Point-Diffraction Ptychography for Microscopy and Interferometry

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Abstract

"Point-diffraction" ptychographic methods use small-area illumination of relatively simple diffracting objects, e.g. in the context of point-diffraction interferometry or spot-scanning microscopy. The resulting interferograms can be adequately sampled with relatively few detector pixels, and the reduced data volume enables the use of faster or more accurate reconstruction algorithms that might not be usable in conventional wide-field ptychography. In one algorithmic approach, "first-principles ptychography", the diffraction object's optical transfer function and the illumination field are simultaneously reconstructed without relying on any assumptions about the internal structure or diffraction mechanisms within the object or illumination optics. This capability would be useful for applications such as interferometric testing of optics for EUV lithography and inspection/metrology.

Introduction

Coherent Diffraction Imaging (CDI, [1]) uses far-field diffraction patterns from an illuminated object to reconstruct the object's spatial image field (amplitude and phase), based on a known illumination field. Point-diffraction interferometry similarly extracts information from diffraction-generated, far-field interferograms, but in this case the diffracting object is known and the illumination field (with optical aberrations) is unknown. Ptychography (scanning CDI [2]) can simultaneously reconstruct both the object and illumination fields from multiple interferograms collected with the object in different positional scan positions. In the context of ptychographic microscopy, the method can be applied as a calibration process to characterize the illumination so that subsequent image reconstructions can be done with the illumination known. In the context of ptychographic interferometry, the diffracting object can be characterized during instrument calibration so that subsequent interferometric testing can be done with the object known.

Point-Diffraction (Small-Spot) Ptychography

Ptychography typically uses broad-area object illumination to generate richly detailed diffraction patterns, which are sampled with multi-megapixel detectors. The object/illumination reconstruction calculations with such large data sets are very computationally intensive and are only practicable with simple optical modeling algorithms. The object is typically modeled using a thin-film approximation. Alternatively, a tomography or "multi-slice" model can be used for thick samples. [3-5] These models do not accurately represent the near-field, volumetric scattering mechanisms within real objects.

Point-diffraction interferometry, by contrast, is conventionally done with the diffracting object at or very close to the focal point of a convergent illumination beam. [6, 7] The relatively small illumination area results in less detailed diffraction patterns and a relaxed pixel density requirement. This can make it possible to use more accurate but computationally intensive algorithms such as Rigorous Coupled-Wave Theory (RCWA, [8]) in ptychographic reconstruction calculations.

Spot-scanning microscopy, the imaging analogue of point-diffraction interferometry, can similarly be implemented as a form of small-spot ptychography in which an inspection surface is raster-scanned across an array of diffraction-limited point illumination spots while the far-field diffraction pattern from each spot is sampled by a position-sensing detector comprising only four sensor elements. [9] The large illumination field and massive detector array of conventional ptychography are replaced by massively parallel point scanning on a dense spatial grid (e.g. ~2 million spots, 20-nm scan step). The relative simplicity of point illumination with quad-cell detectors can greatly simplify the data processing; for example, a simple threshold detection algorithm might be used for defect inspection.

Ptychographic Interferometry and Interferometric Polarimetry

The focus spots in a spot-scanning microscope can be accurately characterized using a ptychographic point-diffraction interferometer (PDI). Point-diffraction interferometry would generally be well suited for testing point-imaging characteristics of high-performance optics such as EUV metrology and lithography projection systems because of its simplicity and high sensitivity, and because the test is performed in basically the same way that the test optic is used. An improved variant of PDI is the Zernike point-diffraction interferometer (aka "Zernike phase-contrast test" [10-15]), which replaces the "point" transmittance aperture with a phase-shifting spot. (A half-cycle optical phase shift is typically used.) This differs from other more complex "phase-shift" PDI systems. [16] If the PDI diffracting aperture is large in relation to the diffraction limit it is similar to a Foucault knife-edge interferometer or the related phase Foucault knife-edge interferometer [13, 17]. These interferometer variants differ only in the diffracting object characteristics. Multiple, interchangeable aperture filters can be used as diffracting objects within the same instrument. For applications requiring polarization measurement, polarizing or birefringent filters can be used and the interferometer can contain polarization-separation optics and multiple detector arrays for sensing different polarization states.

