Refractive lens design and aberration compensation

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Refractive lens design and aberration compensation

Outline:

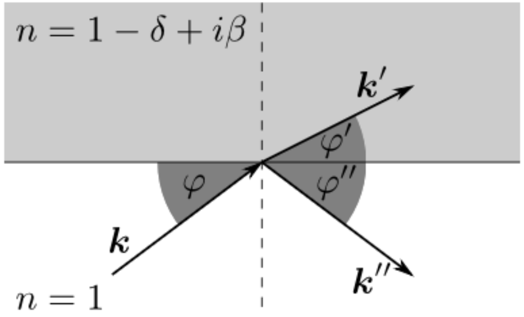
- Refractive index for x rays
- Basic lens properties
- Simple online calculator: lenscalc.desy.de
- Some application examples

- Lens errors and material impurities
- Wavefront measurements
- Design of phase plates for aberration compensation

The refractive index in the x-ray regime

Derived from phenomenological comparison

- scattering from atoms (form factor)
- transmission with refraction through material



Refractive index n: $n(\omega) = 1 - \delta + \mathrm{i}\beta$

$$\delta = \frac{n_a}{2\pi} r_e \lambda^2 \underbrace{\left(Z + f'(\omega)\right)}_{f_1} \qquad \beta = \frac{n_a}{2\pi} r_e \lambda^2 f''(\omega)$$

n_a… Avogagro constant
r_e … Classical e- radius

Snell's law:

$$n \cos \varphi' = \cos \varphi$$

Critical angle:

$$\varphi_c = \arccos n \approx \sqrt{2\delta}$$

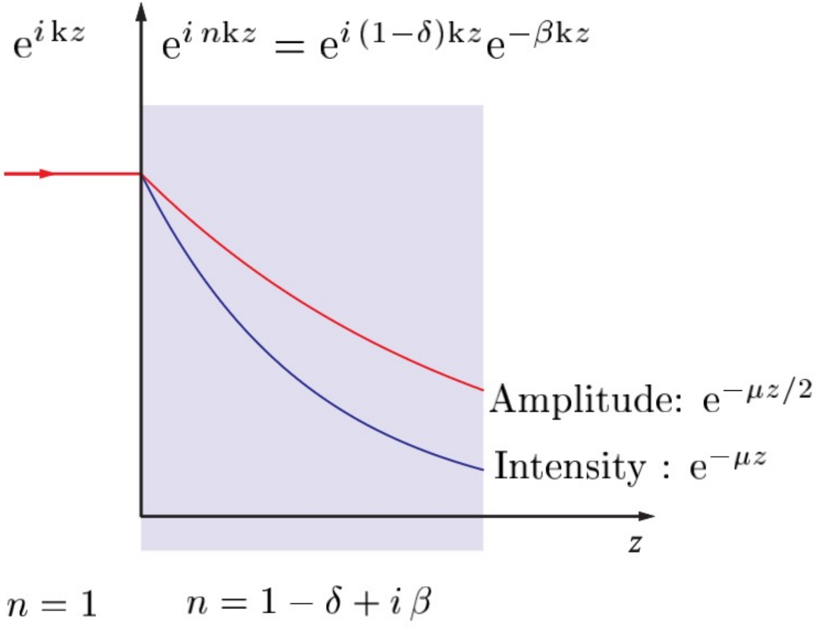
Atomic form factor:

$$f(\boldsymbol{q}, \omega) = \underbrace{f_0(\boldsymbol{q}) + f'(\omega)}_{f_1} + \underbrace{\mathrm{i} f''(\omega)}_{f_2}$$

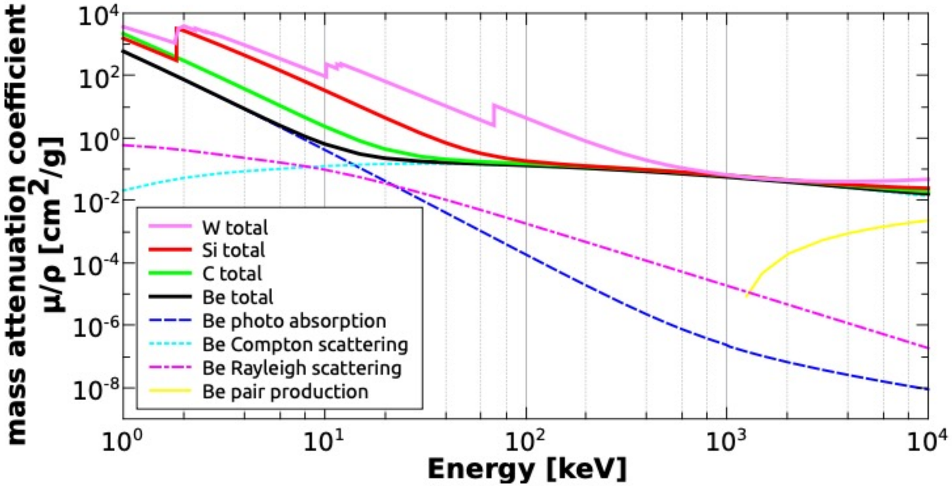
Absorption

Beer-Lambert law

$$I_{\Delta z}(x,y,z) = I_0 \cdot e^{-\int_{z=0}^{\Delta z} dz\, \mu(x,y,z)} \qquad \mu(x,y,z) = \frac{4\pi}{\lambda}\beta(x,y,z)$$



Total attenuation has many contributions:

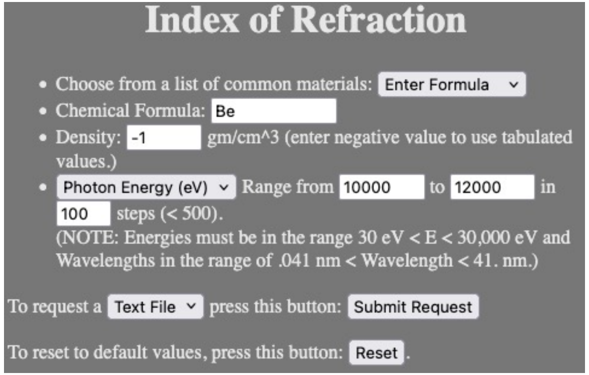


Als-Nielsen: Elements of Modern X-ray Physics

Available resources / library packages

Henke online database: https://henke.lbl.gov

- only up to 30 keV




```
Be Density=1.848
Energy(eV), Delta, Beta
 10000.    3.40754082E-06  1.02839592E-09
 10018.249   3.39512917E-06   1.02188757E-09
 10036.5303   3.38276345E-06   1.01542974E-09
 10054.8457   3.3704423E-06   1.00901842E-09
```

NIST / Chantler database: http://physics.nist.gov/ffast

- up to 433 keV, inconvenient (only f', f'')

Python packages

- periodictable
  - only to 30 keV
  - based on Henke tables
- **xraylib**
  - up to 800 keV
  - bindings to many languages

```
In [40]: from periodictable import xsf

In [41]: Be=xsf.index_of_refraction('Be', energy=10)

In [42]: print(f'delta: {1-np.real(Be)}, beta: {-np.imag(Be)}')
delta: 3.4075426530444375e-06, beta: 7.985610572831211e-10
```

```
In [53]: import xraylib

In [54]: Be=xraylib.Refractive_Index('Be', E=10, density=1.848)

In [55]: print(f'delta: {1-np.real(Be)}, beta: {np.imag(Be)}')
delta: 3.4082724095219064e-06, beta: 1.1788936509214389e-09
```

f'' only photo absorption or total scattering

Typical values for delta/beta and implications for refractive optics

X rays

- $\delta \sim 10^{-6}$
- focusing lens concave
- focal length 5 km
  for lens with R = 1 cm

Concave

$$f_s = \frac{R}{2\delta}$$

- $\mu \sim 1 – 100\ \mathrm{cm}^{-1}$
- attenuation length ~ 10 – 0.1 mm

Visible light

- $|\delta| \sim 0.5$
- focusing lens convex
- focal length 1cm
  for lens with R = 1cm

Convex

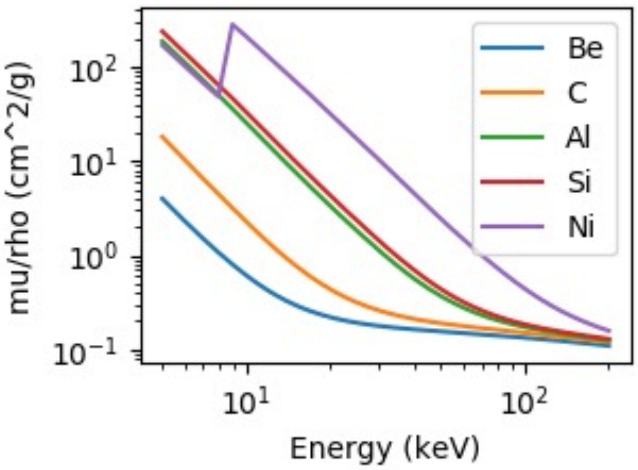
- attenuation 0.001 dB/m
- $\mu \sim 0.0002\ \mathrm{m}^{-1}$
- attenuation length ~ 5 km

