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Accurate characterization of mask defects by combination of phase retrieval and deterministic approach

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Abstract. We present a method to characterize not only shape but also depth of defects in line and space mask patterns. Features in a mask are too fine for a conventional imaging system to resolve them and a coherent imaging system providing only the pattern diffracted by the mask is used. Then phase retrieval methods may be applied, but the accuracy is too low to determine the exact shape of the defect. Deterministic methods have been proposed to accurately characterize the defect, but this requires a reference pattern. We propose to use a phase retrieval algorithm to retrieve the general shape of the mask and then apply a deterministic approach to precisely characterize the defects detected. © The Authors. Published by SPIE under a Creative Commons Attribution 3.0 Unported License. Distribution or reproduction of this work in whole or in part requires full attribution of the original publication, including its DOI. [DOI: [10.1117/1.OE.55.10.103105](https://doi.org/10.1117/1.OE.55.10.103105)]

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1 Introduction

In extreme ultraviolet lithography (EUVL), it is important to detect and characterize mask defects since the presence of defects as small as a few tenths of nanometers is already a critical issue.¹ As the structures of masks present features much finer than the wavelength, a conventional imaging system cannot be used even though methods relying on deep ultraviolet illumination were proposed.²

Coherent diffraction imaging methods^{1,3} have been proposed for defect inspection. However, in this case, mask shape is not directly obtained. Only diffraction patterns are measured, i.e., magnitude of Fourier transforms. Then phase information is lost and phase retrieval techniques should be applied to recover images. The hybrid input-output (HIO) algorithm developed by Fienup⁴ is the most widely used method for reconstructing phase information from the Fourier transform modulus since it enables to avoid local minima. In the case of mask inspection for EUVL, periodic patterns can be reconstructed and defects' widths can be estimated.⁵ However, it was reported that conventional phase retrieval methods, such as HIO algorithm, were not robust to noise.^{6,7} In practical applications, the noise is, therefore, limiting the accuracy.

A deterministic approach can be applied instead of a phase retrieval algorithm in the case where a reference, such as a diffraction pattern of a defect-free mask, is known in addition to the pattern diffracted by the mask under inspection.⁸ In this case, the shape of the defect can be determined precisely as well as its width. However, in practice, reference is not often available. Moreover, even if the theory was derived,⁸ the deterministic approach was only demonstrated with simulations and with defects represented by a single impulse⁹ or linear combination of impulse signals.¹⁰

To make the deterministic approach suitable for practical use, it is necessary to extend its conditions of application.

In this paper, we propose a method that enables to extend the application range of deterministic approach. The principle is to use phase retrieval algorithm to retrieve the shape of the mask and to use it as a reference to determine more precisely depth of defects with the deterministic approach. Since a phase retrieval algorithm is used, the reference profile can be determined and an iterative approach can then be adopted to detect multiple defects. We performed simulations to test our method and demonstrated its effectiveness with experimental results. The experimental demonstration was performed only at a micrometer scale, but imaging systems for mask inspection in EUVL are actually using magnifying systems that scale the diffraction patterns at a scale equivalent to our own data.

2 Problem Considered

2.1 Model of the Defect

We considered the case of a periodic line and space (L/S) stripe mask, presenting a single defect smaller than one complete stripe. The defect is represented by a linear combination of impulse signals. This is shown in Fig. 1.

The aim of this study is to retrieve the position and shape of the defect with the magnitude of the Fourier transform of the mask as the only initial data.

We suppose that the first and last points of the mask have the value x_{\max} . In addition, as the diffraction pattern is symmetrical, we make the choice to assume that the defect is on the first half of the pattern on the left. These assumptions are necessary for the application of the deterministic approach. However, we will see that our method can also be used in the cases where several defects are present on different stripes, as long as they are located on the same half of the profile.

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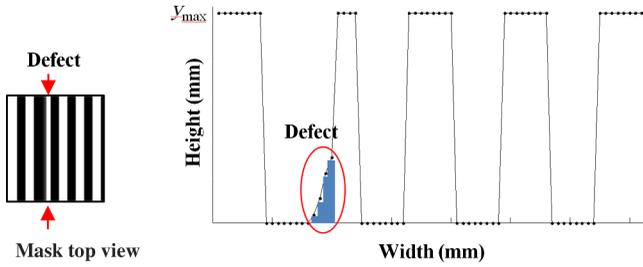


Fig. 1 Top view and profile of the type of mask considered.

2.2 Effect of Defects on the Diffraction Pattern

In the first step, we performed simulations to examine the effect of defects on the diffraction pattern.

The presence of defect induces the energy to spread into secondary orders (See Fig. 2). We can observe that the effect of the defect is more visible when the slope of the defect is abrupt. In practice, it is important to have a dynamic large enough when recording the diffraction patterns so that the secondary peaks can be clearly observed without saturating the main peaks. Deep defects lead to larger changes in the diffraction patterns which are, therefore, easier to detect.

