Fast Track Communication

A single-image method of aberration retrieval for imaging systems under partially coherent illumination

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Received 2 April 2014, revised 30 May 2014
Accepted for publication 4 June 2014
Published 25 June 2014

Abstract

We propose a method for retrieving small lens aberrations in optical imaging systems under partially coherent illumination, which only requires to measure one single defocused image of intensity. By deriving a linear theory of imaging systems, we obtain a generalized formulation of aberration sensitivity in a matrix form, which provides a set of analytic kernels that relate the measured intensity distribution directly to the unknown Zernike coefficients. Sensitivity analysis is performed and test patterns are optimized to ensure well-posedness of the inverse problem. Optical lithography simulations have validated the theoretical derivation and confirmed its simplicity and superior performance in retrieving small lens aberrations.

Keywords: partial coherence in imaging, aberration retrieval, object pattern optimization, optical lithography

PACS numbers: 06.20.-f, 42.30.-d, 42.15.Fr

(Some figures may appear in colour only in the online journal)

1. Introduction

Information of lens aberration of an imaging system is important as it directly affects the intensity distribution in the image plane \cite{1, 2}. Zernike polynomials are commonly used for a mathematical description of lens aberrations \cite{3}. Current approaches of aberration retrieval are broadly classified into two categories: one uses wavefront sensors and the other is based on intensity measurement. A variety of techniques using wavefront sensors have been reported, such as Hartmann–Shack wavefront sensors \cite{4, 5}, and point diffraction interferometers \cite{6, 7}. Though capable of fast and accurate aberration retrieval, these techniques need complex and costly apparatus such as embedded interferometers and micro lens arrays. Due to the advantage of lower cost and easier implementation of tools, techniques based on intensity measurement have been widely used. A common way to retrieve a wavefront aberration uses the intensity point spread function, as in the Extended Nijboer–Zernike approach \cite{8}, and the phase retrieval and phase diversity approach \cite{9, 10}. However, Being limited to optical imaging systems with either fully spatially coherent or completely incoherent sources, such methods are not well suited for systems under partially coherent illumination.

In practice, many imaging systems, such as lithography tools \cite{11} and optical microscopes \cite{12}, are typically partially coherent that are characterized by an optimized source map and a lens pupil function. The imaging process of such partially coherent systems is described by a bilinear model \cite{13}, which entails time-consuming calculations and does not lend
a simple and intuitive relationship between lens aberrations and the resulted images. Previous methods for retrieving lens aberrations in such partially coherent systems involve through-focus image measurements [14, 15] and time-consuming iterative algorithms [16]. In this work, we propose a method for small aberration retrieval in optical imaging systems under partially coherent illumination, which only requires to measure one single defocused image of intensity distribution. A linear formulation is derived in a matrix form that directly relates the measured image to the unknown Zernike coefficients. Consequently, an efficient non-iterative solution is obtained.

2. Theory

According to the Hopkins’ formulation [17], an image intensity \( I(x) \) for a system under partially coherent illumination is characterized by a bilinear transform

\[
I(x) = \iint O(f_1)O^*(f_2)T(f_1, f_2) \cdot e^{-\frac{2\pi i (f_1 - f_2) \cdot x}{\lambda}} df_1 df_2, \tag{1}
\]

where \( x \) is a two-dimensional real vector representing the spatial coordinate, \( f \) is the normalized pupil coordinate, \( O(f) \) is the diffraction spectrum of the object, \( T(f_1, f_2) \) represents effects of lens aberration, which can be represented as

\[
T(f_1, f_2) = \int J(f)H(f + f_1)H^*(f + f_2) df. \tag{2}
\]

Here \( J(f) \) describes the source map in the pupil plane under Kohler illumination, the objective pupil function \( H(f) \) represents effects of lens aberration, which can be represented as

\[
H(f) = P(f) e^{ik \sum z_n R_n(f)}, \tag{3}
\]

where \( k = \frac{2\pi}{\lambda} \) is the wave number, \( \lambda \) is the wavelength of the monochromatic light source, and \( z_n \) is the Zernike index, so that \( z_n \) is the \( n \)th Zernike coefficient and \( R_n \) denotes the \( n \)th Zernike polynomial in normalized coordinate over the pupil plane. \( P(f) \) is the unit disc modulated by a defocus phase factor:

\[
P(f) = \text{cir}(|f|) e^{\frac{ik}{\sqrt{1-N^2}} f^2 - 1}. \tag{4}
\]