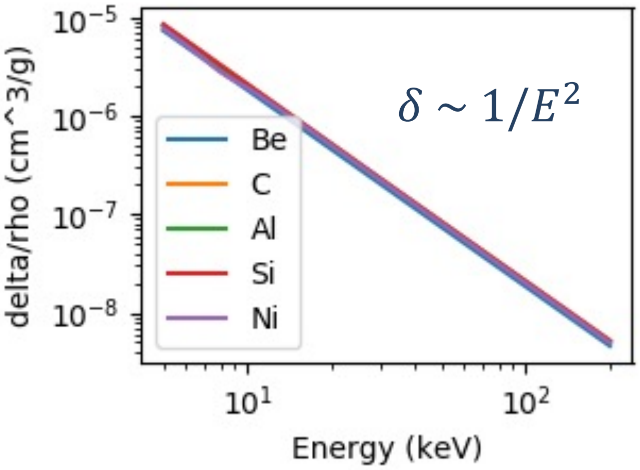
Refractive x-ray optics face the challenge of very weak refraction
in combination with strong absorption

Material considerations for refractive x-ray lenses

- Refractive power only depends on electron density
  $$f_0(q \rightarrow 0) = Z$$
- Strong dependence of absorption on atomic number Z
  $$\sigma_{photo} \sim Z^4/E^3$$

- Best material: high density ρ, low atomic number Z, high purity, fabrication methods



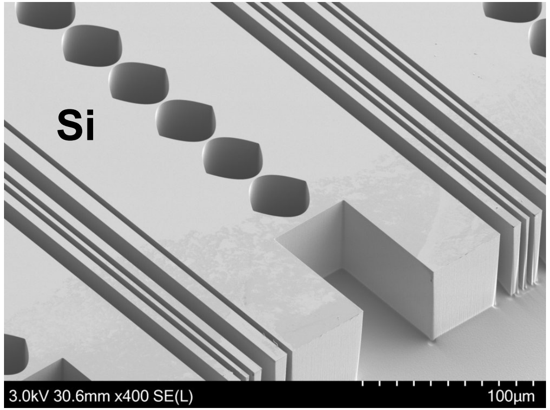


Design consequences and examples

- Small curvatures R in range 10 µm – 1000 µm
- Stacking of multiple lenses

Individually packaged, coin-shaped lenses
Be, Al, C*

Etched one-dimensional lenses
Si, SiC, C*

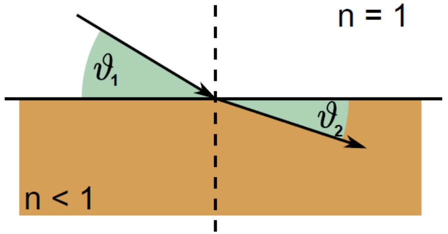


Printed/lithographic plastic lenses

Kubec et al., Nat. Commun. 13(1), (2022)

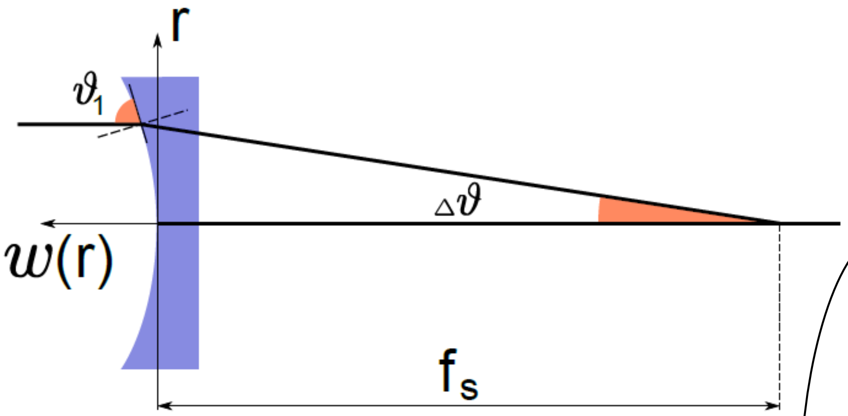
Lens shape

Snell's law:



$$n_1 \cos\vartheta_1 = n_2 \cos\vartheta_2$$

Refraction on single surface into common focal point:



$$\cos\vartheta_1 = (1-\delta)\cos(\vartheta_1 - \Delta\vartheta)$$

paraxial approximation

- $\cos(\vartheta_1 - \Delta\vartheta) = \cos(\vartheta_1)\cancelto{1}{\cos(\Delta\vartheta)} + \sin(\vartheta_1)\cancelto{\Delta\vartheta}{\sin(\Delta\vartheta)}$
- $\delta\sin(\vartheta_1)\,\Delta\vartheta = 0$

$$\Delta\vartheta = \delta\cot\vartheta_1 = \delta\tan(90^\circ - \vartheta_1) = \delta\frac{dw}{dr}$$

thin lens

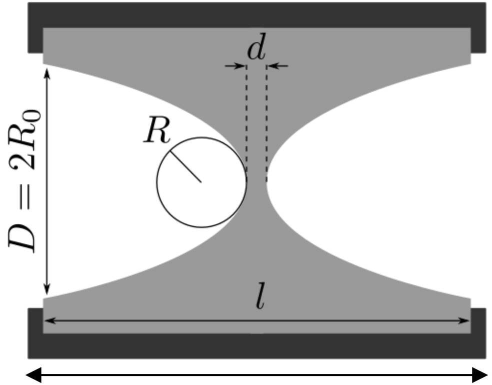
$$w(r) \ll f_s$$

$$\frac{r}{f_s} = \delta\frac{dw}{dr} \quad \Rightarrow \quad w(r) = \frac{r^2}{2 f_s \delta} + c$$

Curvature definition:

$$\frac{d^2\omega}{dr^2} = \frac{1}{f_s\delta} \equiv \frac{1}{R}$$

Basic lens properties



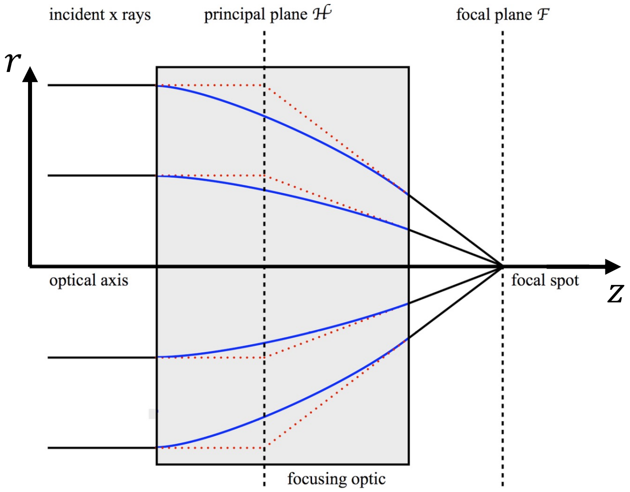
- Focal length: $$f_N = \frac{R}{2N\delta}$$
  N… Number of lenses
- Diffraction-limited spot size: $$d_t = \alpha \cdot \frac{\lambda}{2NA} = \alpha \cdot \frac{\lambda f}{D_{\text{eff}}}$$
  α… aperture-shape dependant: 1.22 (disc) – 0.75 (Gaussian)
  NA… numerical aperture
- Effective aperture: $$D_{\text{eff}} = \sqrt{\frac{1-e^{-a_p}}{a_p}} 2R_0 \qquad a_p = \frac{\mu N R_0^2}{2R}$$
- Transmission (2D lens): $$T_p = \frac{1-e^{-2a_p}}{2a_p} e^{-\mu N d}$$

Thick lens

Defining refractive power: $\omega = \sqrt{\frac{1}{f_s l}}$

Solving harmonic differential equation, boundary conditions: $r(0) = r_0,\ r'(0) = 0$

$$\frac{d^2}{dz^2} r(z) = -\omega^2 r(z) \longrightarrow r(z) = r_0 \cdot \begin{cases} 1 & : z \leq 0 \\ \cos(\omega z) & : 0 \leq z \leq L \\ b + mz & : L \leq z \end{cases}$$



$$\begin{aligned} b &= \cos(\omega L) + \omega L \sin(\omega L) \\ m &= -\omega \sin(\omega L). \end{aligned}$$

Principal plane $\boldsymbol{\mathcal{H}}$: $b + m\, z_H = 1$

Focal plane $\boldsymbol{\mathcal{F}}$: $b + m\, z_F = 0$

Thick lens

Principal plane location:

$$z_H = L + \frac{\cot(\omega L)}{\omega} - \frac{1}{\omega \sin(\omega L)}$$

Focal plane location:

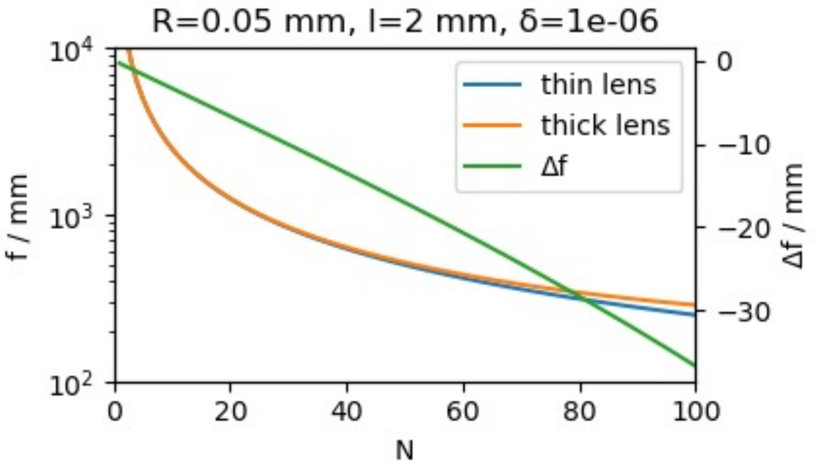
$$z_F = L + \frac{\cot(\omega L)}{\omega}$$

Focal length $f = z_F - z_H$:
$$f = \frac{1}{\omega \sin(\omega L)}$$

Critical lens length, if converging ray intersects optical axis: $\cos(\omega L) = 0$, i.e. $\omega L \geq \pi/2$

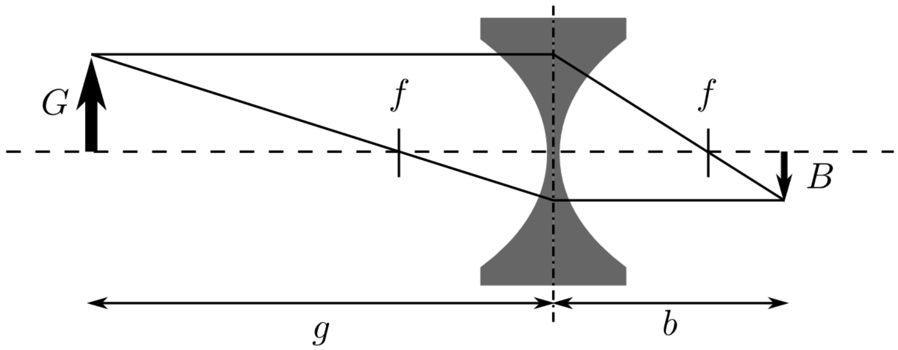
$$L_c = \frac{\pi}{2\omega}$$

$$f_{min} = \frac{1}{\omega \sin(\omega L_c)} = \frac{1}{\omega} = \sqrt{f_s l} = \sqrt{\frac{Rl}{2\delta}}$$



Focus size

Convolution between geometric image size $\boldsymbol{B}$ and diffraction-limit d_t



Lens equation: $\frac{1}{g} + \frac{1}{b} = \frac{1}{f}$

Image size $\boldsymbol{B}$: $B = G \cdot \frac{b}{g}$

Total image size $B_t = \sqrt{B^2 + d_t^2}$

Two contributions:

- Geometric demagnification of source
- Diffraction effects

Beam caustic: $B_t(z) = \sqrt{B_t^2 + 0.5\ln(2)\, D_{eff}^2 \left(\frac{z}{b}\right)^2}$

Two contributions:

- Focus size
- Lens aperture / divergence

Reverse calculation for desired focal length / image distance

Focal length f for given image distance b:

$$\frac{1}{g} + \frac{1}{b} = \frac{1}{f} \longrightarrow f = \frac{bg}{b+g}$$

Required number of lenses N:

$$f_N = \frac{R}{2N\delta} \longrightarrow N = \frac{R}{2f\delta}$$

$$f = \frac{1}{\omega \sin(\omega L)} \longrightarrow N = \frac{1}{\omega L} \arcsin\left(\frac{1}{f\omega}\right)$$

Analytic online calculator

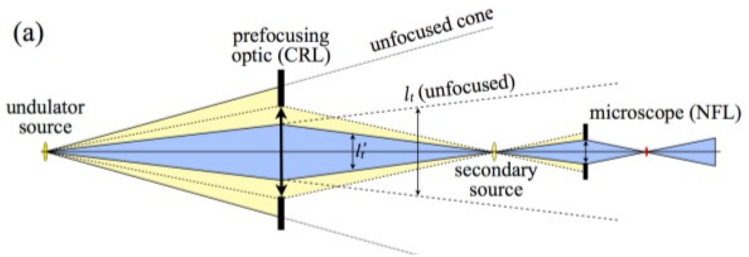
DESY lenscalc: http://lenscalc.desy.de

Covers:
- 2D Focusing (i.e. CRL)
- Crossed 1D focusing (i.e. NFL)
- Combination with 1D / 2D prefocusing

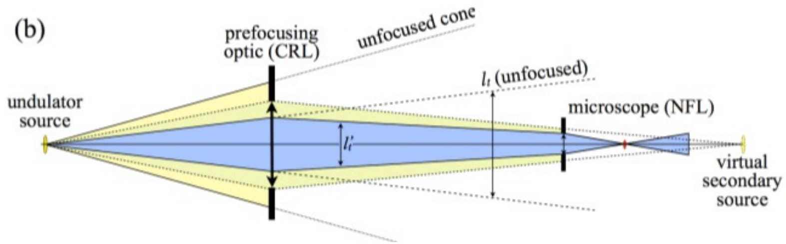
Assumptions/Limitation:
- Beam divergence is neglected
- Full illumination / overfill of lenses
- Gaussian source
- No spatial filtering for prefocus (coherence independent of lens aperture size)

Calculations can be shared/saved with link

Real secondary source:



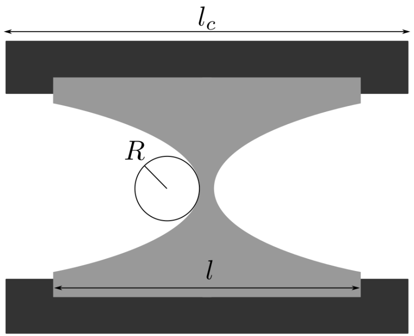
Imaginary secondary source:



Focal spot limit

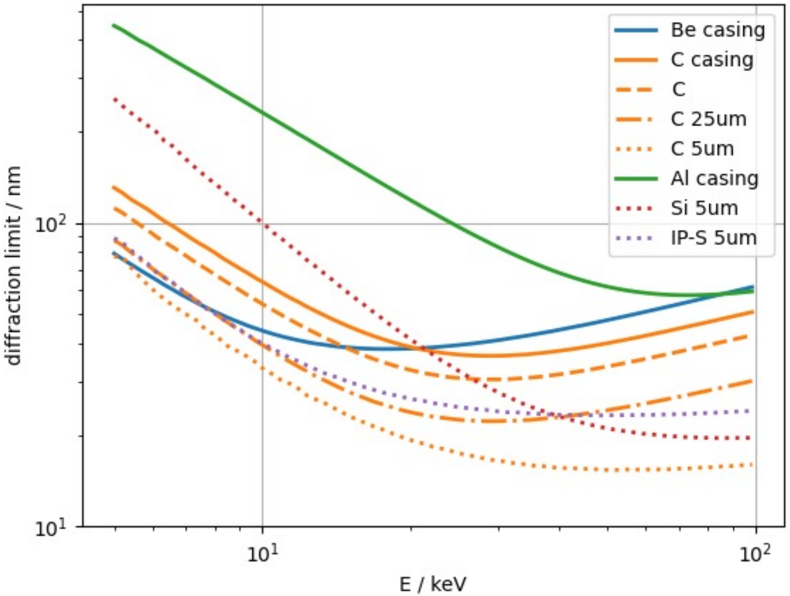
Desirable lens properties

- Fabrication of small curvatures
- Large lens stacks possible
- Minimize gap between lenses: $l_c \approx l$



$$f_{\min} = \sqrt{\frac{R l_c}{2\delta}}$$

achievable focal spot size

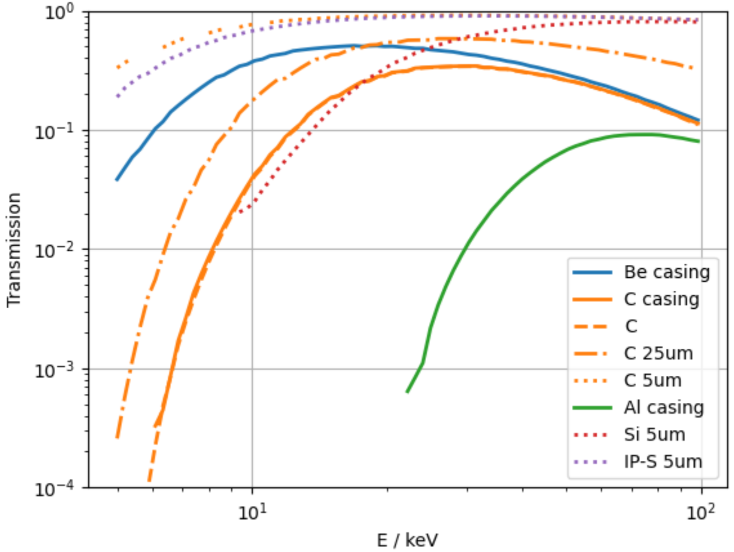


Be/Al/C: 1 mm substrate, 2 mm casing, R = 50 µm
Si/IP-S: 40 µm aperture, R = 5 µm
Working distance ≥ 10 mm