3 Phase Retrieval and Deterministic Methods

3.1 Hybrid Input-Output Algorithm

3.1.1 Principle of the algorithm

The lost phase information can be reconstructed using a phase retrieval algorithm if the diffraction pattern is sampled at a frequency finer than the Nyquist frequency.¹¹ The principle of the method is to go back and forth between the real space and the frequency space, and to apply constraints in each space. Starting from the diffraction pattern and a random phase term, inverse Fourier transform is applied to go back to the real space. Then, a first constraint is applied before going back to the frequency space by Fourier transform. At that point, the phase term is kept, but the amplitude of the new Fourier transform calculated is replaced by

the known diffraction pattern. After several iterations, the phase term converges to a solution and the image in the real space is recovered.

A space constraint can be applied because the support γ of the image to be recovered can be determined. In the case of mask inspection, the size of the mask under inspection is known, the support can, therefore, be determined from the parameters such as pixel pitch of the camera and position of the diffraction order. Several types of constraints have been proposed for the real space.¹² The most basic one is to force to zero all values outside the support of the image. However, it might lead the algorithm to converge to a solution corresponding to a local minimum. The HIO algorithm is the most widely used algorithm as it enables to find the global minimum. Instead of being set abruptly to zeros, values outside the support are gradually reduced by a factor β . This is explained in Fig. 3.

In the case of mask inspection, defects can be detected by reconstructing the mask profile from the diffraction pattern. The illustration shown in Fig. 4 was performed by taking the Fourier transform of a simulated pattern presenting a period of eight pixels. The pattern counted nine stripes, and a defect was introduced on the third stripe. After application of the HIO algorithm, the pattern could be successfully retrieved, and the defect was clearly visible on the top view of the reconstructed mask. However, the question of accuracy in the depth direction should be examined to characterize the shape of the defect.

3.1.2 Application of hybrid input-output for mask inspection

Gerchberg–Saxton¹³ and HIO methods have been adopted in several recent studies^{1,3,5,14–20} for mask inspection in EUVL. Harada et al.^{1,14,17} reported the development of coherent scatterometry microscope to characterize mask defect. Extensive investigations to improve the numerical aperture of the imaging system and the coherence of the synchrotron radiation were reported to improve the lateral spatial resolution. An HIO algorithm was used to reconstruct profiles from the

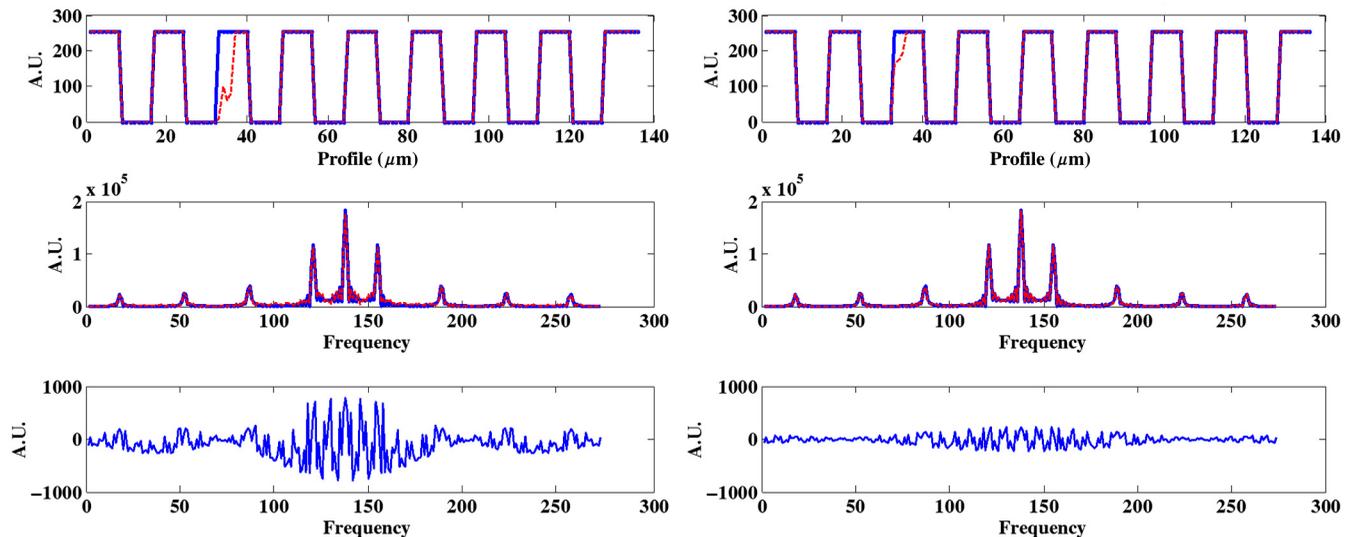


Fig. 2 Effect of defects on the diffraction pattern. The first line represents the mask profile with (red) and without defect (blue), the second line shows the amplitude of the diffraction pattern in one dimension, and the third line represents the subtraction between the two diffraction profiles.

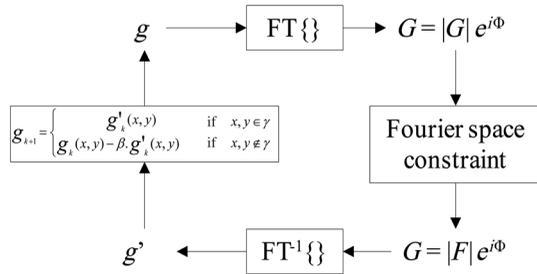


Fig. 3 Principle of the HIO algorithm. The support of the image is noted γ , and $|F|$ is the known amplitude of the Fourier pattern.