Here, \( h \) is the defocus (in nm) of the image plane, \( N \) is the image-side numerical aperture of the projection lens. Substituting equation (3) into equation (2), the TCC function is written as

\[
T(f_1, f_2) = \int J(f)P(f + f_1)P^*(f + f_2) \times e^{i \sum z_n R_n(f + f_1) - \sum z_n R_n(f + f_2)} df. \tag{5}
\]

Since the exponential term inside the integral in equation (5) is expanded as an infinite Taylor series, the TCC function can be further represented as

\[
T(f_1, f_2) = \sum_{n=0}^{\infty} \frac{(ik)^n}{m!} \int J(f)P(f + f_1)P^*(f + f_2) \times \left[ \sum z_n R_n(f + f_1) - \sum z_n R_n(f + f_2) \right] df. \tag{6}
\]

In the case that the unknown aberration is small, we approximate the TCC function by truncating the Taylor series to the linear term:

\[
T(f_1, f_2) = T_0(f_1, f_2) + T_1(f_1, f_2), \tag{7}
\]

where \( T_0(f_1, f_2) \) represents the TCC without aberration:

\[
T_0(f_1, f_2) = \int J(f)P(f + f_1)P^*(f + f_2) df, \tag{8}
\]

and \( T_1(f_1, f_2) \) represents the linearly aberrated TCC, which has the Zernike coefficients \( z_n \) separated from the integrals over the spatial frequency:

\[
T_1(f_1, f_2) = \sum_n z_n B_n(f_1, f_2), \tag{9}
\]

Here we define \( A_n(x) \) as the sensitivity function for the \( n \)th Zernike order, and \( I_0(x) \) and \( A_n(x) \) can both be directly calculated from \( T_0(f_1, f_2) \) and \( B_n(f_1, f_2) \) respectively:

\[
I_0(x) = \iint O(f_1)O^*(f_2)T_0(f_1, f_2) \cdot e^{-\frac{2\pi i (f_1 - f_2) \cdot x}{\lambda}} df_1 df_2, \tag{12}
\]

\[
A_n(x) = \iint O(f_1)O^*(f_2)B_n(f_1, f_2) \cdot e^{-\frac{2\pi i (f_1 - f_2) \cdot x}{\lambda}} df_1 df_2. \tag{13}
\]

Actually, both \( I_0(x) \) and \( A_n(x) \) can be calculated in advance and stored in memory for a given object at a given defocus. This means that for the purpose of aberration retrieval, we only need to measure one defocused image for some specially designed object. In this way, the total image intensity \( I(x) \) in equation (1) is treated as the observed data, and a linear relationship for aberration retrieval is formulated as

\[
\Delta I(x) \overset{\text{def}}{=} I(x) - I_0(x) = \sum_n z_n A_n(x). \tag{14}
\]

To suit numerical calculations, equation (14) is discretized into matrix and vector operations as

\[
\Delta A = A Z, \tag{15}
\]

where \( \Delta A \) is an \( M \times 1 \) vector representing \( M \) discrete samples (pixels) from the image intensity \( \Delta I(x) \), \( Z \) is an \( N \times 1 \) vector of the unknown Zernike coefficients \( \{z_n\} \), and \( A \) is an \( M \times N \) matrix of samples of the sensitivity function \( \{A_n(x)\} \).
is the spectral norm of test patterns, and formulate the optimization problem as sensitivity matrix as the objective function for optimizing the illumination condition. We use the condition number of the patterns differently. Test patterns should be carefully aberration has a unique characteristics and interacts with test object pattern is critical in the aberration retrieval, as each can be solved using the least-square method.

\[ \hat{\mathbf{O}} = \arg \min_{\mathbf{O}} \left[ \text{cond}(\mathbf{A}^* \mathbf{A}) \right] \]

\[ \hat{\mathbf{O}} = \arg \min_{\mathbf{O}} \left[ \| \mathbf{A}^* \mathbf{A} \| \cdot \| (\mathbf{A}^* \mathbf{A})^{-1} \| \right]. \quad (16) \]

where \( \hat{\mathbf{O}} \) represents the optimized object pattern parameters, containing width of each patterns and pitch of adjacent patterns, \( \mathbf{A} \) is the sensitivity matrix of the given object pattern, which can be calculated efficiently from equation (13), \( \mathbf{A}^* \) is the Hermitian conjugate of \( \mathbf{A} \), and \( \| \cdot \| \) is the spectral norm of matrix. A small condition number guarantees fast convergence and a stable solution to the inverse problem. Many multi-parameter optimization algorithms can be used to solve the inverse problem. Here we adopt the Powell algorithm for this purpose [18].