Ptychographic Modeling and Calibration Algorithms

Accurate object modeling, e.g. via RCWA, would be indispensable for applications such as testing high-NA EUV optics. For example, actinic interferometry at wavelength 13.5 nm with a Zernike PDI or phase Foucault knife-edge test might use a diffracting edge formed as a 60-nm step in a ruthenium layer deposited on a thin (e.g., 50-nm) silicon substrate. The 60-nm step is much larger than a 0.55-NA focused beam's waist (13-nm FWHM) and focus depth (35 nm). [18] Furthermore, while a 60-nm step would provide a half-cycle phase shift at near-normal incidence, the phase shift will vary significantly over the full range of incidence angles. The focus beam would also exhibit polarization effects at high incidence angles, which might need to be accounted for in the optical modeling. [19] These factors would require accurate diffraction modeling to reliably measure beam aberrations.

As an alternative to complex near-field diffraction modelling, the ptychographic instrument could simply be represented by a generic optical transfer function, a linear transformation from the illumination field to the detector field at the pixel sensor elements. This "first-principles ptychography" approach would make no assumptions about the illumination optics or the object, other than the assumed linear dependence between the illumination and detector fields. In the context of microscopy, diffraction modeling of the object would be required to determine its structure from its measured optical transfer function, but the calculation would not rely on any assumptions about the illumination optics. In the context of interferometry, the illumination optics would need to be modeled to extract aberration data from the measured illumination field, but no assumptions would need to be made about the object structure. However, the object and illumination optics would both need to be modeled, at least approximately, in the ptychographic reconstruction calculations to provide initial estimates of the illumination field and transfer function, which are computed by an iterative numerical process.

A drawback of first-principles ptychography is that the object transfer function and illumination field cannot be determined from only translational object scans. The process would, at a minimum, require multi-axis rotational scans, and a robust measurement process might require up to 6-axis translational and rotational scanning. (The positional scan coordinates would not necessarily need to be accurately controlled or measured; they can be calculated as part of the reconstruction algorithm. [20, 21]) The measurement might also require data from multiple illumination fields and multiple aperture filters. However, this process would only be required during system calibration.

Interferometric Measurement Processes and Applications

After the interferometer's transfer function has been calibrated, it can be used to sample an optical system's point-imaging performance at multiple image field locations to fully and accurately characterize aberrations and geometry errors of all optical surfaces in the system. In addition to measuring surface form errors, ptychographic interferometry can be used to measure optical alignment errors for all surfaces and also positioning errors in the illumination source point and the diffracting object's location at each scan position.

Ptychographic interferometry would be useful for shop testing and alignment of high-performance optics and for *in situ* aberration testing e.g. for thermal compensation or adaptive optics. The method could be used for manufacturing EUV and X-ray mirrors in two ways: A test using a long wavelength (UV or visible) would be used for aberration measurement in the surface figuring process (before reflective coatings have been applied to the mirrors), and then the operating EUV or X-ray wavelength would be used for final test and alignment.

A spot-scanning microscope could be calibrated by using a ptychographic interferometer as a primary accuracy standard. Potential applications for spot-scanning microscopy include actinic EUV mask inspection, wafer inspection, defect review, metrology, and wafer alignment (for accurate field stitching and overlay).

Algorithm Approach

Following is a conceptual outline of the reconstruction algorithm approach (or one possible approach), assuming coherent illumination and neglecting polarization effects and the finite size of detector pixels.

The illumination field $A^{(\mathrm{illum})}(\mathbf{x})$, as a function of position $\mathbf{x}$, comprises an integral superposition of plane waves of the form

$$A^{(\mathrm{illum})}(\mathbf{x}) = \iint_{\mathbf{f}|=1/\lambda} \tilde{A}^{[\mathrm{illum}]}(\mathbf{f}) \exp(i\,2\,\pi\,\mathbf{f}\bullet\mathbf{x})\,d\Omega \tag{1}$$

where $\mathbf{x}$ and $\mathbf{f}$ are spatial position and spatial frequency vectors, which have the following coordinate representations relative to coordinate basis vectors $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$, and $\hat{\mathbf{e}}_3$,

$$\mathbf{x} = x_1\,\hat{\mathbf{e}}_1 + x_2\,\hat{\mathbf{e}}_2 + x_3\,\hat{\mathbf{e}}_3, \quad \mathbf{f}_j = f_{j,1}\,\hat{\mathbf{e}}_1 + f_{j,2}\,\hat{\mathbf{e}}_2 + f_{j,3}\,\hat{\mathbf{e}}_3 \tag{2}$$

The illumination traverses the object in the $\hat{\mathbf{e}}_1$ direction, and the $f_{j,1}$ frequencies are all positive and are defined by the condition $|\,\mathbf{f}\,|=1/\lambda$,

$$f_{j,1} = \sqrt{1/\lambda^2 - f_{j,2}{}^2 - f_{j,3}{}^2} \tag{3}$$

where λ is the illumination wavelength. The integral in Eq. (1) is a two-dimensional integral over a portion of the sphere $|\,\mathbf{f}\,|=1/\lambda$, and the differential $d\Omega$ is a solid angle element on the integration sphere. (In numerical implementations, the integral in Eq. (1) can be approximated as a sum over a finite set of discrete frequencies $\mathbf{f}$.)