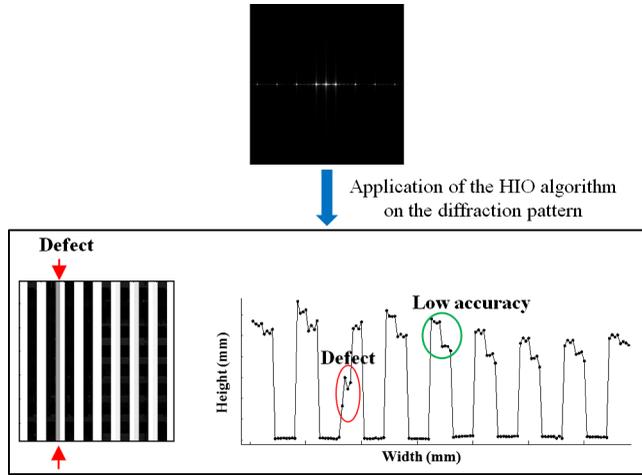


Fig. 4 HIO algorithm enables to retrieve the global shape of the mask pattern, but accuracy is too low to determine precisely the depth of the defect.

diffraction patterns and they presented good correlation with SEM measurements. Widths of the defects were characterized with a high precision. However, it is difficult to estimate the accuracy in depth.

We performed simulations to investigate the application of an HIO algorithm for reconstruction of the mask profile. To illustrate this problem in a simple way, we consider a diffraction pattern composed of diffraction orders presenting a narrow Gaussian shape. The Fraunhofer diffraction of the pupil induces an aura around the light spots.¹⁴ As a result, the image recovered with phase retrieval method is actually the desired profile multiplied by the shape of the pupil. This phenomenon is illustrated in Fig. 5 with two diffraction patterns that are exactly the same except for the width of the diffraction aura.

To recover the final shape of the mask, it is necessary to normalize the output of the HIO algorithm by the pupil of the system. One problem that arises is that when the widths of the diffraction orders are too large, the support area tends to move out of the center, as in Fig. 5(e). Harada et al.¹⁴ applied a strategy to optimize the support area gradually with the number of iterations. The general shape of the mask could then be retrieved. However, if the width of the defects can be estimated, it is more difficult to quantify the error made in the depth direction. In practical cases, the pupil may not be exactly a Gaussian, but the results are very similar.

Another issue is that convergence of the HIO algorithm tends to be disturbed in the presence of noise. Because

constraints in the real and Fourier space cannot be exactly satisfied at the same time, the algorithm has a tendency to oscillate between several solutions instead of converging to a unique solution. Several enhancements have been proposed to make the HIO algorithm more accurate and especially more robust to noise.^{7,21,22} For instance, Rodriguez et al.⁷ suggested adding an additional filter operation before application of the constraint in real space.

In spite of the different attempts to improve the robustness of the HIO algorithm, it is difficult to precisely evaluate the accuracy that it can provide in the depth dimension. Thus, an alternative method should be proposed to precisely characterize the shape of the defects in addition to their width. It is important to develop a method to improve the defect modeling and, thus our understanding of defects.

3.2 Deterministic Approach

An alternative solution to phase retrieval is to use a deterministic approach.¹⁰ However, additional information such as a reference diffraction pattern is required. We note $x(n)$ the defect-free mask pattern, $y(n)$ the profile of the mask with a defect, and $h(n)$ the defect represented by a linear combination of impulse signals. We can write

$$\begin{cases} y(n) = x(n) - h(n) \\ h(n) = \sum_{i=1}^M A_i \delta(n - n_i) \end{cases} \quad (1)$$

We can note that the coefficients A_i are all assumed to be positive. If a defect is located at a position n_0 , the deterministic approach can be applied only if $y(n_0) < x(n_0)$.

The only initial known data are the magnitude of the Fourier transform of $x(n)$ and $y(n)$, respectively, noted $X(\omega)$ and $Y(\omega)$. Then the autocorrelation of the signals can be obtained by taking the reverse Fourier transform of the diffraction pattern

$$\begin{cases} r_x(n) = \text{FT}^{-1}[|X(\omega)|^2] = x(n) * x(-n) \\ r_y(n) = \text{FT}^{-1}[|Y(\omega)|^2] = y(n) * y(-n) \end{cases} \quad (2)$$

Using Eqs. (1) and (2), the quantity r_{xy} is defined as follows:

$$\begin{aligned} r_{xy}(n) &= r_x(n) - r_y(n) \\ &= r_x(n) - [x(n) - h(n)] * [x(-n) - h(-n)] \\ &= \sum_{i=1}^M A_i x(-n + n_i) + \sum_{i=1}^M A_i x(n + n_i) - r_h(n). \end{aligned} \quad (3)$$