A flowchart of the proposed aberration retrieval method is shown in figure 1, which highlights two key technical aspects. An aberration retrieval model is first established, serving as the theoretical basis for efficiently calculating the sensitivity matrix. An object pattern optimization algorithm based on sensitivity analysis is another important module for designing optimal test patterns whose images are sensitive to Zernike aberrations.

3. Numerical results

We take a projection lithography tool as an example partially coherent system and apply the proposed method. The considered tool has a partially coherent illumination with wavelength \( \lambda = 193 \) nm, projection lens with NA = 0.8, and operates at defocus \( h = 180 \) nm. Figure 2 depicts a typical image intensity of a two-level \( 0/\pi \) phase-shift object pattern with the width of central contact 210 nm, the width of surrounding contact 80 nm, the pitch between central and surrounding contact 85 nm, and the simulation range \([-500 \text{ nm}, 500 \text{ nm}]\), under a quadrupole source \( \sigma_{\text{out}}/\sigma_{\text{in}} = 0.8/0.4/45^\circ \) and lens aberration shown below in figure 5(a). The normalized intensity error is on the order of \( 10^{-4} \), which justifies the use of linear approximation.

From equation (13), each element of the sensitivity matrix \( \mathbf{A} \) has a compact analytic expression as a function of \( \mathbf{x} \) under fixed test patterns \( \mathbf{O}(\mathbf{f}) \), which serves an analytic kernels for measuring the Zernike coefficients. A suitable amount of defocus is desired so that odd aberrations lead to lateral shifts and even aberrations interact with defocus to distort images. Figure 3 depicts the first fifteen analytic kernels for retrieving aberrations from \( z_2 \) to \( z_{16} \) as \( A_i(\mathbf{x}) \) (\( i = 2, 3, \ldots, 16 \)) is the \( i \)th row of the matrix \( \mathbf{A} \) in equation (15). A quadrupole source with \( \sigma_{\text{out}}/\sigma_{\text{in}} = 0.8/0.4/45^\circ \) was set, and an object pattern shown in figure 2 was used. As expected, the analytic kernels have the same symmetry properties as the corresponding Zernike polynomials. In addition, with the help of defocus, the sensitivities to even aberrations \( (A_4(\mathbf{x}), A_6(\mathbf{x}), A_8(\mathbf{x}), A_{10}(\mathbf{x}), A_{12}(\mathbf{x}), A_{14}(\mathbf{x}) \) and \( A_{16}(\mathbf{x}) \) in figure 3) are in similar magnitudes as those to the odd aberrations \( (A_2(\mathbf{x}), A_3(\mathbf{x}), A_5(\mathbf{x}), A_7(\mathbf{x}), A_9(\mathbf{x}), A_{11}(\mathbf{x}), A_{13}(\mathbf{x}) \) and \( A_{15}(\mathbf{x}) \) in figure 3), which facilitates reliable retrieval of both the even and odd aberrations with only one single intensity measurement.

It is customary to represent aberrations of lens pupils by Zernike coefficients, which weight the corresponding Zernike polynomials that form a complete and orthogonal basis over the interior of the unit circle. There the Zernike representation affords a linear relationship between the Zernike coefficients and the point-wise aberration of pupil phase. Analogously, equations (13) and (14) establish a similar linear map between the Zernike coefficients and the image intensity points, through our derived analytic kernels. Although the analytic kernels are not necessarily orthogonal, they incorporate and condense information of the illumination source and test patterns, so to lend a simple and compact linear equation,
which is amenable to an efficient and robust solution and sensitivity analysis.

As the test patterns should be carefully designed and optimized to be most effective under a given illumination condition, figure 4 shows some of the results of our optimization simulation. We used two kinds of source: one was set as a traditional one with \( \sigma = 0.8 \), and the other a quadrupole one with \( \sigma_{out}/\sigma_{in}/\theta = 0.8/0.4/45^\circ \). There are four kinds of object patterns shown in the figure, which fall into two types: binary objects shown as black-and-white diagrams, and \( 0/\pi \) phase-shift objects as gray-scale diagrams. In this figure, original object patterns are in the first row, object patterns after optimization with a traditional source are in the second row, and with a quadrupole source in the third row.

