Effect of tilt on zone plate performance

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Outline

Introduction

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Focusing X-Rays

- Ref. index$\rightarrow$ complex,slightly < 1
- Zone plates$\rightarrow$ monochromatic diffractive optics.
- Alternate rings of low/high ref. index materials placed such that outgoing waves interfere constructively.

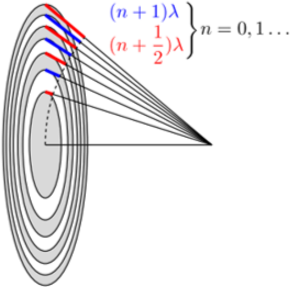
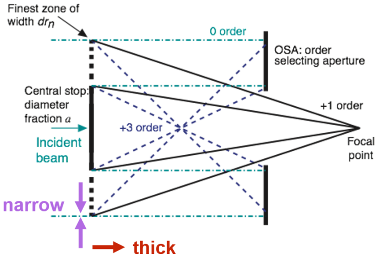


Illustration of zone plate [1]

[1] Jacobsen [2019]

Factors affecting efficiency & resolution

- Spatial resolution limited to finest, outermost zone width.[2]
- Zones must be thick enough along beam direction to produce a phase shift of π, several um at hard x-ray energy.[3]



Efficiency & resolution for first order focus[4]

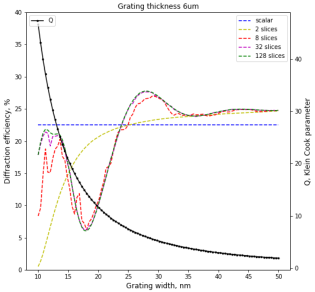
[2] Baez [1952]; Myers Jr. [1951]

[3] Kirz [1974]

[4] Jacobsen [2019]

Scalar theory is not enough

- Scalar approximation assumption → interaction between x-rays and the optic can be treated as one-step diffraction.
- Klein-Cook param. : Q_{K-C} indicator of "diffraction regime"[5].



Volume effects in 1d gratings

[5] Klein und Cook [1967]

Outline

Need for tilt misalignment study [8]

- As aspect ratios of zone plates go up[6] , degradation of performance due to tilt misalignment becomes more prominent.
- Analytic limits[7] from literature do not account for volume diffraction effects.

[6] Chang und Sakdinawat [2014]; Li et al. [2017a]; Parfeniukas et al. [2017]

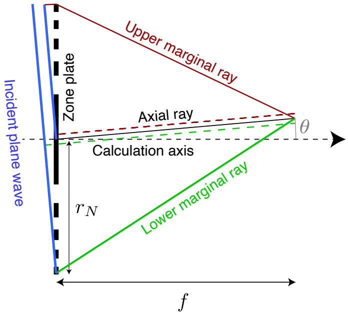
[7] Myers Jr. [1951]; Young [1972]

[8] Tilting zones to local bragg angle is not considered here.

Analytic limits

Analytic limits

- Based on path length deviation (from no tilt) between marginal, axial ray[9] $\rightarrow \ell'_u, \ell'_l$.
- Simplified expressions for path length deviation
  - $\ell_u = (\ell_0) + \ell_c\theta - \ell_a\theta^2$
  - $\ell_l = (\ell_0) + \ell_c\theta + \ell_a\theta^2$
- $\ell_0 \rightarrow$ convergence to focus, $\ell_c \rightarrow$ coma, $\ell_a \rightarrow$ astigmatism & field curvature[10].



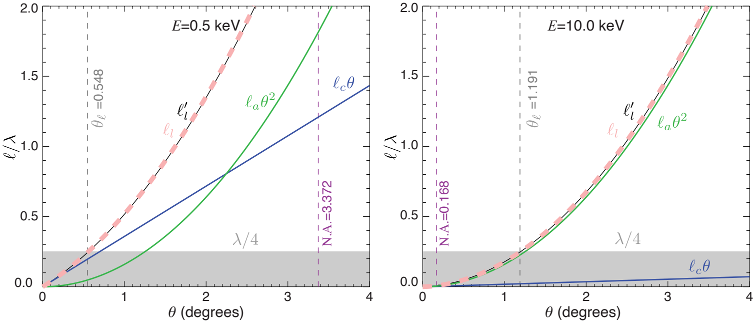
Path length schematic.

[9] Myers Jr. [1951]; Young [1972]

[10] referred to hereafter as astigmatism only.

