gratings is preset in order to have a maximum sensitivity of overlay metrology. The part of the overlay we are concerned with is the dislocation arising from misalignment in the process. The total overlay for the overlaid linear gratings is defined as $\Delta x=\epsilon$ in rad. In Fig. 3 the $L$ and $S$ denote the linewidth and line spacing of the linear gratings, respectively, and the geometric parameters of the sample are listed in Table I.

If we take the $L/S=1/1$, pitch=800 nm, offset bias $=0$ nm, and $\lambda=633$ nm, the results of simulation are shown in Fig. 4, where the $x$ axis gives the phase difference and $y$ axis represents the diffractive efficiency. Signatures corresponding to overlay from 0 to 400 nm are shown in Fig. 4. For example, the 150 nm signature means the overlay is 150 nm. A maximum efficiency difference between the two adjacent signatures occurs at a certain phase difference. For example, if the overlay is in the range from 50 to 100 nm, the maximum efficiency difference is 2.8715% at a phase difference of 0.178 rad. The maximum efficiency differences for the overlay from 0 to 400 nm with an interval of 50 nm are listed in Table II, where we find the largest one is 3.3368% corresponding to the overlay from 100 to 150 nm. Thus, we

![Image](image_url)

**TABLE I.** Geometric parameter of the sample.

<table>
<thead>
<tr>
<th>Material</th>
<th>thickness</th>
<th>$n$</th>
<th>$k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top layer</td>
<td>Photosist</td>
<td>850 nm</td>
<td>1.624</td>
</tr>
<tr>
<td>Inter layer</td>
<td>Polysilicon</td>
<td>200 nm</td>
<td>3.926</td>
</tr>
<tr>
<td>Bottom layer</td>
<td>SiO$_2$</td>
<td>50 nm</td>
<td>1.463</td>
</tr>
<tr>
<td>Substrate</td>
<td>Silicon</td>
<td>—</td>
<td>3.867</td>
</tr>
</tbody>
</table>

**TABLE II.** Phase difference vs the maximum efficiency difference for a 50 nm range. The phase difference is calculated from the optical path difference caused by the mirror moving.

<table>
<thead>
<tr>
<th>Overlay (nm)</th>
<th>Maximum efficiency difference (%)</th>
<th>Phase difference (rad)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0–50</td>
<td>1.1910</td>
<td>0.122$\pi$</td>
</tr>
<tr>
<td>50–100</td>
<td>2.8715</td>
<td>0.178$\pi$</td>
</tr>
<tr>
<td>100–150</td>
<td>3.3368</td>
<td>0.233$\pi$</td>
</tr>
<tr>
<td>150–200</td>
<td>2.7563</td>
<td>0.250$\pi$</td>
</tr>
<tr>
<td>200–250</td>
<td>2.2571</td>
<td>0.256$\pi$</td>
</tr>
<tr>
<td>250–300</td>
<td>2.4712</td>
<td>0.294$\pi$</td>
</tr>
<tr>
<td>300–350</td>
<td>2.5014</td>
<td>0.322$\pi$</td>
</tr>
<tr>
<td>350–400</td>
<td>0.9243</td>
<td>0.256$\pi$</td>
</tr>
</tbody>
</table>
can preset an offset bias between 100 and 150 nm for overlaid linear gratings to get the maximum sensitivity of the overlay metrology. In our simulation, the sensitivity of the overlay metrology is referred to the global maximum value of the efficiency difference for the interval of 10 nm of the overlap between the upper and lower linear gratings. Therefore, in Table II, the SOM_{10 nm} is 0.667 (the value of 3.3367% must be divided by 5, corresponding to the interval of 10 nm of the overlaid linear gratings).

IV. OPTIMIZING THE PARAMETERS

In the process of making linear gratings, we can optimize the parameters of linear gratings for higher sensitivity. The parameters which could change without any effect on the process of making chips are the pitches and \( L/S \) ratio of the overlaid gratings. We sample the total range of the interested parameters by searching the grid and find the optimum solution range. Then, we shrink the searching range of parameters and increase the sampling resolution. Finally the optimum parameters could be found.