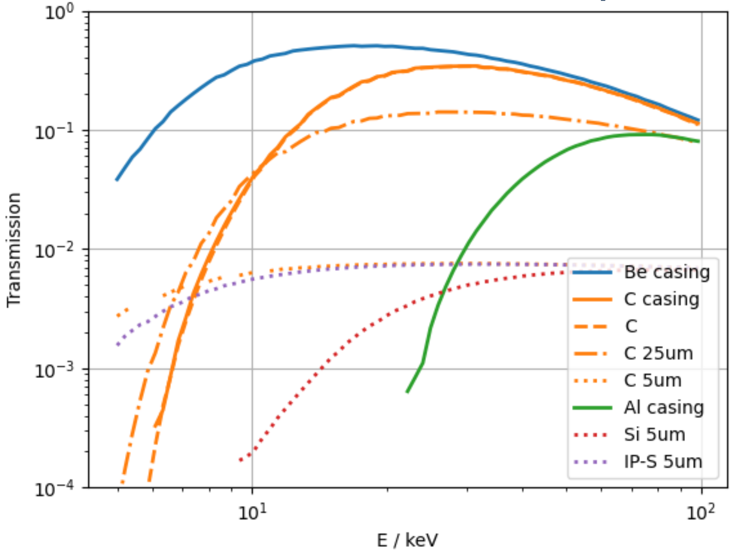
Performance for 100 nm focus

- Reduced transmission with diamond compared to beryllium
- Etched/printed lenses only viable, if beam can be tuned to aperture
- Large aperture lenses only viable, if lateral coherence high enough

raw lens transmission



lens transmission scaled to aperture

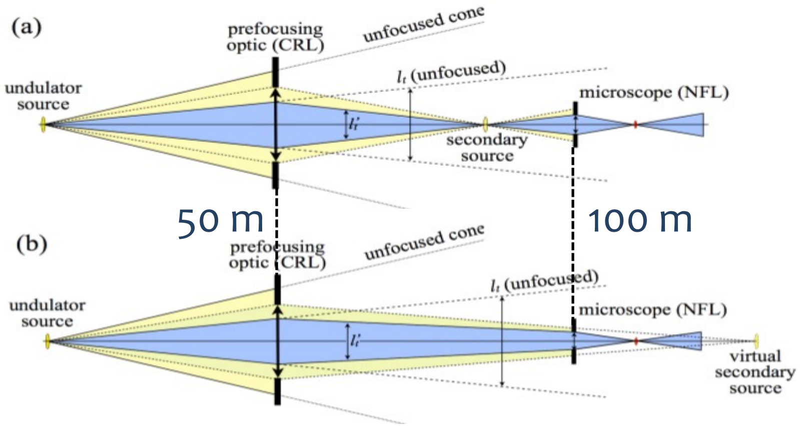


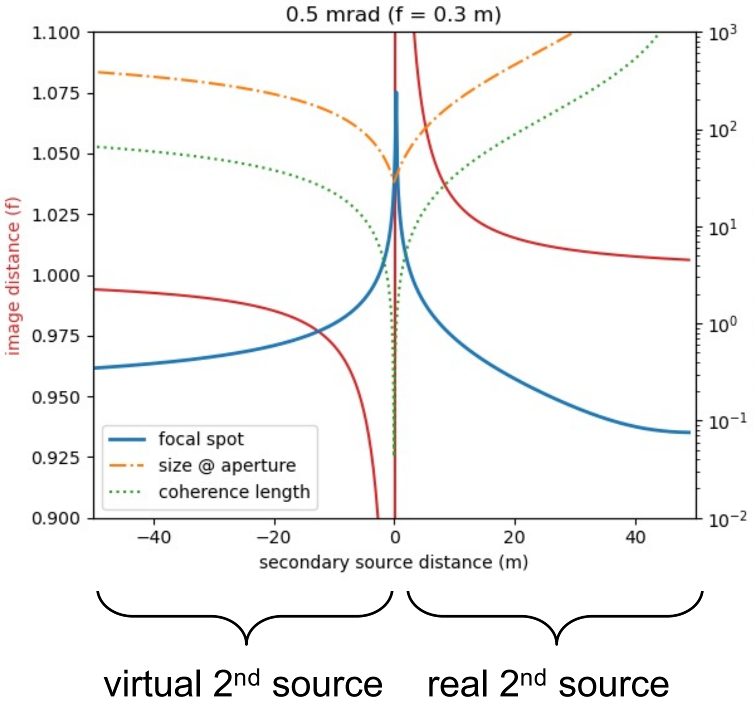
Example: Zoom lens system

Limits for flexible focal spot size change with 2-stage focusing at Petra IV

Conditions

- Prefocus at 50 m
- Full beam on prefocusing lens (0.7 mm)
- Experiment / main lens at 100 m
- Main lens: 300 µm aperture, f = 0.3 m

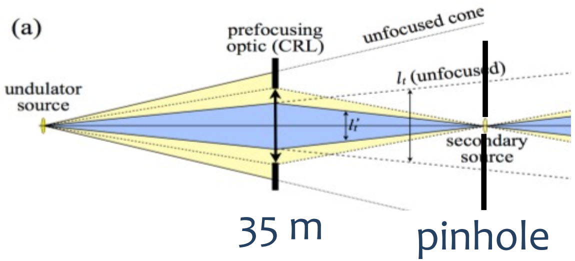


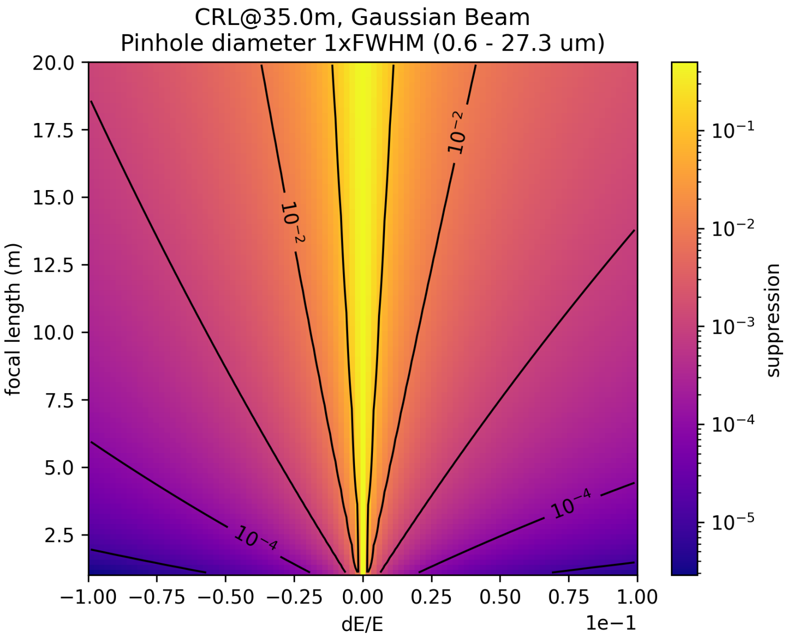


CRL as monochromator

Setup

- CRL @ 35 m, aperture matching beam size
- Variable focal length 1 m – 20 m
- Pinhole in focus for $dE/E = 0$
- Pinhole size = FWHM focus size





Beam caustic: $B_t(z) = \sqrt{B_t^2 + 0.5\ln(2)\, D_{eff}^2 \left(\frac{z}{b}\right)^2}$

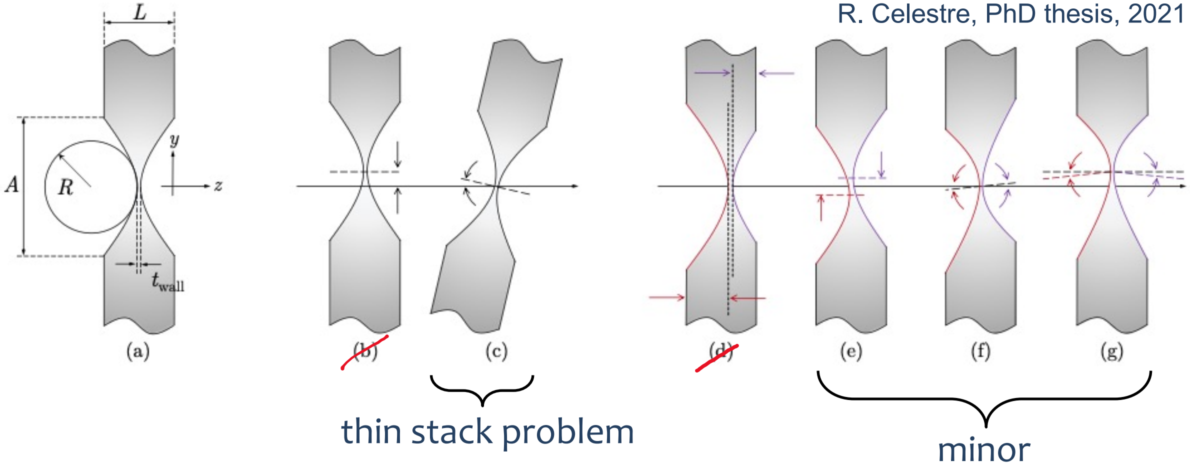
Lens errors and aberration measurement / compensation

Lens aberration, wavefront measurements

Not discussed here: Induced aberration due to mechanical misalignment

- Transverse position error (stacking errors or lens eccentricity)
- Tilt errors

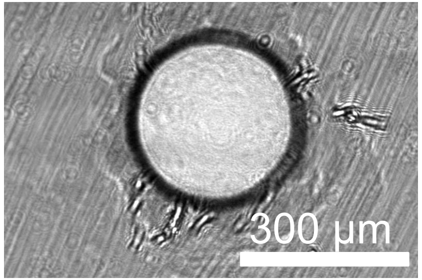
R. Celestre, PhD thesis, 2021



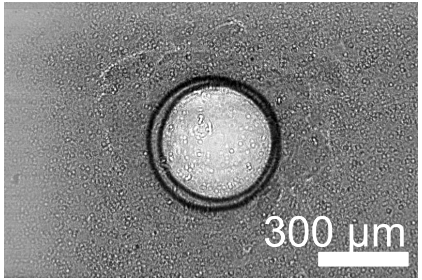
Focus on lens error due to fabrication limitations to create a parabolic lens shape.