**Figure 3.** Analytic kernels for measuring aberrations.

**Figure 4.** Optimization results of some object patterns, with (a)–(d) as four kinds of object patterns.
histogram in the bottom shows the condition numbers of the sensitivity matrices of object patterns above. In the legend, ‘B’ is short for a binary object pattern, ‘P’ for a phase-shift object pattern, ‘T’ for a traditional source, ‘Q’ for a quadrupole one, ‘O’ for original, and ‘A’ for after optimization. Therefore, ‘B-T-O’ means the condition number of the original binary object pattern with a traditional source, etc. It is noted from the histogram that the condition number of sensitivity matrix becomes much smaller after optimization, and the results are different under different sources. We utilized the combination of phase-shift object and a quadrupole source shown in figure 2 as an example for the demonstration of our aberration retrieval method. Theoretically lens aberration should be express as the sum of infinite orthogonal Zernike polynomials, and this method is applicable up to any high-order Zernike term. However, for practical applications, the aberrations are expressed as the sum of finite Zernike terms up to z_n plus a much smaller residual aberration which is the sum of infinite Zernike terms higher than z_n, where n is the highest concerned order. To guarantee the accuracy, the aberrations should be measured up to a sufficient high-order Zernike term [19], which is usually the 37th order for practical lithography tools, where the 37th Zernike term is actually the 49th Zernike term [1, 3]. In these simulations, to guarantee that equation (15) is over-determined and can be solved by the least-square method accurately, for measuring unknown Zernike coefficients up to the 37th (49th) order, the discretized number M is set to be 81×81.

Figure 5 depicts one of the simulation results with an optimized object shown in figure 2. An unknown aberration as shown in figure 5(a) is induced by setting the Zernike coefficients z_2 to z_37 (z_40) with a random value in the range of [-15 mλ, 15 mλ], which leads to the aberration in the range of [-60 mλ, 60 mλ]. Figure 5(b) depicts the wavefront of the retrieved Zernike coefficients up to the 37th (49th) order, while figure 5(c) shows the difference between retrieved and unknown wavefront. The absolute error in figure 5(c) is 1.61 mλ, which is decreased by 1.1 mλ compared to the error of retrieval using the original object, indicating a satisfactory accuracy for aberration retrieval.

To further evaluate the accuracy and effective range of the proposed method, we performed another series of simulations with unknown aberrations in different ranges. Figure 6 shows the absolute error for different ranges of input aberrations. It is clear that the proposed method achieves a very good accuracy on the order of mλ’s when the input aberrations are small (less than 60 mλ), and the retrieval error increases significantly as the magnitude of aberration increases. When the aberration range is smaller than 50 mλ, the absolute error is less than 1.5 mλ. However, if the aberration range surpasses 80 mλ, the absolute wavefront error sharply increases to the order of 10 mλ, which is unacceptable for the aberration retrieval application. This simulations demonstrate that the proposed linear formulation works best under the condition of small aberrations.

4. Conclusion

In conclusion, a method is proposed for small aberration retrieval in optical imaging systems under spatially partially coherent illumination using one single measurement of defocused image of an object containing optimized test patterns. Numerical results are presented to verify the theoretical derivation and demonstrate the efficacy of test pattern optimization. The proposed method of aberration retrieval is simple to implement and yields superior performance in retrieving small lens aberrations.

In the proposed method, the effective source intensity distribution and the NA are treated as known system parameters for sensitivity analysis, test patterns optimization and aberration retrieval. In practical applications, however, there are imaging systems that do not have all the system parameters known or given. To ensure accurate aberration retrieval, it is best to have such system parameters measured or calibrated in advance. Inevitably, uncertainty in such measured system parameters will propagate to the retrieved Zernike coefficients. There are interesting questions and
challenges for further investigations, regarding error or uncertainty analysis and optimizations of the measurement procedures as well as the data processing algorithms to minimize errors in the final results.

Acknowledgements

This work was funded by the National Natural Science Foundation of China (grants 91023032 and 51005091), the Specialized Research Fund for the Doctoral Program of Higher Education of China (20120142110019), the National Science and Technology Major Project of China (2012ZX02701001), and the Program for Changjiang Scholars and Innovative Research Team in University of China.

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