For the structure of Fig. 3 we change the pitch from 1000 to 1800 nm with the interval of 10 nm and the \( L/S \) ratio changes from \( L/S=5/5 \) to \( 8/2 \). The simulation results are shown in Fig. 5, where the \( x \) axis is the pitch of linear gratings and the \( y \) axis is the SOM_{10 nm}. As the \( L/S \) ratio changes from \( L/S=5/5 \) to \( 8/2 \), the peak location of SOM_{10 nm} moves from pitch=1160 nm to pitch=1260 nm and then goes back to pitch=1040 nm. The maximum value of SOM_{10 nm} is 1.76 if the \( L/S=7/3 \) and pitch=1150 nm. In order to find more accurate parameters, we shrink the searching range of simulation. Then, we change the pitches from 1000 to 1300 nm with intervals of 5 nm and the \( L/S \) ratio of simulation from 60/40 to 80/20. We find that the maximum value of SOM_{10 nm} becomes 1.8287 at point B \( (L/S=64/36, \text{pitch}=1215 \text{ nm}) \). Point A is the submaximum value of SOM_{10 nm}, which is from optimizing parameters in the long range [see Fig. 5(c)].

![FIG. 5. Simulation results of optimizing parameters in the long range. The pitch of the grating changes from 1000 to 1800 nm with the interval of 10 nm and the \( L/S \) ratio changes from \( L/S=5/5 \) to \( 8/2 \). The peak location of SOM_{10 nm} moves from pitch=1160 nm (a) to pitch=1260 nm (b) and then goes back to pitch=1040 nm (d). The optimum SOM_{10 nm} is found at pitch=1150 nm (c).](image)

![FIG. 6. Simulation results of optimizing parameters in the short range. The pitch changes from 1000 to 1300 nm with an interval of 5 nm and the \( L/S \) ratio changes from 60/40 to 80/20. The maximum value of SOM_{10 nm} is 1.8287 at point B \( (L/S=64/36, \text{pitch}=1215 \text{ nm}) \). Point A is the submaximum value of SOM_{10 nm}, which is from optimizing parameters in the long range [see Fig. 5(c)].](image)

TABLE III. Optimum parameters of overlaid gratings for the interferoscat-

terometer and the angular scatterometer.

<table>
<thead>
<tr>
<th>Pitch (nm)</th>
<th>( L/S ) ratio</th>
<th>Offset bias (nm)</th>
</tr>
</thead>
</table>
| Interfero-
| scatterometer | 1215 | 64/36 | 300 |
| Angular
| scatterometer | 460 | 48/52 | 395 |

at phase difference \( =1.667 \pi \text{ rad} \) at angle=14.3°.
in this range, the average value of the DDE is 4.9\% for the interferoscatterometer and 3.3\% for the angular scatterometer. Thus, the sensitivity of the interferoscatterometer is 47.3\% larger than that of the angular scatterometer in the $\varepsilon$ range from +50 to −50 nm as shown in Fig. 8.

V. EXPERIMENT AND RESULTS

We fabricated a sample for tests of the interferoscatterometer. The parameters of the upper and lower linear gratings are listed in Table I for the material and thickness and the optimum parameters of the gratings designed for in the interferoscatterometer are shown in Table III. However, after fabrication, we find that the real structures of the gratings are a little different from the designed structures. The real parameters of the structures were measured by atomic force microscopy (AFM) and ellipsometer and are listed in Table IV. The size of the sample is 85 $\mu$m × 65 $\mu$m, which is big enough to meet the infinite boundary condition.\(^{14}\) We measured the overlay of the sample with the interferoscatterometer.

The sample was measured consecutively 20 times in order to obtain the repeatability of the interferoscatterometry overlay measurements. The distribution of the overlay is from 432 to 435 nm and the peak is at 433 nm. The precision (3$\sigma$ or $\sigma$ is the standard deviation) of the interferoscatterometry measurement is 1.95 nm. The measured signature and the result of RCWA fitting for the mirror moving distance of four periods are shown in Fig. 9. In this figure, the real circles are the values measured by the interferoscatterometer and the real line is the fitting result by the RCWA. The method that we used for extraction of the overlay is the library-based methodology. First, linear gratings data, thin-film data, and sidewall angle data are used to obtain a collection of structures for the library-based methodology. Then, we can calculate and create the library of signatures of the diffractive efficiency from the collected structures by the RCWA. Finally, we calculate the root mean square (rms)
between the measured signature and the library signatures and find the closest signature in the library to the measured signature. The overlay, \( \Delta x \), of the sample which is extracted from the library-based methodology is 433 nm and then the error is 133 nm.

After the sample was measured by the interferoscatterometer, we observed the cross section of the sample with scanning electron microscope (SEM). The picture taken from SEM is shown in Fig. 10, from which a total overlay of 402 nm can be seen. There is a difference of 31 nm from the result given by our library-based methodology. The error could be mainly from the fact that we do not collect enough structures in the library to approach the measured signature exactly. For example, the sidewall angle in the library is from 0° to 5°, but the shape of sidewall is supposed to be straight and symmetric. In fact, the sidewall is bent and asymmetric as shown in Fig. 10.

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