The detector pixels are labeled with index j and the field amplitude on pixel j, denoted $A_j^{(\mathrm{pixel})}$, is a linear function of the illumination wave amplitudes sampled at some reference point $\mathbf{x} = \mathbf{x}^{(\mathrm{ref})}$,

$$A_j^{(\mathrm{pixel})} = \iint_{\mathbf{f}|=1/\lambda} L_j(\mathbf{f})\,\tilde{A}^{[\mathrm{illum}]}(\mathbf{f}) \exp(i\,2\,\pi\,\mathbf{f}\bullet\mathbf{x}^{(\mathrm{ref})})\,d\Omega \tag{4}$$

The signal S_j acquired from pixel j is proportional to $|\,A_j^{[\mathrm{pixel}]}\,|^2$,

$$S_j = \eta_j\,|\,A_j^{[\mathrm{pixel}]}\,|^2 \tag{5}$$

where η_j is a conversion efficiency. (The signals are normalized to a direct measure of the illumination source power.) $A_j^{(\mathrm{pixel})}$ and $L_j(\mathbf{f})$ can be scaled to absorb the efficiency factor $(A_j^{(\mathrm{pixel})} \leftarrow \sqrt{\eta_j}\, A_j^{(\mathrm{pixel})}, L_j(\mathbf{f}) \leftarrow \sqrt{\eta_j}\, L_j(\mathbf{f}))$, so we can assume without loss of generality that $\eta_j = 1$.

$$S_j = | A_j^{(\mathrm{pixel})} |^2 \quad (\eta_j = 1) \tag{6}$$

Also, the phase of $A_j^{(\mathrm{pixel})}$ can similarly be absorbed in a complex scaling factor $(A_j^{(\mathrm{pixel})} \leftarrow c_j\, A_j^{(\mathrm{pixel})}, L_j(\mathbf{f}) \leftarrow c_j\, L_j(\mathbf{f}), | c_j | = 1)$, so we can constrain $A_j^{(\mathrm{pixel})}$ to be real-valued and non-negative,

$$\mathrm{Im}(A_j^{(\mathrm{pixel})}) = 0, \quad A_j^{(\mathrm{pixel})} \geq 0 \tag{7}$$

The reference position $\mathbf{x}^{(\mathrm{ref})}$ is not explicitly specified, but its three coordinates can be implicitly constrained by the condition that $\tilde{A}^{[\mathrm{illum}]}(\mathbf{f})$ is real-valued for three specific, linearly independent frequencies $\mathbf{f}$.

Within these constraints, the problem is to determine the amplitudes $\tilde{A}^{[\mathrm{illum}]}(\mathbf{f})$ and coefficients $L_j(\mathbf{f})$ from the signals S_j. (In numerical implementations $\mathbf{f}$ is finitely discretized, L becomes a matrix operator, and $\tilde{A}^{[\mathrm{illum}]}$ is a vector; so the number of unknowns is finite.) A single interferogram defined by Eq. (4) does not contain sufficient information to determine the unknowns, but they can be resolved by combining Eq. (4) with a constraining optical model for the detector and/or illumination optics, or with additional information from interferograms acquired at different detector positions as described below.

The linear coefficients $L_j(\mathbf{f})$ in Eq. (4) represent the optical transfer function of a detector system, which includes an aperture filter, the pixel array, and any intervening optics. If the detector position is changed by translational displacement vector $\Delta\mathbf{x}$ (with the illumination field stationary) then Eq. (4) will apply to the field amplitudes sampled at $\mathbf{x} = \mathbf{x}^{(\mathrm{ref})} + \Delta\mathbf{x}$,