High-frequency errors and material defects

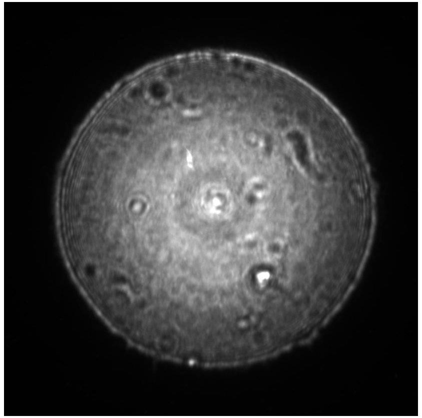
1x Be IF-1



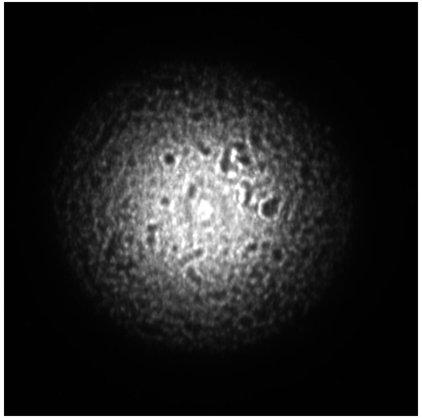
1x Be IS50M



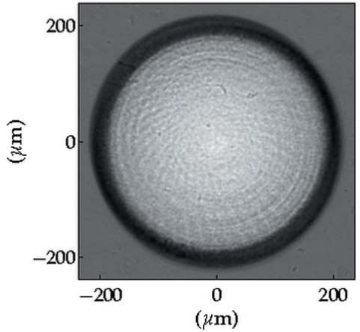
20x Be IS50M far field



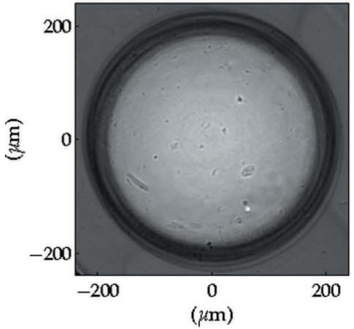
20x Be IS50M far field



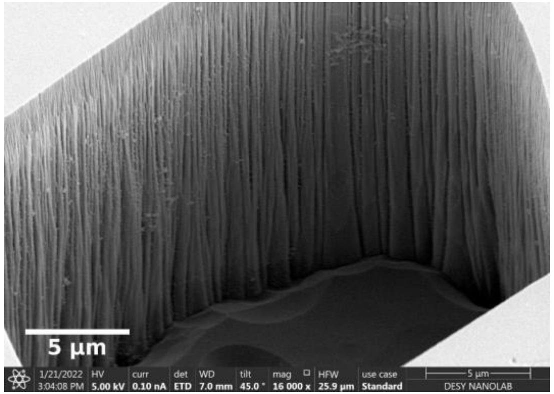
unpolished C*



polished C*



etched C* lens



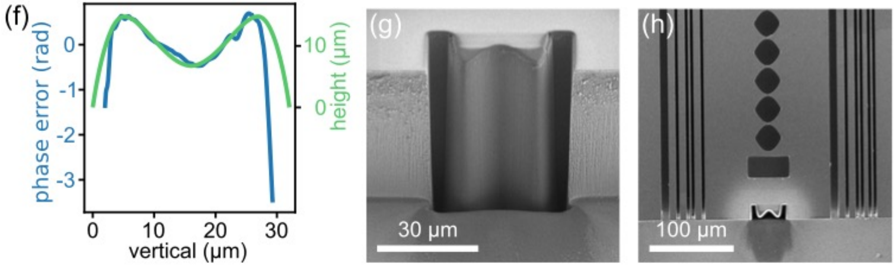
Celestre et al., J. Synchrotron Rad. 29, 629-643 (2022)

Typical fabrication errors

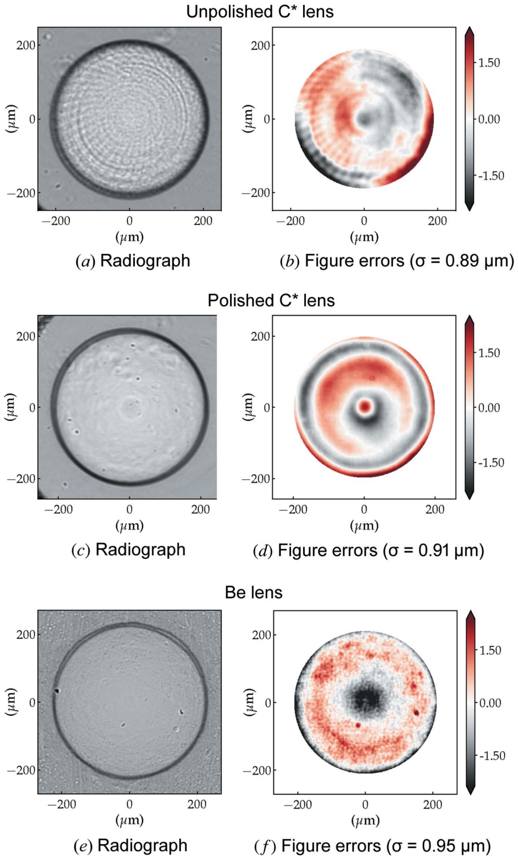
- ~~Stamp positioning/guiding errors~~
- Stamp to press metallic lens deformed
- Metallic material relaxes after pressing

- Ablation process unstable / random
- Laser positioning errors

- Etching errors: Slanted side wall, under-etched mask



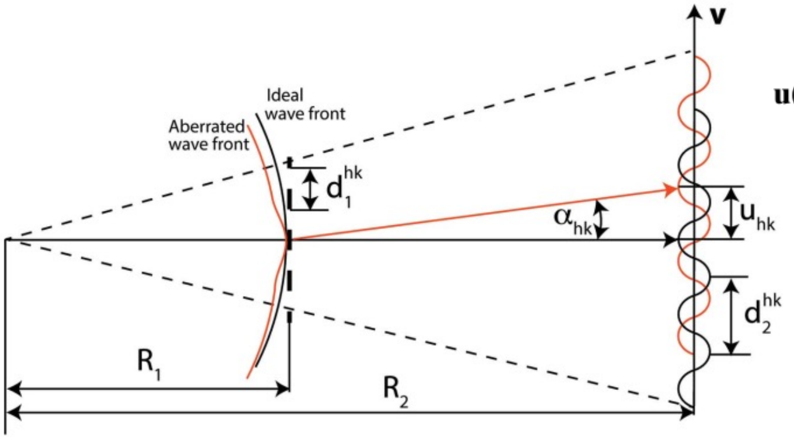
Seiboth et al., Appl. Phys. Lett. 122(24), (2023)