The term r_{xy} is the superposition of several terms. The first term is composed of the signal $x(-n)$ translated by $-n_i$ and multiplied by A_i . The second term is symmetric to the first one and the last term is a negative term corresponding to the autocorrelation of $h(n)$. The extreme points of r_{xy} have the value $A_i x(N)$. Then, as we assume that the extreme values of the signal x both have the value x_{\max} , we have $r_x(N) = x(1) \times (N) = x_{\max}^2$. As a result, we can deduce that $x(N) = \sqrt{r_x(N)}$ and, therefore, obtain $A_1 = r_{xy}(N) / x_{\max}$. Once this quantity is derived, the contribution brought by the first component of the defect can be removed by subtracting the quantity $A_1 x(N-1) \text{rect}(n_1 - N + 1, n_1) + A_1 x(N-1) \text{rect}(-n_1, N - 1 - n_1)$ from r_{xy} . A_2 and the other components A_i can then be recursively deduced. The procedure

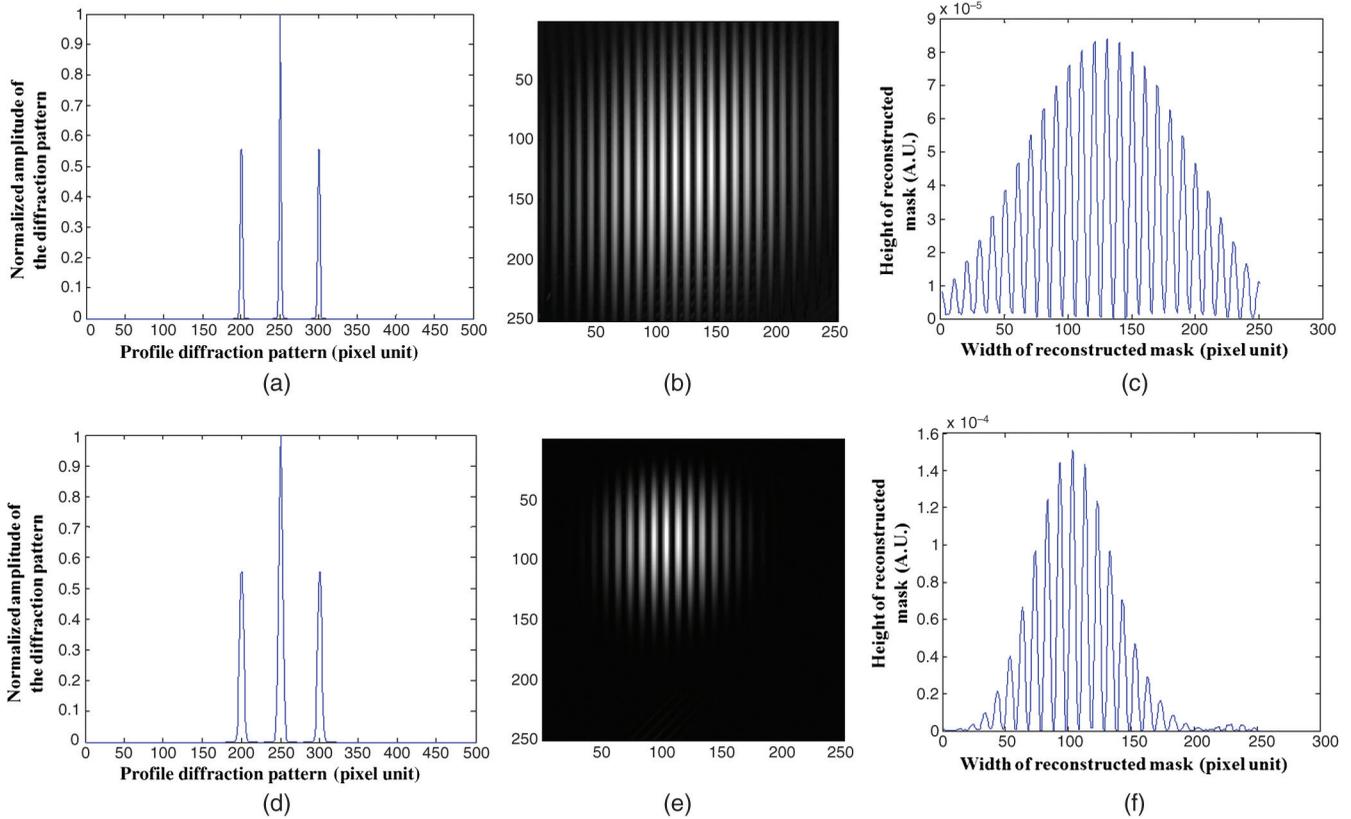


Fig. 5 Masks (b) and (e) are recovered from diffraction patterns with (a) narrow and (b) medium spots width, i.e., respectively. Only a one-dimensional (1-D) profile of the diffraction patterns is illustrated. The profiles (c) and (f) are 1-D illustration of the mask (b) and (e), respectively.

is completed when all contributions have been removed from r_{xy} , i.e., when the resulting signal $r_{xy}(n) - \sum_{i=1}^M A_i x(N-1) \text{rect}(-n_i, N-1-n_i) - \sum_{i=1}^M A_i x(N-1) \text{rect}(-N+1+n_i, n_i)$ does not have positive values.

At this stage, the defect $h(n) = \sum_{i=1}^M A_i \delta(n-n_i)$ can be estimated. Then another procedure should be applied to determine the shape of the signal $x(n)$. However, the determination of $h(n)$ is enough to apply our proposed method.