Expected behavior

- $\frac{\ell_a \theta^2}{\ell_c \theta} \propto \frac{\theta}{N.A.}$, $N.A. \rightarrow$ numerical aperture.
- RQW limit[11]: $\theta_c < \frac{1}{2N\, N.A.} \mid \theta_a < \frac{1}{\sqrt{3N}}$, $N \rightarrow$ number of zones.



Path length terms

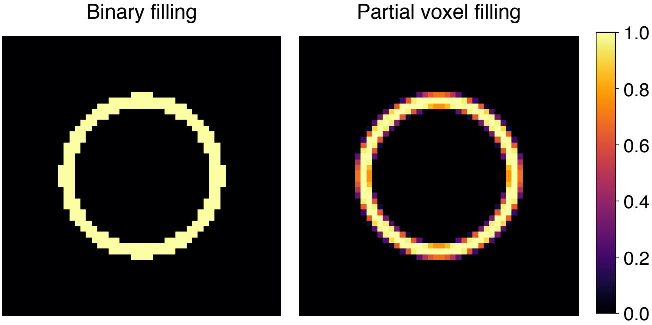
11 Rayleigh Quarter Wave Criterion

Implementation

Outline

Partial Filling

- Binary fill on a smaller pixel grid, then downsample!



Partial fill

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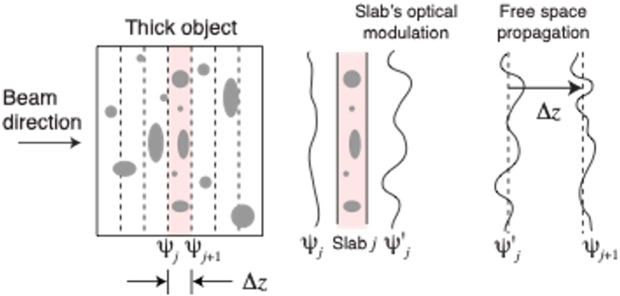
Multislice

- "Slice" the object into multiple thin sections[12].
- Agrees with rigorous coupled wave theory[13].



Multi-slice schematic [14]

[12] Cowley und Moodie [1957], Ishizuka und Uyeda [1977], also known as beam prop. meth. Van Roey et al. [1981]

[13] Li et al. [2017b]

[14] Jacobsen [2019]

Algorithm 1: Optic simulation using the multislice method.

```
/* initialize                         */
ψ(x, y) ← 1
/* diffraction within optic           */
for n=1,N do
    SliceDiff(n)
    PropShort(Δ_z)
end
/* Propagate exit wave by a focal
   length f to the focal plane        */
PropLong(f)
```

Procedure SliceDiff(n)

/* Apply refractive effect of slice using */

$\psi(x, y) = \psi(x, y) \odot \exp\left[i \frac{2\pi\Delta_z}{\lambda} \left(\delta(x, y) + i\beta(x, y)\right)\right]$;

return;

Procedure PropShort(Δ_z)

/* Free space propagation from source s to destination d plane */

$\psi_s(x, y) \xrightarrow{\mathcal{F}} \Psi(u, v)$;

$\Psi(u, v) = \Psi(u, v) \odot \exp\left[-i \frac{2\pi\Delta_z}{\lambda} \sqrt{1 - \lambda^2(u^2 + v^2)}\right]$;

$\Psi(u, v) \xrightarrow{\mathcal{F}^{-1}} \psi_d(x, y)$;

return;

Procedure PropLong(f)

/* Free space propagation from source s to destination d plane */

$\psi'(x, y) = \psi_s(x, y) \odot \exp\left[-i \frac{2\pi f}{\lambda} \sqrt{x_s^2 + x_s^2 + f^2}\right]$;

$\psi'(x, y) \xrightarrow{\mathcal{F}} \Psi'(x, y)$;

$\Psi_d(x, y) = \Psi'(x, y) \odot \exp\left[-i \frac{2\pi f}{\lambda} \sqrt{x_d^2 + x_d^2 + f^2}\right]$;

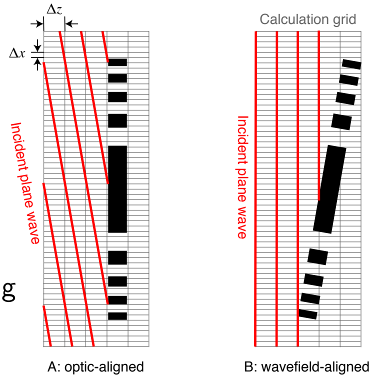
$\psi_d(x, y) = \frac{i\Delta_x^2}{\lambda f} \Psi_d(x, y)$;

return;

Outline

Approaches to simulating tilt misalignment

- Two methods to simulating tilt.
  - Optic aligned.
  - Wavefiled aligned.
- Optic aligned → simple, but limited to cases where output grid can capture focus.
- Wavefiled aligned → time consuming but no limit on tilt angle.