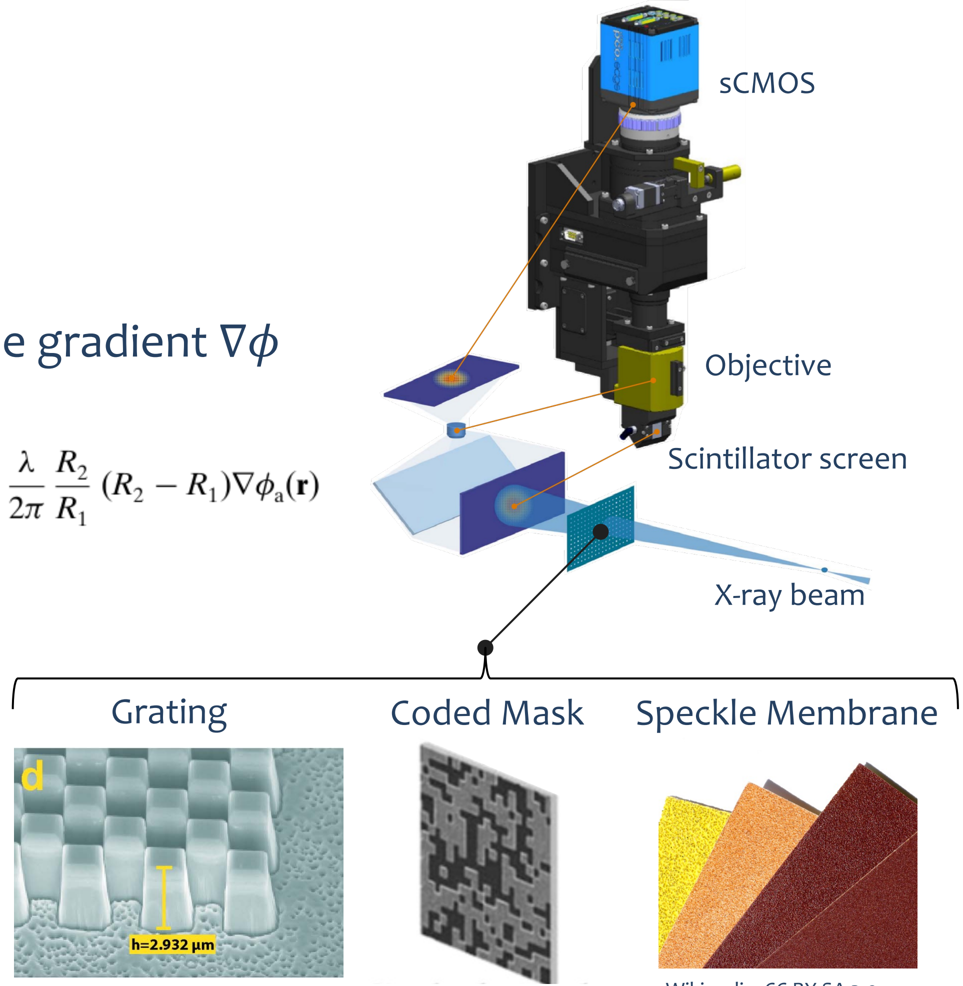
Celestre et al., J. Synchrotron Rad. 29, 629-643 (2022)

Near-field measurements

- Typically based on phase contrast
- Low coherence requirements
- Flat and divergent beams
- Displacement of features **u** ⟶ Phase gradient $\nabla\phi$



$$\mathbf{u}(\mathbf{r}) \simeq \frac{\lambda}{2\pi}\frac{R_2}{R_1}(R_2 - R_1)\nabla\phi_a(\mathbf{r})$$



Wikipedia, CC BY-SA 3.0

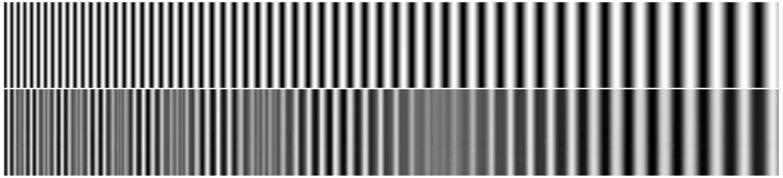
Liu et al., J. Synchrotron Rad. 27(2), 2020
Seaberg et al., J. Synchrotron Rad. 26(4), 2019
Frith et al., Rev. Sci. Instrum. 94(4), 2023
Berujon et al., J. Synchrotron Rad. 22(4), 2015

Near-field measurements

Feature size and contrast on detector depend on:

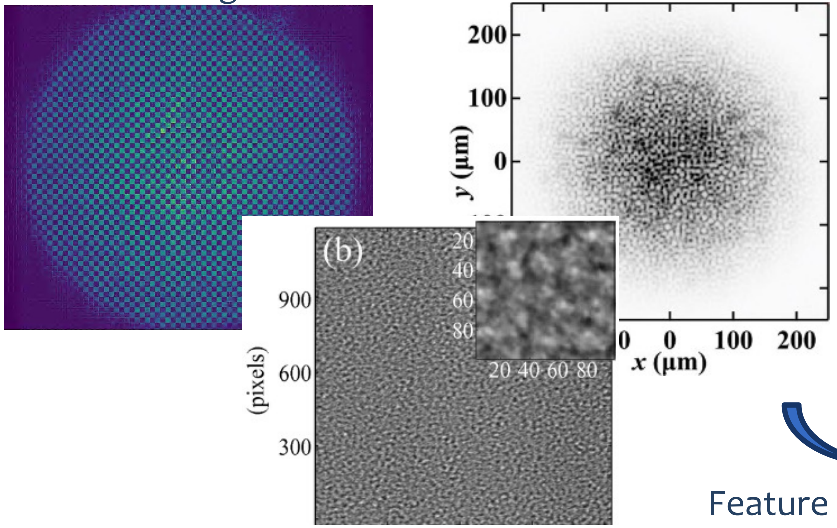
- Pattern feature size
- Pattern feature phase shift
- Pattern – Detector distance

modulation transfer of phase contrast



Grating

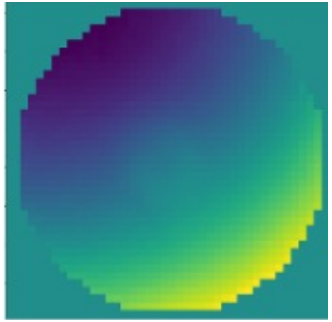
Coded Mask



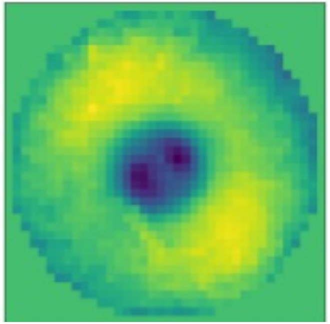
Speckle Membrane

Feature displacement in x/y direction

x/y phase gradient



Phase error

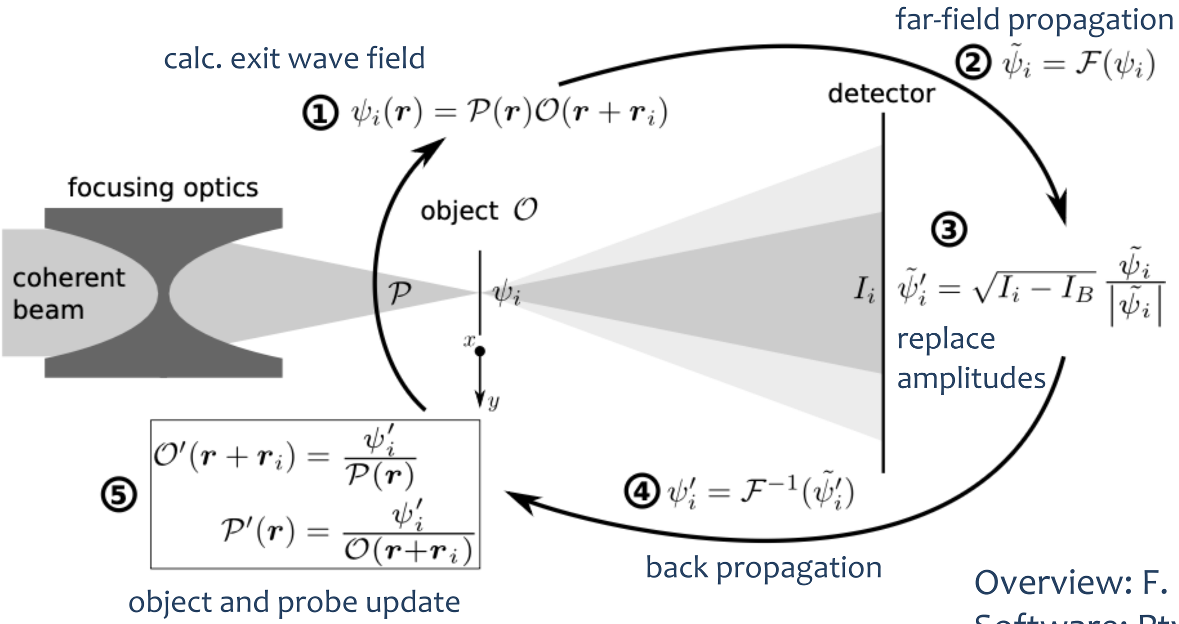


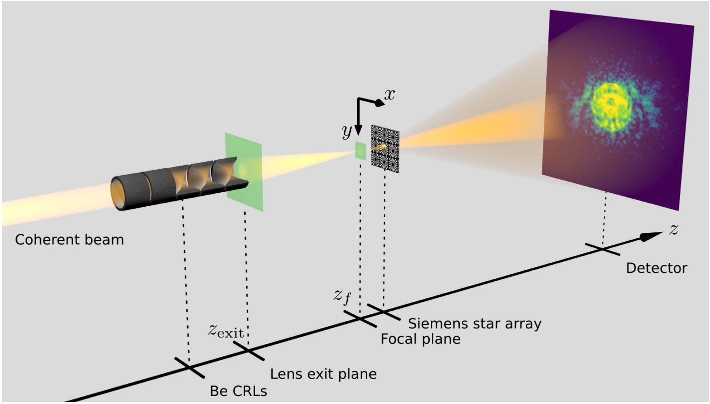
Numerical integration

- least-square minimization
- Fourier transform based

Far-field measurements

- Ptychography: Coherent scanning method, requires a confined beam
- Arbitrary test object: Strong phase shift and diverse feature orientation optimal
- Far-field detector: High dynamic range, low noise, and small pixelsize