4 Proposed Method

4.1 General Principle

As we have seen previously, phase retrieval enables to recover the shape of the mask with the diffraction pattern as the only initial data, but the accuracy is low. On the other hand, the deterministic approach provides detailed information on the defect but requires an additional reference pattern. We propose to use the result of phase retrieval as a reference for the deterministic approach. In this way, we can completely characterize the defect without the need for any reference. The proposed procedure is illustrated in Fig. 6.

4.2 Determination of the Reference Signal

We propose to use the profile obtained with the phase retrieval algorithm as a reference. However, the profile pattern is not defect free. Thus, we suggest retrieving the global shape of the L/S mask by applying a threshold filter on the result obtained by phase retrieval. With this operation, the profile is divided into “line values” and “space values.”

First, the signal given by the HIO algorithm is normalized by its maximum value, as its accuracy is too low to rely on numerical values. The original diffraction pattern enables to calculate the autocorrelation signal r_y , and, therefore, enables to extract the real maximum value y_{\max} ($=x_{\max}$). Then scaling signal can be done easily after shape extraction.

In the case where a real reference pattern is used, the reference profile presents correct line and space values since it is from a defect-free pattern. However, since the result obtained by phase retrieval is not retrieved from a defect-free pattern, two situations can occur after the threshold operation. If the defect has a small depth, a line value will be attributed in the reference profile as if it was defect free [see Fig. 7(a)]. However, if the defect is too deep, i.e., under the threshold value, a space value will be attributed to the reference profile instead of a line value. These two cases are illustrated in Fig. 7.

In the second case [see Fig. 7(b)], the reference pattern is different from a defect-free pattern because a space value is obtained instead of a line value. It is equivalent to have negative coefficient A_i in the model of $h(n)$. A deterministic approach cannot work directly in this situation because the signal r_{xy} defined in Eq. (3) is supposed to be negative, except for the defect contributions that are assumed to be positive. The iterative loops to determine h from r_{xy} stops when the signal obtained after subtraction of defects' contributions becomes negative. Therefore, defects with negative coefficients cannot be detected in this way. To detect defects with negative coefficients, it is necessary to modify a little definition of the parameters according to the equation below:

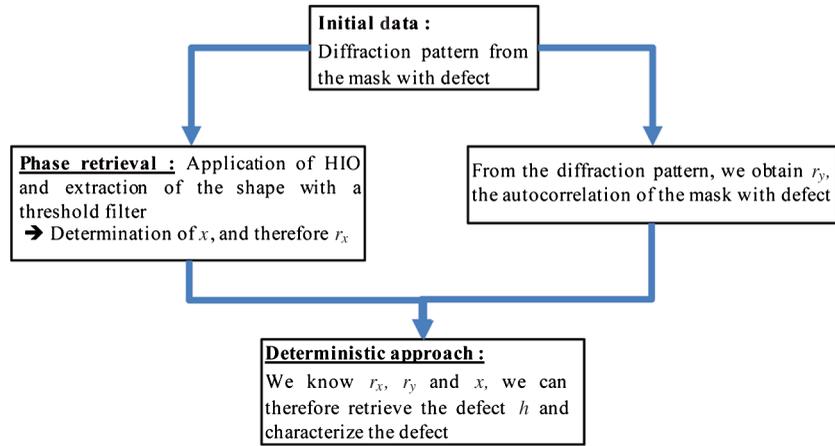


Fig. 6 Proposed method combining phase retrieval and deterministic approach.

$$\begin{cases} y(n) = x(n) - h(n) \\ r_{xy}(n) = r_x(n) - r_y(n) \end{cases} \rightarrow \begin{cases} y(n) = x(n) + h(n) \\ r_{xy}(n) = r_y(n) - r_x(n) \end{cases} \quad (4)$$

In the original definition of the parameters, the signal r_{xy} is negative and defects can be identified because they produce positive contributions. By applying the modifications described in Eq. (4), the signal r_{xy} becomes a positive quantity. Defects with negative coefficients can, therefore, be detected. However, defects with positive coefficients are no longer detected.

Three cases are then possible at each point: no defect, defect with negative coefficient (deep defects), or defect with positive coefficient (small defects). Once the shape is extracted, the problem consists of determining which case we are in so that we can apply the deterministic approach correctly and characterize the defect accurately.

Because deep defects are equivalent to having a negative coefficient A_i , we will refer to them as “negative defects” in the following. Similarly, defects with a small depth will be referred to as “positive defects.”