Tilt schematic

Optic aligned approach

- Apply a phase of $\frac{2\pi}{\lambda} x \tan(\theta)$ at each pixel.

Algorithm 2: Optic-aligned approach.

```
/* For each angle in range of interest                   */
for i=1,K do
    /* initialize                                        */
    AddPhase(θ)
    /* diffraction within optic                          */
    for n=1,N do
        SliceDiff(n)
        PropShort(Δ_z)
    end
    /* Propagate exit wave by a focal length f to the focal
       plane                                             */
    PropLong(f)
end
Procedure AddPhase(θ)
    /* Apply phase to mimic tilt misalignment            */
    ψ(x, y) ← 1
    φ_x = (2πΔ_z / λ) tan(θ)x
    ψ(x, y) = ψ(x, y) ⊙ exp[iφ_x]
    return
```

Wavefield aligned approach

- Reduce the size of 2D grid to essential area.
- Duplicate slices along propagation direction to create isotropic grid.
- Rotate zone plate relative to grid.
- Collapse the grid back along the propagation direction.

Algorithm 3: Wavefield-aligned approach.

```
/* Reduce the pattern down to
   essential area.                */
Reduce (pattern)
/* For each angle in range of
   interest                       */
for i=1,K do
    Rotate (pattern_reduced)
    /* For each slice in a zone
       plate at a given tilt
       misalignment perform
       multislice simulation      */
    for n=1,N do
        Extract (pattern_reduced)
        SliceDiff(n)
        PropShort(Δz)
    end
    PropLong(f)
end
```

```
Procedure Reduce (pattern)
    /* Extract relevant part of zone plate                    */
    /* choose and save appropriate parameters viz.
       number of slices, step size along propagation
       direction                                              */
    pattern →pattern_reduced ;
    return;
Procedure Rotate (pattern_reduced)
    /* Rotate zone plate pattern                              */
    /* Expand the number of slices along direction of
       propagation to form an isotropic three
       dimensional grid.                                      */
    pattern_reduced --Expand--> pattern_isometric;
    /* Rrotate along axis of rotation                         */
    pattern_isometric --Rotation--> pattern_isometric;
    /* reduce number of slices to number of slices for
       propagation.                                           */
    pattern_isometric --Collapse--> pattern_reduced;
    return;
Procedure Extract (pattern_reduced)
    /* Extract zone plate pattern at slice, expand back
       to grid size neede for propagation.                    */
    pattern_reduced →pattern ;
    return;
```

Outline

Parameter \ Regime	Soft X ray	Hard X ray
Photon energy	0.5 keV	10 keV
Outermost zone width dr_N	21.09 nm	21.07 nm
Diameter $2r_N$	58.90 µm	58.88 µm
Pixels N_x	55,296	55,296
Input array pixel size Δ_x	4.73 nm	4.73 nm
Output array pixel size Δ'_x	4.73 nm	4.74 nm
Focal length f	0.5 mm	10 mm
Numerical aperture N.A.	3.372°	0.168°
Bragg tilt angle[15] $\theta_{\mathrm{B}}(r_N)$	1.687°	0.084°
Aberration tilt limit θ_l	0.548°	1.191°
Max tilt θ_f for optic-alig. approach	10.90°	0.75°
Optimum thickness $t_{\mathrm{zp,opt}}$	0.098 µm	1.975 µm
t_{zp} for $Q = 0.333$	0.038 µm	0.759 µm
t_{zp} for $Q = 3.333$	0.381 µm	7.594 µm
t_{zp} for $Q = 10$	1.142 µm	22.782 µm