Overview: F. Pfeiffer, Nat. Photon. 12(1), 2018
Software: Ptypy, PyNX, PtyLab, CDTools, PtychoShelves, …

Phase plate design

1-2: Wave field retrieval (see slides before): ψ

3:

- Reconstructed wavefield is numerically propagated (Fresnel propagator)

$$\psi_{exit} = \mathbb{K}_{\Delta z}\psi$$

- Removal of spherical wave and other unrelated phase errors (i.e. tilt)

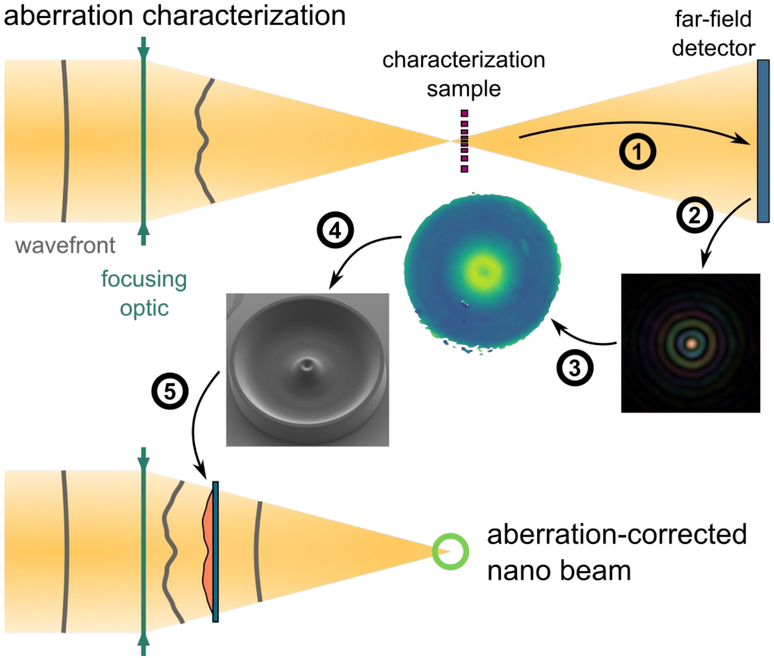
$$\psi_{\varepsilon} = \psi_{exit} e^{-ik(\sqrt{\Delta z^2 + x^2 + y^2} - \Delta z)}$$

4:

- Conversion of phase shift into height profile

$$\arg(\psi_{\varepsilon}) = -\varphi_{PP} = k\delta z_{PP}$$

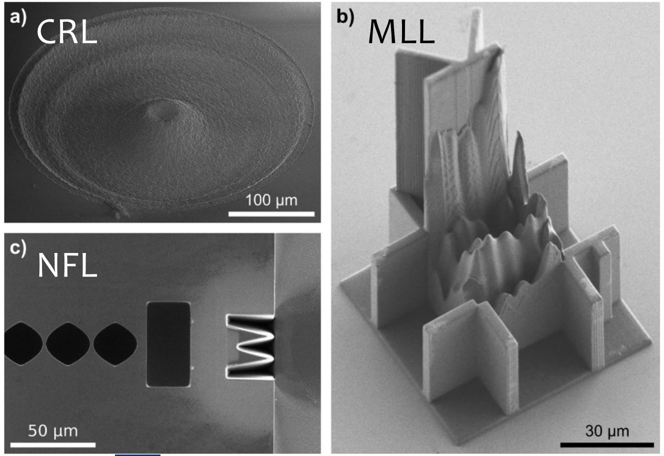
5: Install and align

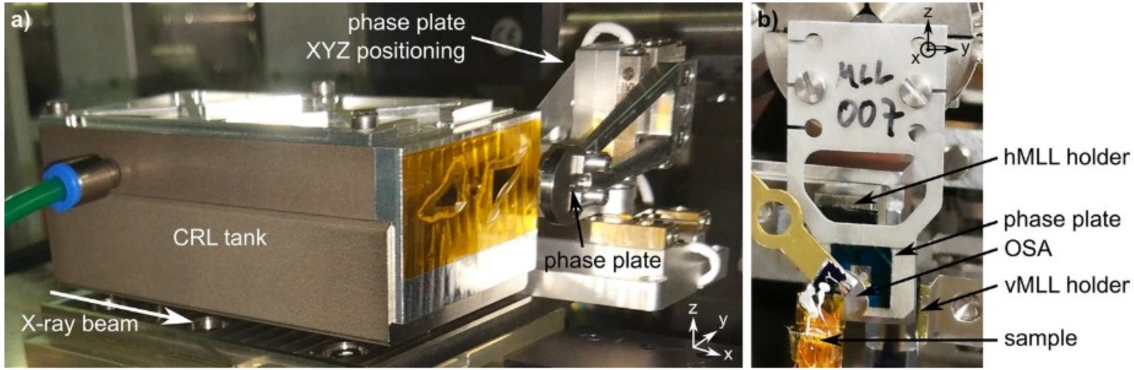


Seiboth, Synchrotron Radiation News, 2022

Alignment…

- Positioning requirements depend on frequency of aberration features
- CRL typical: < 5 µm

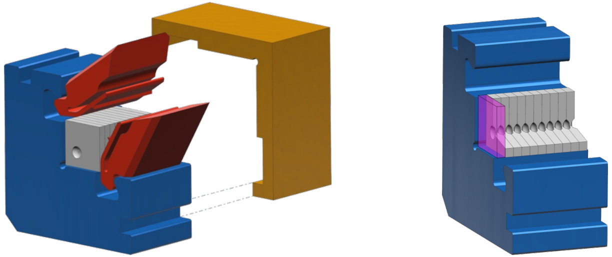




Seiboth, Synchrotron Radiation News, 2022

Pre-aligned, monolithic assembly concept for large-aperture CRLs:

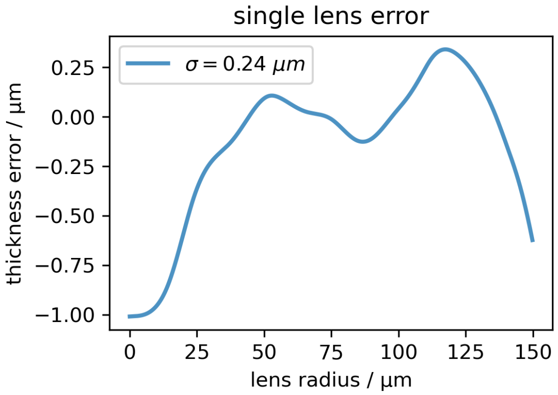
Lens Cube

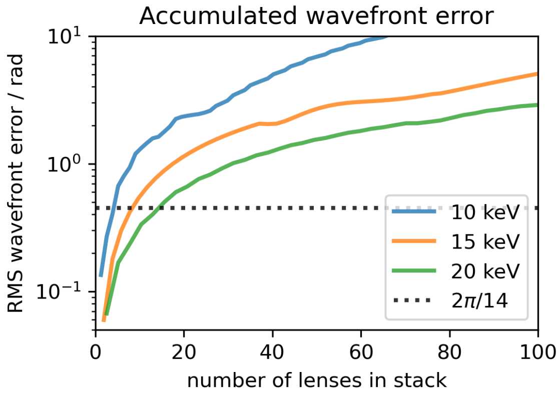


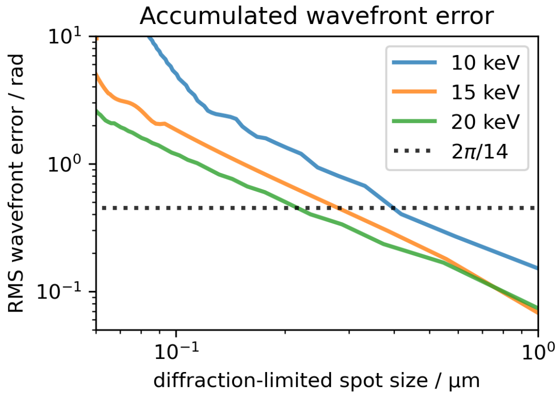
Wang et al., Opt. Express 33(11), 2025

Aberration compensation is required for sub-micron beams

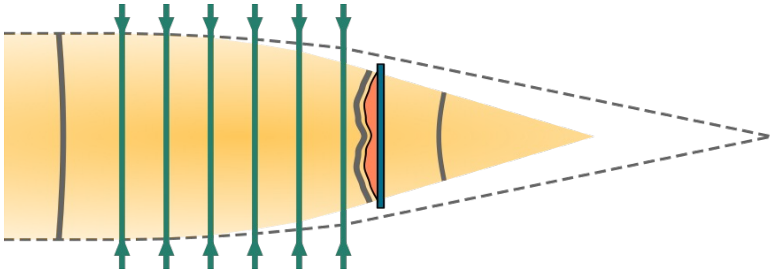
Numerical example with a typical CRL error profile for R = 50 µm / D = 300 µm lenses