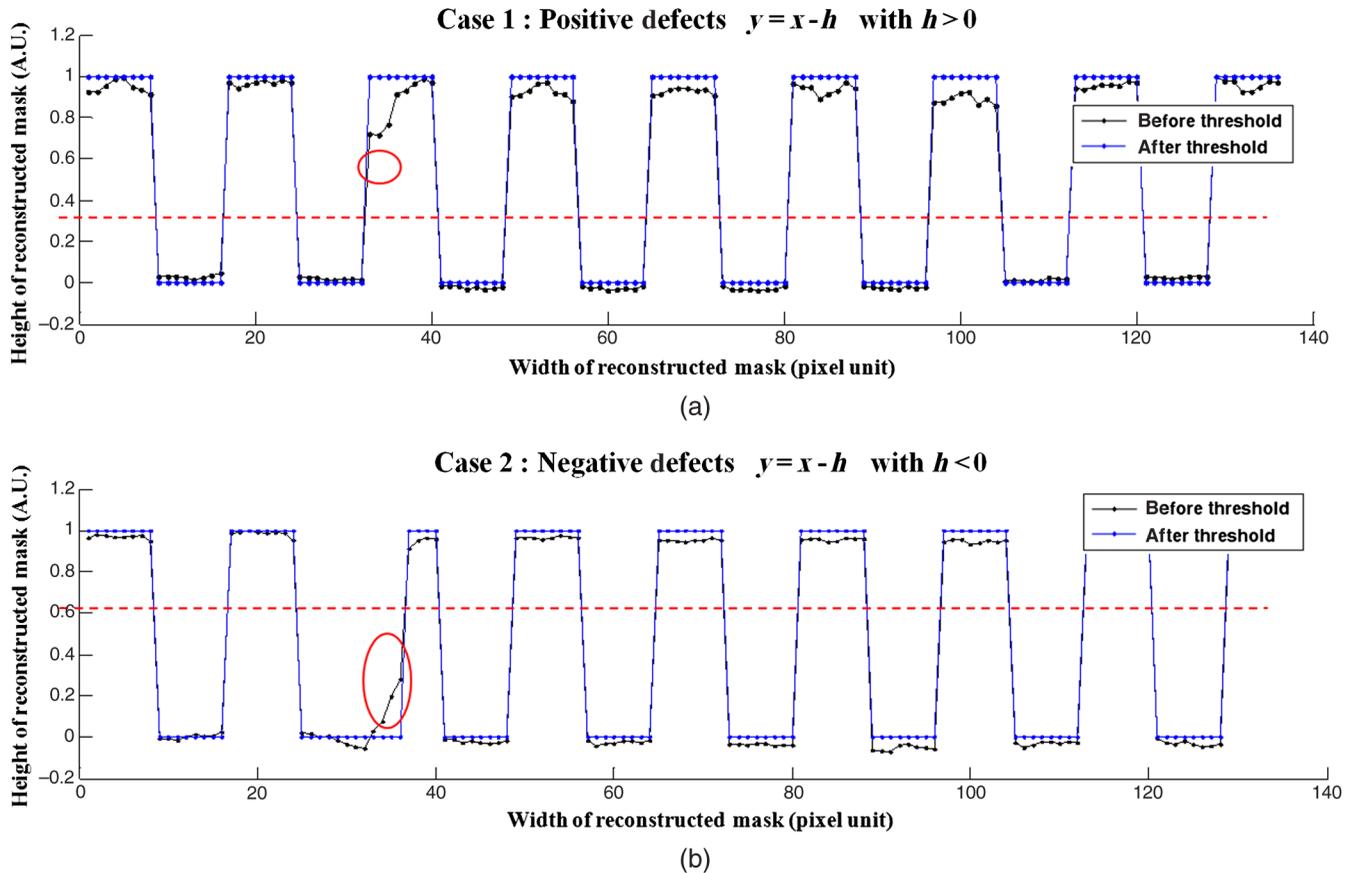


Fig. 7 After application of the HIO algorithm, a threshold filter is applied to obtain the reference profile. Since the pattern is not defect free, two cases may happen depending if the defect is (a) above or (b) under the threshold value (red line).

