Through-Focus Point-Spread Function Evaluation for Lens Metrology using the Extended Nijboer-Zernike Theory

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1 Introduction

Lens metrology is of utmost importance in the field of optical lithography; both at the delivery stage and during the lifetime of the projection objective, a very high imaging quality should be guaranteed. Frequent on-line tests of the optical quality are required and they should be well adapted to the environment in which the objective has to function, viz. a semiconductor manufacturing facility. The most common method for high-precision lens characterization is at-wavelength optical interferometry [1]. A first limitation for applying this method can be found in the availability of an appropriate coherent source at the desired wavelength. The second problem is the reference surface that is needed in virtually all interferometric set-ups. For these reasons, there has been much interest in lens quality assessment by directly using the intensity distribution in the image plane. A reconstruction of the complex pupil function of the objective from a single intensity measurement is generally not possible. A combined intensity measurement in the image plane and the pupil plane, if possible, can give rise to an improved reconstruction method. More advanced methods use several through-focus images but it is not possible to guarantee the uniqueness of the aberration reconstruction in such a numerical 'inversion' process [2]-[4]. In this paper we give an overview of a new method that is based on an analysis of the through-focus images of a pointlike object using a complex pupil function expansion in terms of Zernike polynomials. While the original analysis of the diffracted intensity by Nijboer and Zernike, using the orthogonal circle polynomials, was limited to a close region around the image plane, the so-called Extended Nijboer-Zernike (ENZ) theory offers Bessel series expressions for the through-focus intensity distribution over a much larger range. Good convergence for the through-focus intensity is obtained over a range of typically 10 to 15 focal depths. For high-quality projection lenses, this is typically the range over which relevant intensity variations due to diffraction are observed and the information from this focal volume is used for the reconstruction of both the amplitude and phase of the complex pupil function of the lens. In a recent development, the theory has been extended to incorporate vector diffraction problems so that the intensity distribution in the focal volume of an imaging system with a high (geometrical) aperture (e.g. $\sin\alpha=0.95$) can be adequately described. From this analysis one can basically also extract the so-called 'polarization aberrations' of the imaging system. As it was mentioned previously, the starting point in all cases is a pointlike object source that is smaller than or comparable to the diffraction limit of the optical system to be analyzed. A sufficient number of defocused images serves to create three-dimensional 'contours' of the intensity distribution that are then used in the reconstruction or retrieval scheme.

In Section 2 we briefly describe the basic features of the extended Nijboer-Zernike theory, followed in Section 3 by a presentation of its implementation in the retrieval problem for characterizing the lens quality. In Section 4 we present experimental results and in Section 5 we give some conclusions and an outlook towards further research and developments in this field.

2 Basic outline of the Extended Nijboer-Zernike theory

To a large extent, the imaging quality of an optical system is described by the properties of the complex (exit) pupil function. In Fig.1 we have shown the geometry corresponding to the exit pupil and the image plane. The cartesian coordinates on the exit pupil sphere are denoted by μ and ν and the pupil radius is ρ_0 . The distance from the centre E_0 of the exit pupil to the centre P_0 of the image plane is R. The cartesian coordinates on the exit pupil sphere are normalized with respect to the pupil radius. The real space coordinates (x,y) in the image plane are normalized with respect to the diffraction unit λ/s_0 where s_0 is the numerical aperture of the imaging system and these coordinates are then denoted by (X, Y). In an analogous way, the axial coordinate z is normalized with respect to the axial diffraction unit, $u = \lambda / \{1 - (1 - s_0^2)^{1/2}\}$ and denoted by *Z*. As usually, the diffraction calculations are carried out using polar coordinates, (ρ, ϑ) for the pupil coordinates and (r, φ, z) for the image plane coordinates. The complex pupil function is written as

$$B(\rho, \mathcal{G}) = A(\rho, \mathcal{G}) \exp\{i\Phi(\rho, \mathcal{G})\} , \qquad (2.1)$$

with $A(\rho, \vartheta)$ equal to the lens transmission function and $\Phi(\rho, \vartheta)$ the aberration function in radians of the objective.



