Effect of tilt on zone plate performance

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Outline

Introduction

Outline

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.

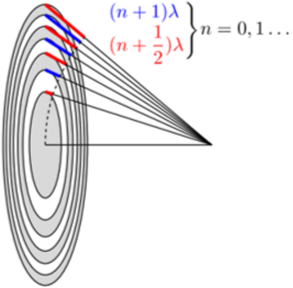
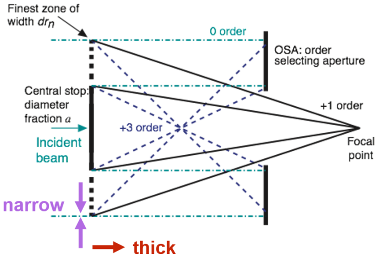


Illustration of zone plate [1]

[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]

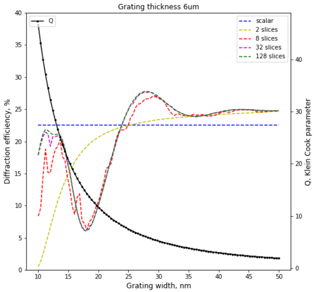
[2] Baez [1952]; Myers Jr. [1951]

[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]

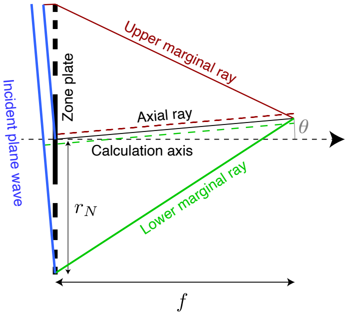
[7] Myers Jr. [1951]; Young [1972]

[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].



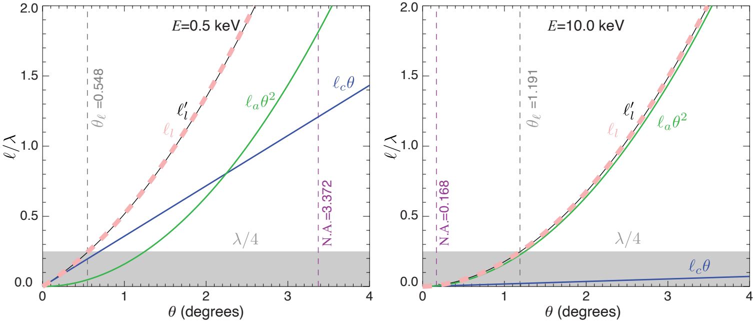
Path length schematic.

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

[10] referred to hereafter as astigmatism only.

Expected behavior

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



Path length terms

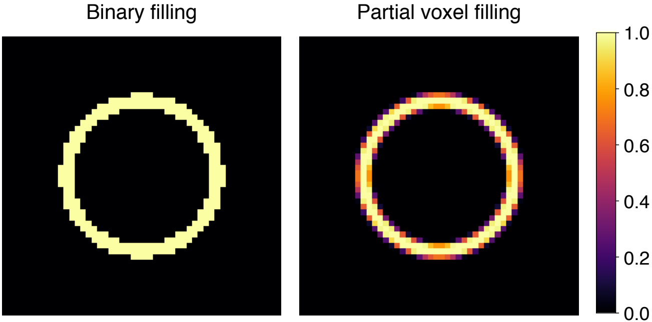
[11] Rayleigh Quarter Wave Criterion

Implementation

Outline

Partial Filling

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



Partial fil

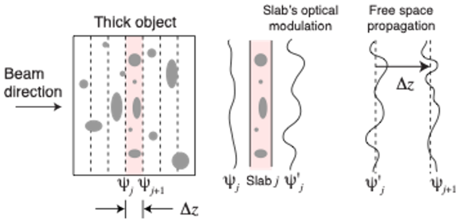
Outline

Multislice

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

Algorithm 1: Optic simulation using the multislice method.