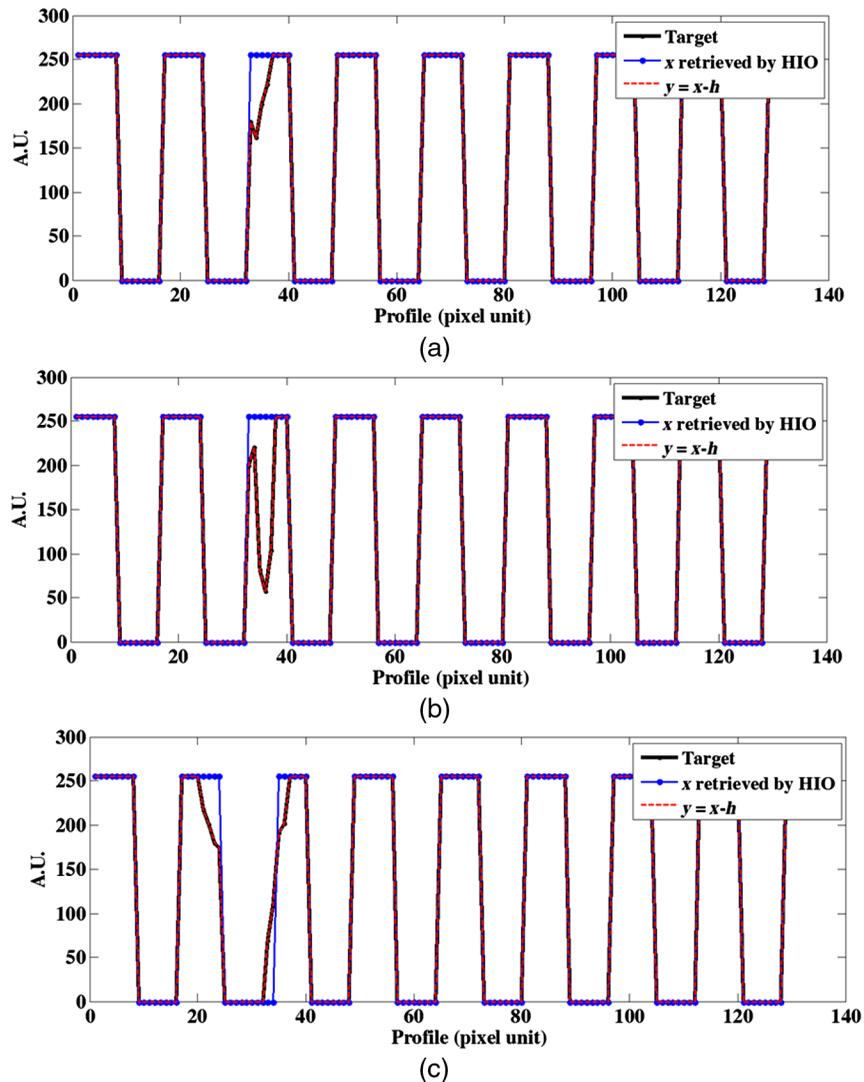


Fig. 8 Example of defect characterization with our proposed method. Several cases were tested including (a) small defect, (b) defect with both positive and negative components, and (c) defects on two different stripes.

The case described in Fig. 7(b) cannot happen when the reference is really a defect-free pattern, but it is necessary to consider this possibility in this situation. One solution to avoid this case would be to set a low threshold value and to consider that we have a reference equivalent to a defect-free pattern. However, very deep defects would still not be detected, and errors in the borders between line and space areas could occur because of the low threshold value. Moreover, we will see in the following that the consideration of the two cases enables to extend the deterministic approach to detection of multiple defects as well as the detection of defects present not only in the line area, but also in the space area.

4.3 Detection of Defects

The deterministic approach may be applied in two ways. In the first case, the method is applied directly and positive defects may be determined. In the second case, modification mentioned in Eq. (4) is made and negative defects are extracted. If the defect is composed of only one type of defect, positive or negative, we can apply the two methods

in parallel. In one case, the defects will be detected, and in the other case, no defect will be found. Then we can keep only the results where defects are detected.

This approach is not efficient if both types of defect are present at the same time in the pattern. A deterministic approach works by detecting contributions of the defect one by one, from A_1 to A_M . If only the first coefficients from A_1 to A_m (with $1 \leq m < M$) are positive, e.g., with a change of sign for A_{m+1} , only the first positive coefficients from 1 to m will be detected. Further contributions will be either incorrect or not detected. Indeed, as contributions from negative coefficients are not removed, even further positive coefficients will not be retrieved with the proper numerical value.

To enable the detection of the full defect, we successively apply the deterministic approach. Each time, we apply it to detect positive and negative defects in parallel and obtain two results $h_+(n)$ and $h_-(n)$. Then, as only the first contribution detected can be trusted, we extract A_1 as being the contribution detected the earliest in $h_+(n)$ and $h_-(n)$, as follow:

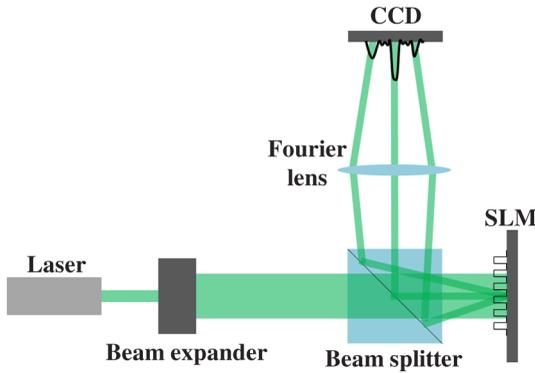


Fig. 9 Experimental setup. Different mask profiles are displayed on the SLM and the patterns diffracted are acquired with a CCD camera.

$$\begin{cases} n_+ = \{n, h_+(n) \neq 0\} \\ n_- = \{n, h_-(n) \neq 0\} \end{cases} \rightarrow n_1 = \min(n_+, n_-) \rightarrow A_1 \\ = \begin{cases} h_+(n_1) & \text{if } n_1 \in n_+ \\ h_-(n_1) & \text{if } n_1 \in n_- \end{cases} \quad (5)$$

Note that if $n_1 \in n_-$, coefficient A_1 is negative. Once this value is determined, we update the reference pattern by adding the defect contribution: $x(n_1) = x(n_1) - A_1$. Then we can apply this method again iteratively until no defect contribution is detected.

In the original deterministic method, the profile $x(n)$ is not known and can be retrieved only after the full determination of the defect $h(n)$. It is, therefore, not possible to apply this iterative approach. Detection of defects is then restricted to the case where all the coefficients A_i have the same sign. Thus, it is not possible to detect defects in space and line areas at the same time. With our approach, it is possible to detect all kind of defects with the restriction

that all defects are supposed to be located on the first half of the profile.

We tested our defect detection method with several shape of defects and managed to reconstruct the mask pattern $y(n)$ each time. A few examples of reconstructions are given in Fig. 8.