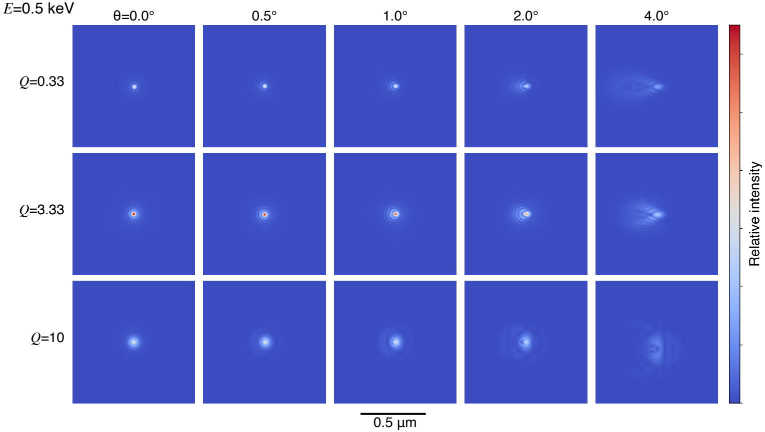
[15] For outermost zones

Results

Outline

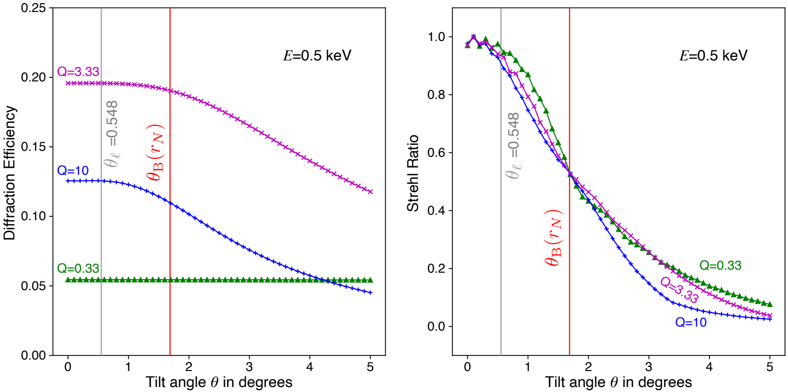
Qualitative performance

- Coma predicted.



Focal Profile

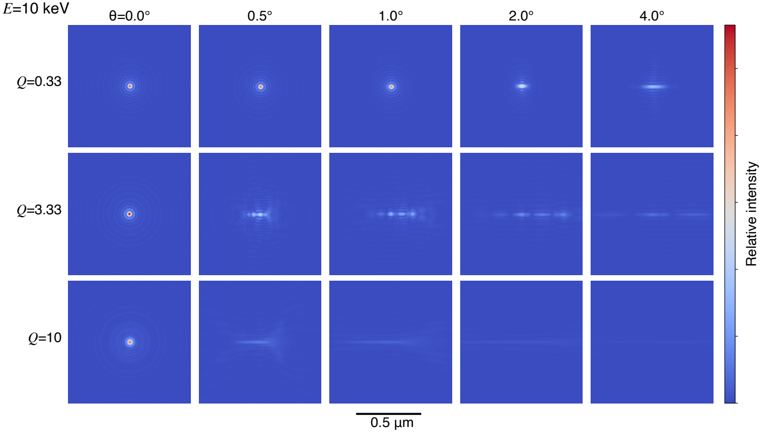
Quantitative performance



Outline

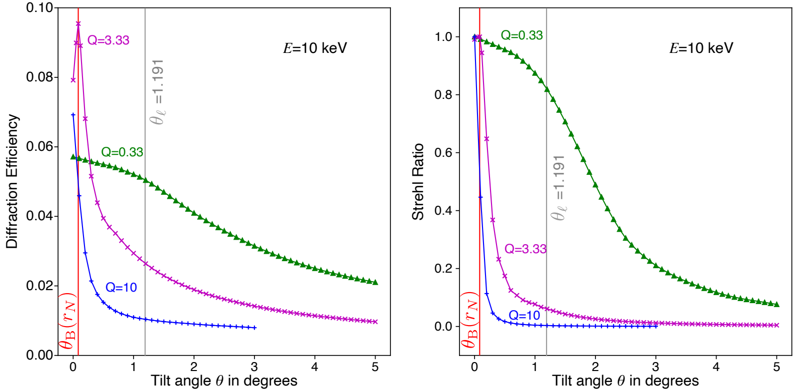
Qualitative performance

- Astigmatism predicted.



Focal Profile

Quantitative performance



Summary

- Systematic study of tilt misalignment conducted.
- Simple analytic models can predict misalignment limits and behavior for thin zone plates.
- Waveguide effects are important for thick zone plates.

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Backup

Programming details

- Implemented in Python3 using the scientific python stack : NumPy,SciPy
- FFT's via pyFFTW
- numexpr for pointwise multiplication
- libvips for 3D rotations
- HDF5 for I/O

Waveguide effects at no tilt