Downstream mounted phase plate: Measurement possible, chromatic problems

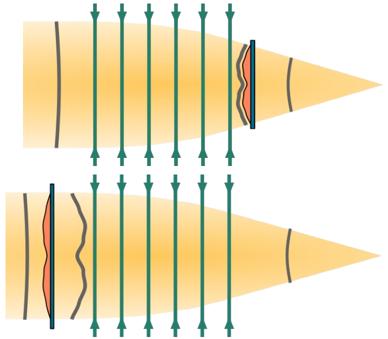


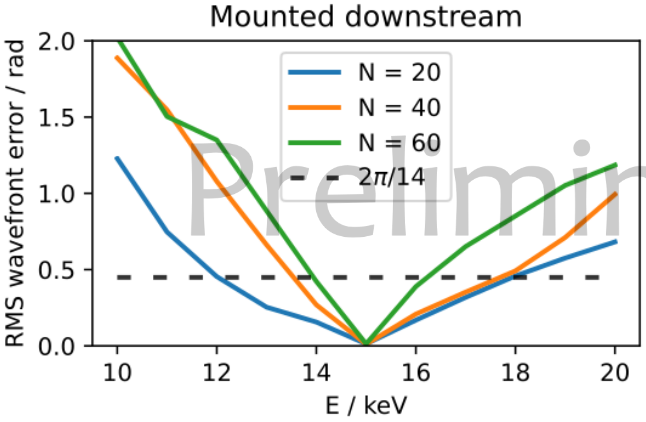
Energy change leads to change in

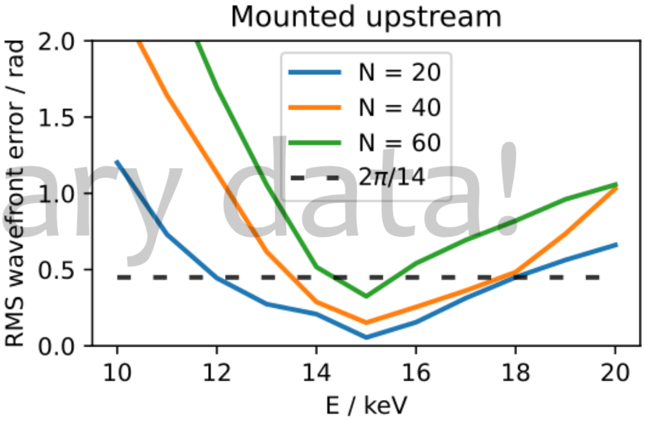
- Beam convergence
- Aberration signature
- Beam size

Behavior of upstream vs. downstream phase plates

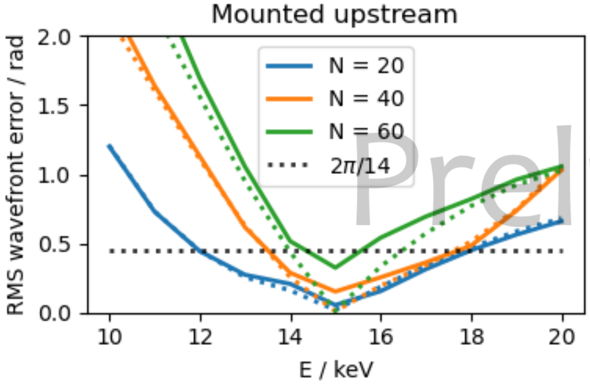
- PP for E_0=15 keV

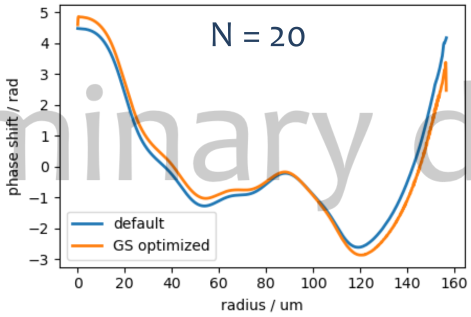


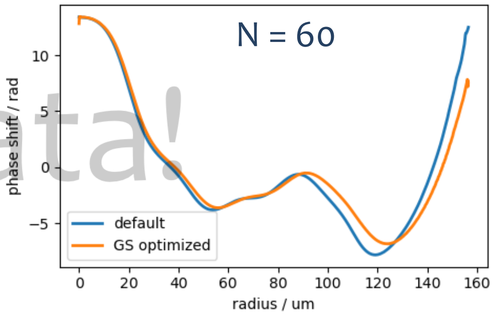




- Upstream phase plate optimized with GS algorithm (dashed lines)



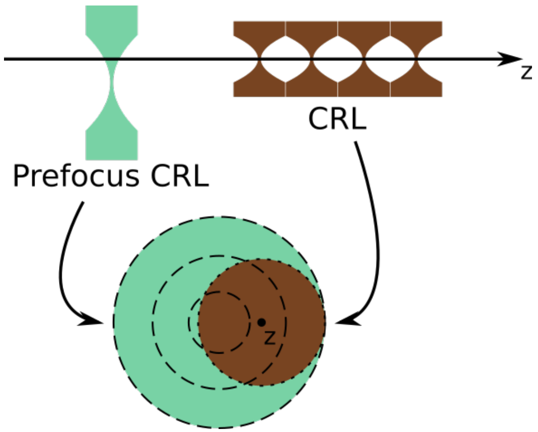


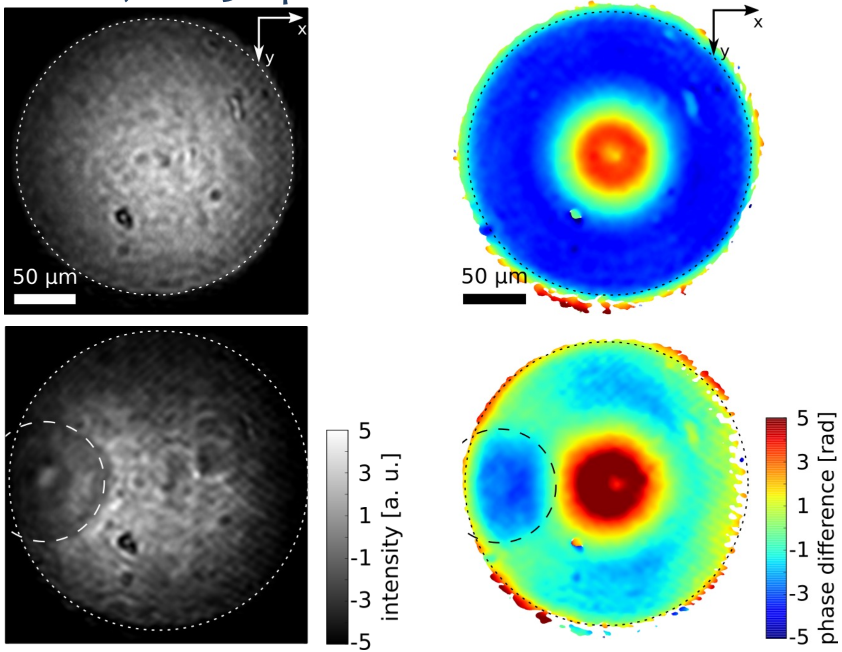


Influence of upstream optics

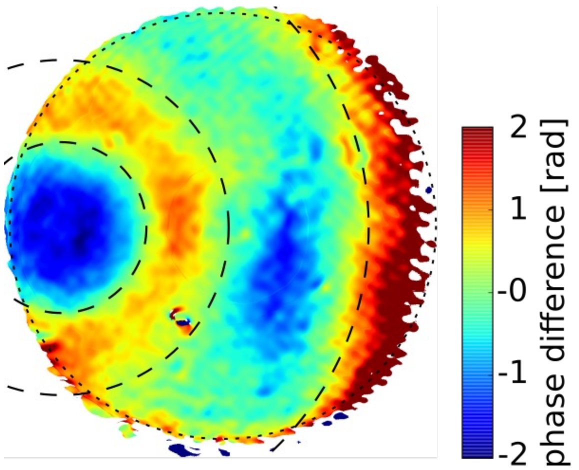
Example for prefocusing at LCLS / MEC

- E = 8.2 keV
- N = 7, R = 500 µm CRLs 4 m upstream
- N = 20, R = 50 µm CRLs





phase difference



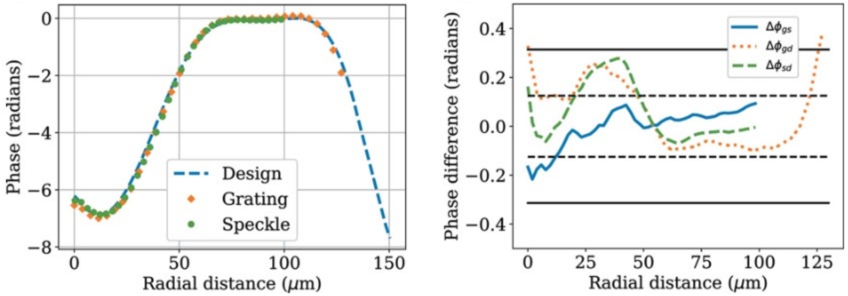
Conclusions

- Analytical calculations give valuable estimations and boundary conditions
- First guess for setting up a beamline on Oasys
- Lens equation applicable to other imaging optics

- Aberrations of a beamline / optical components can be measured by various methods
- Confidence in measurements / results needs to be established

- Alignment is crucial

Questions?



Seaberg et al., J. Synchrotron Rad. 26(4), 2019