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



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]

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 */

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

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

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

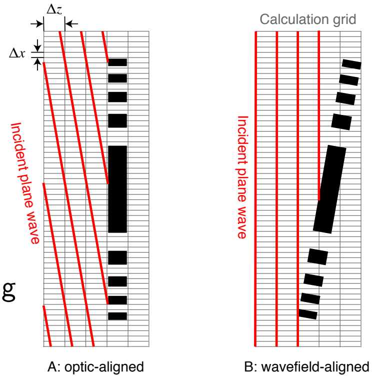
$\psi_d(x,y) = \frac{i\Delta_x^2}{\lambda f}\Psi_d(x,y)$;

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

Optic aligned approach

Algorithm 2: Algorithm for the optic-aligned approach.

```
/* initialize                                        */
AddPhase(θ)
/* diffraction within optic                          */
for n=1,N do
    SliceDiff(n)
    PropShort(Δz)
end
/* Propagate exit wave by a focal length f to the focal plane
   */
PropLong(f)
Procedure AddPhase(θ)
    /* Apply phase to mimic tilt misalignment         */
    ψ(x,y) ← 1
    φx = (2πΔz/λ) tan(θ)x
    ψ(x,y) = ψ(x,y) ⊙ exp[iφx]
    return
```

Procedure steps in math form:

$\psi(x,y) \leftarrow 1$

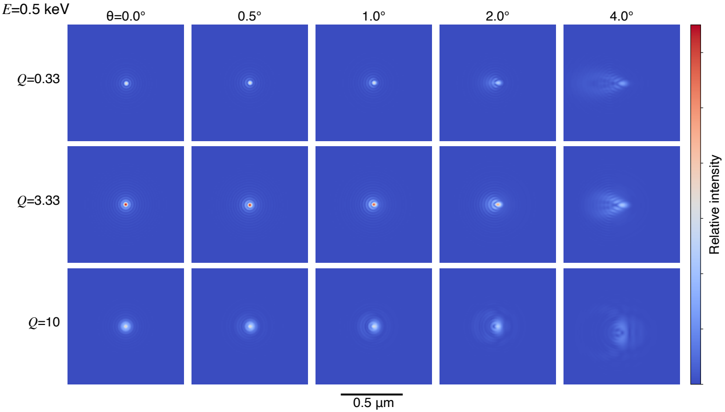
$\varphi_x = \frac{2\pi\Delta_z}{\lambda}\tan(\theta)x$

$\psi(x,y) = \psi(x,y) \odot \exp[i\varphi_x]$

Results

soft x-ray

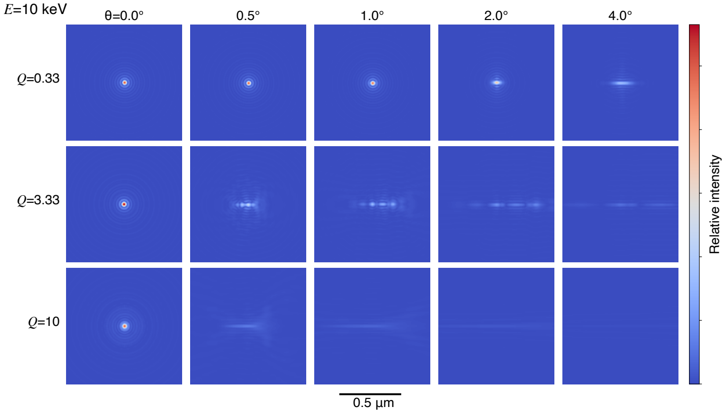
- Coma predicted.



Partial fil

hard x-ray

- Astigmatism predicted.



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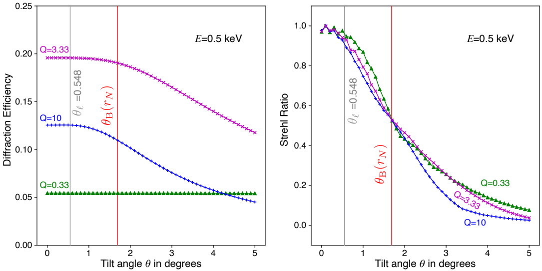
soft x-ray

- Limit agrees with analytic expectation.



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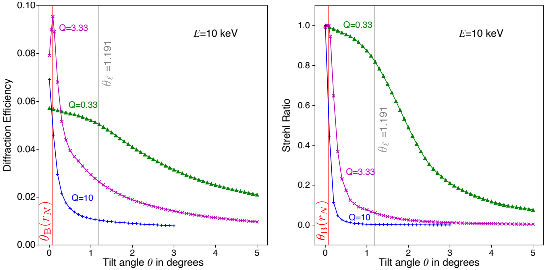
hard x-ray

- Limit agrees with analytic expectation.