Figure 1: The choice of coordinates in the pupil and the image space.

The point-spread function in image space is obtained from Fourier optics [5] and is written as $U(r, \varphi; f) =$

$$(r,\varphi,f) =$$

$$\frac{1}{\pi} \int_{0}^{2\pi} \int_{0}^{1} \exp\{if\rho^{2}\} B(\rho, \theta) \exp\{i2\pi r\rho\cos(\theta - \varphi)\} \rho d\rho d\theta,$$
(2.2)

where the defocusing parameter *f* has been included to allow throughfocus evaluation of the image space amplitude. The calculation of $U(r,\varphi;f)$ can be done in a purely numerical way but the Nijboer-Zernike theory has shown that a special representation of $B(\rho, \vartheta)$ in terms of the Zernike polynomials allows an analytical solution for f=0. It has turned out that for nonzero values of *f*, as large as $\pm 2\pi$, a well-converging series expression for Eq.(2.2) can be found [6] and this solution has proven to be very useful and effective [7] once we are confronted with the inversion problem described in the introduction.

2.1 Zernike representation of the pupil function

The common way to introduce Zernike polynomials in the pupil function representation is to put the amplitude transmission function $A(\rho, \vartheta)$ equal to unity (a frequently occurring situation in optical systems) and to apply the expansion only to the phase aberration function $\Phi(\rho, \vartheta)$ according to

$$B(\rho, \vartheta) = \exp\{i\Phi(\rho, \vartheta)\} \approx 1 + i\Phi(\rho, \vartheta) = 1 + i\sum_{n,m} \alpha_n^m Z_n^{[m]}(\rho, \vartheta) \quad ,$$

$$(2.3)$$

with

$$Z(\rho, \mathcal{G}) = R_n^{|m|}(\rho) \exp(im\mathcal{G}) \quad . \tag{2.4}$$

The radial polynomial $R_n^{|m|}(\rho)$ is the well-known Zernike polynomial of radial order *n* and azimuthal order |m| (with $n - |m| \ge 0$ and even) and the azimuthal dependence is represented by the complex exponential function $\exp(im \theta)$. To represent all possible cosine and sine dependences in the Zernike polynomial expansion, the summation over n,m for the representation of $\Phi(\rho, \theta)$ has to be extended to both positive and negative values of *m* up to a chosen maximum value of |m|.

In our analysis of the through-focus amplitude we prefer to use a Zernike polynomial expansion for the complete pupil function $B(\rho, \theta)$ and this leads to the following expression

$$B(\rho, \vartheta) = A(\rho, \vartheta) \exp\{i\Phi(\rho, \vartheta)\} = \sum_{n,m} \beta_n^m Z_n^{[m]}(\rho, \vartheta) \quad , \tag{2.5}$$

where the coefficients β now represent both the amplitude and phase of the complex pupil function. For sufficiently small values of the β -coefficients, an unequivocal reconstruction of the separate functions $A(\rho, \vartheta)$ and $\Phi(\rho, \vartheta)$ is feasible.

2.2 Amplitude distribution in the focal region

The extended Nijboer-Zernike theory preferably uses the general representation of the complex pupil function according to Eq.(2.5) and from this expression the amplitude in the focal plane is obtained as

$$U(r,\varphi;f) = \sum_{n,m} \beta_n^m U_n^m(r,\varphi;f) , \qquad (2.6)$$

with the functions $U_n^m(r,\varphi;f)$ given by

$$U_n^m(r,\varphi;f) = 2i^m V_n^m(r,f) \exp(im\varphi) .$$
(2.7)
The expression for $V_n^m(r,f)$ reads

$$V_{n}^{m}(r,f) = \begin{cases} \int_{0}^{1} \exp(if\rho^{2}) R_{n}^{m}(\rho) J_{m}(2\pi r\rho)\rho d\rho & m \ge 0, \\ (-1)^{m} \int_{0}^{1} \exp(if\rho^{2}) R_{n}^{|m|}(\rho) J_{|m|}(2\pi r\rho)\rho d\rho & m < 0. \end{cases}$$
(2.8)