$$\begin{aligned} A_j^{(\mathrm{pixel},\Delta\mathbf{x})} &= \iint_{|\mathbf{f}|=1/\lambda} L_j(\mathbf{f})\, \tilde{A}^{[\mathrm{illum}]}(\mathbf{f}) \exp(i\, 2\pi\, \mathbf{f} \bullet (\mathbf{x}^{(\mathrm{ref})} + \Delta\mathbf{x}))\, d\Omega \\ &= \iint_{|\mathbf{f}|=1/\lambda} L_j^{(\Delta\mathbf{x})}(\mathbf{f})\, \tilde{A}^{[\mathrm{illum}]}(\mathbf{f}) \exp(i\, 2\pi\, \mathbf{f} \bullet \mathbf{x}^{(\mathrm{ref})})\, d\Omega \end{aligned} \tag{8}$$

where

$$L_j^{(\Delta\mathbf{x})}(\mathbf{f}) = L_j(\mathbf{f}) \exp(i\, 2\pi\, \mathbf{f} \bullet \Delta\mathbf{x}) \tag{9}$$

The "$\Delta\mathbf{x}$" superscripts represent the transformed pixel amplitudes $A_j^{(\mathrm{pixel},\Delta\mathbf{x})}$ and coefficients $L_j^{(\Delta\mathbf{x})}$ under translation of the detector. The corresponding signals are

$$S_j^{(\Delta\mathbf{x})} = | A_j^{(\text{pixel},\Delta\mathbf{x})} |^2 \tag{10}$$

The detector can be scanned over a three-dimensional range of displacement vectors $\Delta\mathbf{x}$ to provide additional information without increasing the number of unknowns (except that the vectors $\Delta\mathbf{x}$ might not be accurately controlled and can be included with the unknowns).

Even with translational scanning Eq. (8) is insufficient to resolve the unknowns without a constraining model because an arbitrary function of $\mathbf{f}$ can be shifted between $L_j(\mathbf{f})$ and $\tilde{A}^{[\text{illum}]}(\mathbf{f})$ without affecting the integral (e.g., $L_j(\mathbf{f}) \leftarrow L_j(\mathbf{f}) / u(\mathbf{f})$, $\tilde{A}^{[\text{illum}]}(\mathbf{f}) \leftarrow u(\mathbf{f})\,\tilde{A}^{[\text{illum}]}(\mathbf{f})$). However, it may be possible to eliminate the model dependence and realize first-principles ptychography by using additional information from rotational scans. If the detector is first translated by displacement $\Delta\mathbf{x}$, and is then rotated around the coordinate origin by rotation operator R, then the pixel amplitudes are described by the following generalization of Eq. (8),

$$\begin{aligned} A_j^{(\text{pixel},\Delta\mathbf{x},R)} &= \iint_{|\mathbf{f}|=1/\lambda} L_j(R^{-1}\,\mathbf{f})\,\tilde{A}^{[\text{illum}]}(\mathbf{f}) \exp(i\,2\,\pi\,\mathbf{f} \bullet (\mathbf{x}^{(\text{ref})} + \Delta\mathbf{x}))\,d\Omega \\ &= \iint_{|\mathbf{f}|=1/\lambda} L_j^{(\Delta\mathbf{x},R)}(\mathbf{f})\,\tilde{A}^{[\text{illum}]}(\mathbf{f}) \exp(i\,2\,\pi\,\mathbf{f} \bullet \mathbf{x}^{(\text{ref})})\,d\Omega \end{aligned} \tag{11}$$

where

$$L_j^{(\Delta\mathbf{x},R)}(\mathbf{f}) = L_j(R^{-1}\,\mathbf{f}) \exp(i\,2\,\pi\,\mathbf{f} \bullet \Delta\mathbf{x}) \tag{12}$$

The "R" superscripts represent the transformed pixel amplitudes $A_j^{(\text{pixel},\Delta\mathbf{x},R)}$ and coefficients $L_j^{(\Delta\mathbf{x},R)}$ after rotation of the detector. The rotation operator is defined by three Euler angles, which can be included with the unknowns.

The measurement robustness and stability can be improved by combining data from multiple detector systems and multiple illumination fields. With M detector systems and N illumination fields combined pairwise, the number of unknowns (not counting scan coordinates) is a linear function of M and N (e.g. $a\,M + b\,N$), whereas the number of constraining equations defined by Eq. (11) is proportional to $M\,N$, so the equations become highly overdetermined with large M and N and can be solved by least-squares error minimization.

In practice, the multiple detectors can all be the same apparatus, but with different aperture filters. The calibration algorithm can be modified to allow translation and rotation of only the filter, not the entire detector apparatus. The multiple illumination fields can be generated by using a set of quick-change, far-field transmission masks. The algorithm can also be generalized to accommodate partial coherence and polarization effects.

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