Our proposed method enables to accurately reconstruct mask profiles without the need for a reference pattern. In addition, the flexibility is improved in respect to the original deterministic approach. Since the first step using the HIO algorithm gives us not only the autocorrelation r_x , but also the profile x , an iterative approach could be adopted. As a result, even multiple defects located on different stripes can be detected.

It can be noted that since the reference pattern is obtained with a threshold operation, the reference is a perfectly flat shape. Real patterns may present a given rugosity and we can, therefore, expect detection of very small defect contributions everywhere in the mask. To avoid detection of rugosity, the loop of deterministic approach was actually slightly modified. Instead of detecting contributions in the signal r_{xy} that are strictly positive, the loop for defect detection is set to detect only contributions superior to a small value ϵ that was set empirically. This adjustment enabled to filter defects of very small sizes.

5 Experimental Results

An experimental setup was designed to demonstrate the feasibility of our proposed method. We used a laser beam emitting at 532 nm to illuminate a spatial light modulator (SLM) displaying a mask pattern. The diffraction pattern was then acquired by a camera through a Fourier lens. Our experimental setup is described in Fig. 9. The SLM used was a liquid crystal on silicon device (Syndiant Co., model

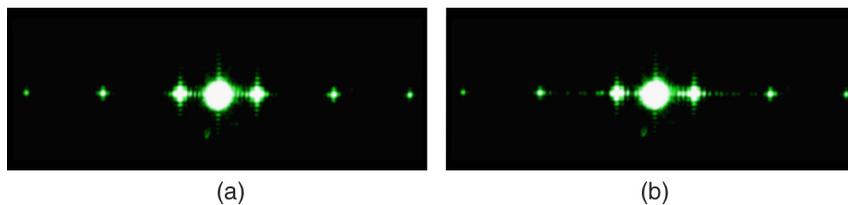


Fig. 10 Diffraction pattern from (a) a defect-free mask and (b) a mask presenting a defect.

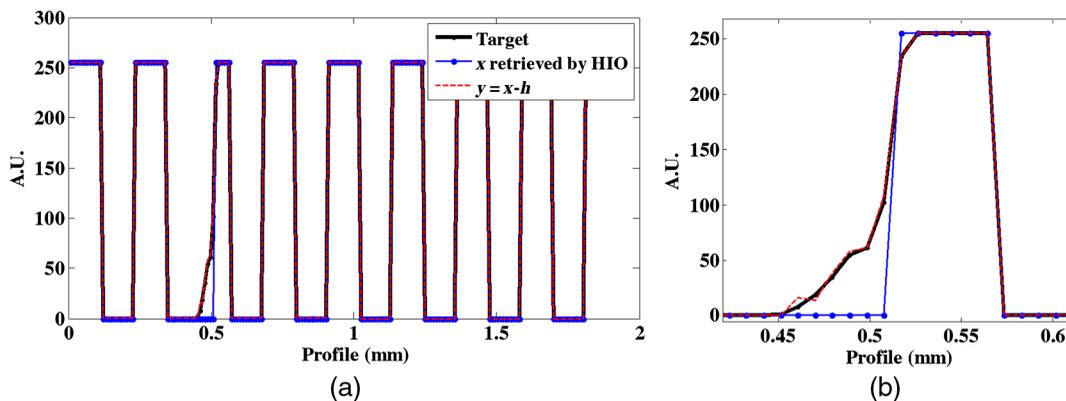


Fig. 11 Example of the total profile reconstruction from the diffraction pattern captured by CCD (a), with a zoom at the defect location (b).

SYL2061) presenting a resolution of 1024×600 pixels with a pitch of $9.4 \mu\text{m}$. The pattern displayed had a period of eight pixels, i.e., $75.2 \mu\text{m}$. The Fourier lens had a focal length of 250 mm and focused the light on the CCD (Imaging Source Co, model DFK 23GP031) that had 2048×1536 pixels with a pitch of $2.2 \mu\text{m}$.

When a pattern with a defect is displayed, we can observe that the energy is spread in secondary orders compared to the case without a defect, as illustrated in Fig. 10. This is in accordance with the simulations presented in Sec. 2.2.

By applying our proposed method, we could obtain the general profile by HIO and then recover every component of the defect iteratively (See Fig. 11).

We performed our test with patterns as large as a few micrometers displayed with an SLM so that we could easily control the profile to be retrieved. In future work, it would be necessary to test this approach with a real mask, especially to examine the sensitivity to noise.

6 Conclusion

It is difficult to quantify the accuracy in depth of the phase retrieval method because the result is strongly linked to the shape of the pupil of the recording system and the illumination beam. The deterministic approach was proposed for accurate characterization, but the theory derived can be applied only in restricted cases. Moreover, no experimental results were reported. We demonstrated an innovative method, which relies on the combination of phase retrieval algorithm and the deterministic approach. Defects in the L/S mask pattern can be precisely characterized in position and depth, and only one diffraction pattern is needed. Our proposed method can be applied for the detection of multiple defects, either bumps or pits. The feasibility of our approach was demonstrated with experimental data at the microscale. In further work, application of this method should be tested with a real mask for EUVL and precise investigations should be performed to examine the influence of noise and to determine the exact limitations in accuracy. This method is expected to provide information necessary to understand the formation of defects in mask pattern and, therefore, contribute to the development of high-quality masks.

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