It is a basic result of the Extended Nijboer-Zernike theory that the function $V_n^m(r, f)$ can be analytically written as a well-converging series expansion over the domain of interest in the axial direction, say $|f| \le 2\pi$. The integrals in (2.8) are given by

$$\exp(if)\sum_{l=0}^{\infty} \left(\frac{-if}{\pi r}\right)^{l} \sum_{j=0}^{p} u_{lj} \frac{J_{|m|+l+2j+1}(2\pi r)}{(2\pi r)},$$
(2.9)

where p = (n - |m|)/2 and q = (n + |m|)/2. The coefficients u_{ij} are given by

$$u_{ij} = (-1)^{p} \frac{|m| + l + 2j + 1}{q + l + j + 1} \binom{|m| + j + l}{l} \binom{j + l}{l} \binom{j + l}{p - j} / \binom{q + l + j}{l}, \quad (2.10)$$

where the binomial coefficients '*n* over *k*' are defined by n!/(k!(n-k)!) for integer *k*,*n* with $0 \le k \le n$ and equal to zero for all other values of *k* and *n*.

2.3 Intensity distribution in the focal region

The intensity distribution is proportional to the squared modulus of the expression in Eq.(2.6) and can be written as

$$I(r,\varphi;f) = \left|\sum_{n,m} \beta_n^m U_n^m(r,\varphi;f)\right|^2$$
(2.11)

and in a first order approximation we obtain

$$I_{a}(r,\varphi;f) \approx \left|\beta_{0}^{0}\right|^{2} \left|U_{0}^{0}(r,\varphi;f)\right|^{2} + 2\sum_{n,m} \operatorname{Re}\left\{\beta_{0}^{0}\beta_{n}^{m^{*}}U_{0}^{0}(r,\varphi;f)U_{n}^{m^{*}}(r,\varphi;f)\right\}$$
$$= 4\left|\beta_{0}^{0}\right|^{2} \left|V_{0}^{0}(r,f)\right|^{2} + 8\beta_{0}^{0}\sum_{n,m} \operatorname{Re}\left\{i^{-m}\beta_{n}^{m^{*}}V_{0}^{0}(r,f)V_{n}^{m^{*}}(r,f)\exp(-im\varphi)\right\}$$
(2.12)

where the second summation sign Σ' excludes (n,m)=(0,0).

The approximated expression $I_a(r,\varphi;f)$ neglects all quadratic terms with factors $\beta_n^m \beta_n^{m^**}$ in them which is reasonable if in the pupil function expansion the term with β_0^0 , assumed to be >0, is the dominant one.

3 Retrieval scheme for the complex pupil function

In this section we develop the system of linear equations that allows to extract the Zernike coefficients from the measured through-focus intensity function. We suppose that in a certain number of defocused planes (typically 2N+1 with N is e.g. 5) the intensity has been measured. A typical step of the defocus parameter from plane to plane is e.g. $4\pi/(2N+1)$. The discrete data in the defocused planes are interpolated and, if needed, transformed from a square to a polar grid so that they optimally fit the retrieval problem. After these operations we effectively have the real measured intensity function $I(r,\varphi;f)$ at our disposal for further analysis.