Partial fil

Acknowledgements

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References I

[Baez 1952] Baez, Albert V.: A study in diffraction microscopy with special reference to X-rays. In: *Journal of the Optical Society of America* 42 (1952), Nr. 10, S. 756–762. – URL http://www.opticsinfobase.org/abstract.cfm?uri=josa-42-10-756. – ISBN 0030-3941

[Chang und Sakdinawat 2014] Chang, Chieh ; Sakdinawat, Anne: Ultra-high aspect ratio high-resolution nanofabrication for hard X-ray diffractive optics. In: *Nature Communications* 5 (2014), Juni, S. 4243

[Cowley und Moodie 1957] Cowley, J M. ; Moodie, A F.: The scattering of electrons by atoms and crystals. I. A new theoretical approach. In: *Acta Crystallographica* 10 (1957), Oktober, Nr. 10, S. 609–619

[Ishizuka und Uyeda 1977] Ishizuka, K. ; Uyeda, N.: A new theoretical and practical approach to the multislice method. In: *Acta Crystallographica A* 33 (1977), September, Nr. 5, S. 740–749

[Jacobsen 2019] Jacobsen, Chris: *X-ray Microscopy*. Cambridge, UK : Cambridge University Press, 2019. – ISBN 9781107076570

[Kirz 1974] Kirz, J: Phase zone plates for X-rays and the extreme UV. In: *Journal of the Optical Society of America* 64 (1974), Nr. 3, S. 301–309. – ISBN 0030-3941

References II

[Klein und Cook 1967] KLEIN, W R. ; COOK, B D.: Unified Approach to Ultrasonic Light Diffraction. In: *IEEE Transactions on Sonics and Ultrasonics* 14 (1967), Juli, Nr. 3, S. 123–134

[Li et al. 2017a] LI, Kenan ; WOJCIK, Michael J. ; DIVAN, Ralu ; OCOLA, Leonidas E. ; SHI, Bing ; ROSENMANN, Daniel ; JACOBSEN, Chris: Fabrication of hard x-ray zone plates with high aspect ratio using metal-assisted chemical etching. In: *Journal of Vacuum Science & Technology B* 35 (2017), Nr. 6, S. 06G901. – URL `http://avs.scitation.org/doi/10.1116/1.4991794`. – ISSN 2166-2746

[Li et al. 2017b] LI, Kenan ; WOJCIK, Michael J. ; JACOBSEN, Chris: Multislice does it all : calculating the performance of nanofocusing x-ray optics. In: *Optics Express* 25 (2017), Nr. 3, S. 185–194. – ISSN 1094-4087

[Myers Jr. 1951] MYERS JR., Ora E.: Studies of Transmission Zone Plates. In: *American Journal of Physics* 19 (1951), Nr. 6, S. 359–365. – URL `http://link.aip.org/link/?AJP/19/359/1{&}Agg=doi`. – ISSN 00029505

References III

[Parfeniukas et al. 2017] PARFENIUKAS, Karolis ; GIAKOUMIDIS, Stylianos ; VOGT, Ulrich ; AKAN, Rabia: High-aspect ratio zone plate fabrication for hard x-ray nanoimaging. In: *Proceedings SPIE* 10386 (2017), S. 103860S. – URL `https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10386/2272695/High-aspect-ratio-zone-plate-fabrication-for-hard-x-ray/10.1117/12.2272695.full`. ISBN 9781510612297

[Van Roey et al. 1981] VAN ROEY, J. ; DONK, J. van der ; LAGASSE, P. E.: Beam-propagation method: analysis and assessment. In: *Journal of the Optical Society of America* 71 (1981), Jul, Nr. 7, S. 803–810. – URL `http://www.osapublishing.org/abstract.cfm?URI=josa-71-7-803`

[Young 1972] YOUNG, M: Zone Plates and Their Aberrations. In: *Journal of the Optical Society of America* 62 (1972), Nr. 8, S. 972–976

Backup

Algorithm 3: Optic simulation using the multislice method.

```
/* initialize */
```
$\psi(x,y) \leftarrow 1$
```
/* 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;