3.1 Azimuthal decomposition

We first carry out a Fourier decomposition of the measured intensity distribution according to

$$X^{m}(r,f) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} I(r,\varphi;f) \exp(im\varphi) d\varphi.$$
(3.1)

Our task is to match the measured function $I(r,\varphi;f)$ to the analytical intensity function $I_a(r,\varphi;f)$ of Eq.(2.12) in the focal volume by finding the appropriate coefficients β_n^m . The harmonic decomposition of $I_a(r,\varphi;f)$ yields

$$X_{a}^{m}(r,f) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} I_{a}(r,\varphi;f) \exp(im\varphi) d\varphi$$

$$= 4\delta_{m0} \left|\beta_{0}^{0}\right|^{2} \psi_{0}^{0}(r,f) + 4\beta_{0}^{0} \sum_{n\neq0} \left[\beta_{n}^{m^{*}} \psi_{n}^{m^{*}}(r,f) + \beta_{n}^{-m} \psi_{n}^{-m}(r,f)\right].$$
(3.2)

Here we have used the shorthand notation

 $\psi_n^m(r,f) = i^m V_0^{0*}(r,f) V_n^m(r,f).$ (3.3)

We now have at our disposal the harmonic decomposition of both the measured data set and the theoretically predicted intensity distribution that depends on the unknown β_n^m -coefficients. These coefficients can be evaluated by solving for each harmonic component *m* the approximate equality

$$X_{a}^{m}(r,f) = X^{m}(r,f).$$
(3.4)

Our preferred solution of the 2m+1 equations is obtained by applying a multiplication with $\psi_n^m(r,\varphi)$ and integrating over the relevant region in the (r,f)-domain (inner product method). In this way, we get a system of linear equations in the coefficients β_n^m that can be solved by standard methods.

4 Experimental results

The ENZ aberration retrieval scheme has been applied to a projection system that allows, in a controlled way, the addition or subtraction of a certain amount of a specific aberration. In this way, by controlled adjustment of the lens setting, we were able to execute two sets of consecutive measurements and detect the aberrational change between them. In Fig.2 we show the results of these measurements where each time a certain amount of extra aberration has been introduced (50 $m\lambda$ in rms-value). It can be seen that the measured aberration values correspond quite well to the changes in the objective predicted by the mechanical adjustments. The through-focus intensity contours have been obtained by a large number of recorded pointspread images at different dose values. For a fixed resist clipping level, we can track the various intensity contours from the developed resist images that are automatically analyzed by an electron microscope. The accuracy of the method can be checked by a forward calculation of the point-spread function intensity using the retrieved pupil function. The measured and reconstructed intensity distributions show differences of 1% at the most. At this moment, the accuracy in the reconstructed wavefront aberration is of the order of a few $m\lambda$ in *rms* value.

5 Conclusions and outlook

The Extended Nijboer-Zernike theory for point-source imaging has been applied to a lens metrology problem and has proven to be a versatile and accurate wavefront measurement method in an environment where e.g. classical interferometry is difficult to implement. The wavefront retrieval process requires a reliable measurement of the through-focus intensity distribution. In our case, for a moderate NA projection lens (NA=0.30), we have used a large number of defocused resist images with widely varying exposure values. Automated resist contour evaluation of the developed images with an electron microscope yields an accurate representation of the through-focus intensity distribution. With the aid of the reconstructed exit



pupil function, the point-spread image of the aberrated projection lens

Figure 2: Bar diagrams of the measured change in aberration value for three specific aberration types (spherical aberration, coma and astigmatism) using the retrieval method according to the Extended Nijboer-Zernike theory. The black bars indicate the reference aberration values, the white bars the values corresponding to the detuned systems (all values in units of $m\lambda$ rms aberration).

can be calculated and we have observed a fit to better than 1% in intensity between the measured and calculated through-focus intensity distributions.

Recent research has focused on the incorporation of high-NA vector diffraction into the *ENZ*-theory [8], on the effects of image blurring due to latent resist image diffusion during the post-exposure bake and on the influence of lateral smear by mechanical vibrations [9]. All these effects tend to obscure the real lens contribution to image degradation and they have to be taken into account in the retrieval process.

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