Wave-Optical Modeling of Hard X-Ray Transmission Optics

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Wave-Optics of Hard X-Rays

Own code as part of “tomo”-package

- paraxial free-space wave propagation
- arbitrary thin transmission objects
- some thick objects (using parabolic wave equation)
    - refractive lenses
    - volume zone plates
    - waveguides
    - gratings
- partial coherence included by propagation of ensemble of modes
- numerics based on LAPACK and FFTW

Free Propagation of X-Rays

Fresnel-Kirchhoff integral (paraxial approx.):

$$\psi_z(\vec{x},\omega) = -\frac{ie^{ikz}}{2\lambda z}\int \psi_0(\vec{x}',\omega)\cdot \exp\left\{ik\frac{(x-x')^2+(y-y')^2}{2z}\right\}dx'dy'$$

Convolution with integral kernel:

$$K_z(x,y) := -\frac{ie^{ikz}}{2\lambda z}\cdot \exp\left\{ik\frac{x^2+y^2}{2z}\right\}$$

Numerical implementation: (convolution theorem)

$$\tilde{\psi}_0 = FFT(\psi_0) \longrightarrow \tilde{\psi}_z = \tilde{\psi}_0\cdot \tilde{K}_z \longrightarrow \psi_z = IFFT(\tilde{\psi}_z)$$

$$\tilde{K}_{z,\omega}(\vec{\xi}) = e^{ikz}\cdot \exp\left\{-\frac{iz}{2k}\left|\vec{\xi}\right|^2\right\}$$

Far-field: rewrite Fresnel-Kirchhoff-integral

$$\psi_z(\vec{x},\omega) = -\frac{ie^{ikz}}{2\lambda z}\int \psi_0(\vec{x}',\omega)\cdot \exp\left\{ik\frac{(x-x')^2+(y-y')^2}{2z}\right\}dx'dy'$$

phase in exponent:

$$\frac{(x-x')^2+(y-y')^2}{2z} = \frac{x^2+y^2}{2z} - \frac{xx'+yy'}{z} + \frac{x'^2+y'^2}{2z}$$

$\uparrow$ only coords. in target plane (first term)

$\uparrow$ only coords. in source plane (last term)

$$\psi_z(\vec{x},\omega) = -\frac{ie^{ikz}}{2\lambda z}\exp\left\{ik\frac{x^2+y^2}{2z}\right\}\int\left[\psi_0(\vec{x}',\omega)\cdot\exp\left\{ik\frac{x'^2+y'^2}{2z}\right\}\right]\cdot\exp\left\{i\vec{\xi}\vec{x}'\right\}dx'dy'$$

where $\vec{\xi} = \frac{k}{z}\begin{pmatrix} x \\ y \end{pmatrix}$

Transmission Through Thin Object

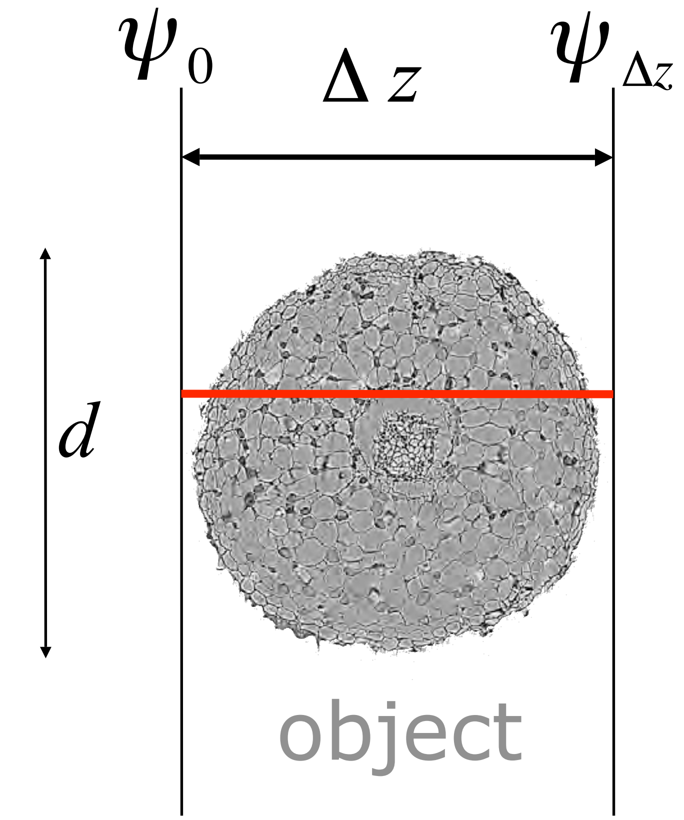
Refraction (elast. scattering), absorption, and attenuation by Compton-scattering described by:

$$n(x,y,z) = 1 - \delta(x,y,z) + i\beta(x,y,z)$$

Thin object:

- no multiple scattering (1. Born approx.)
- no propagation effects inside object

$$\psi_{\Delta z}(x,y) = T_{\Delta z}(x,y) \cdot \psi_0(x,y)$$

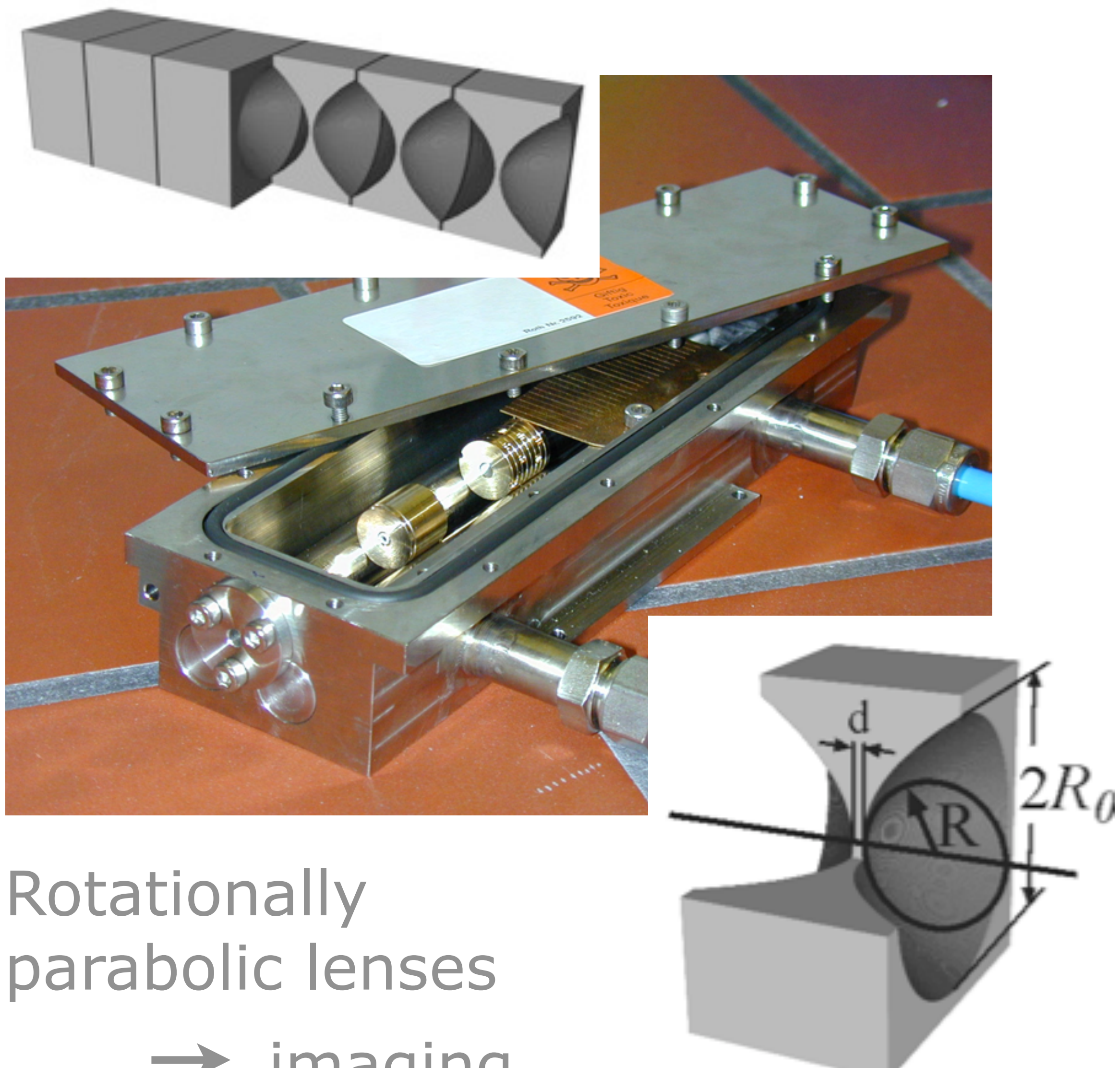


Transmission function:

$$T_{\Delta z}(x,y) = e^{ik\int n dz} = e^{ik\Delta z} \cdot e^{-ik\int \delta dz} \cdot e^{-k\int \beta dz}$$

Transmission Optic: Refractive X-Ray Lenses

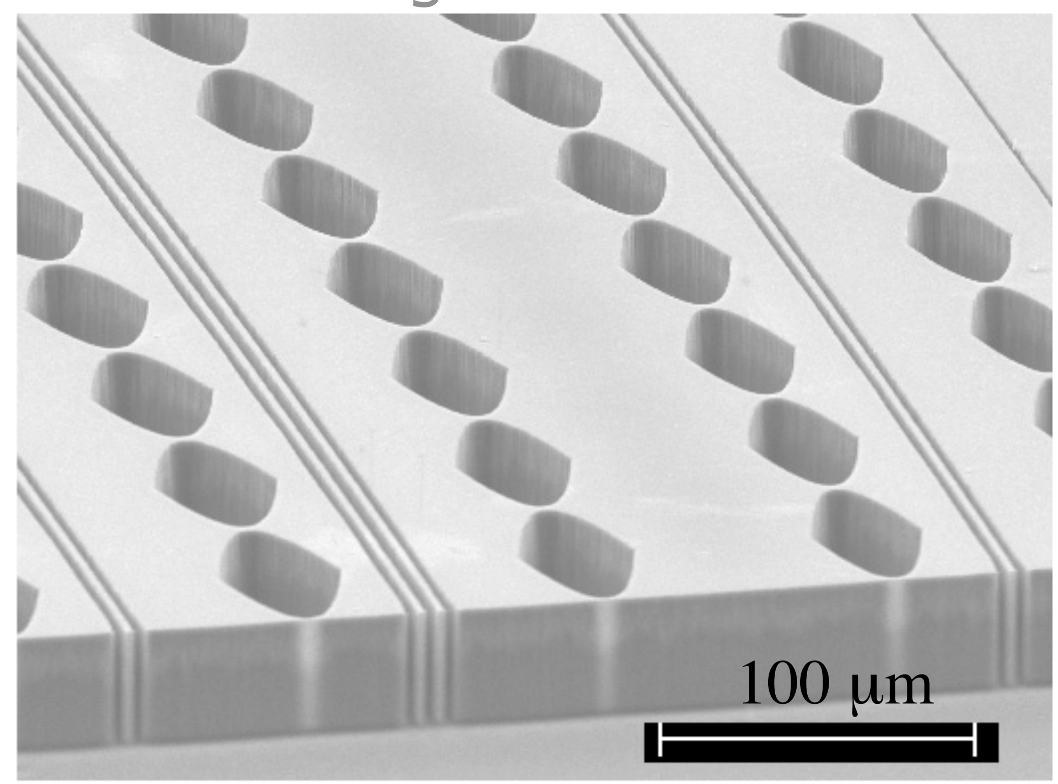
Many different realizations, e. g.:



Rotationally parabolic lenses

→ imaging

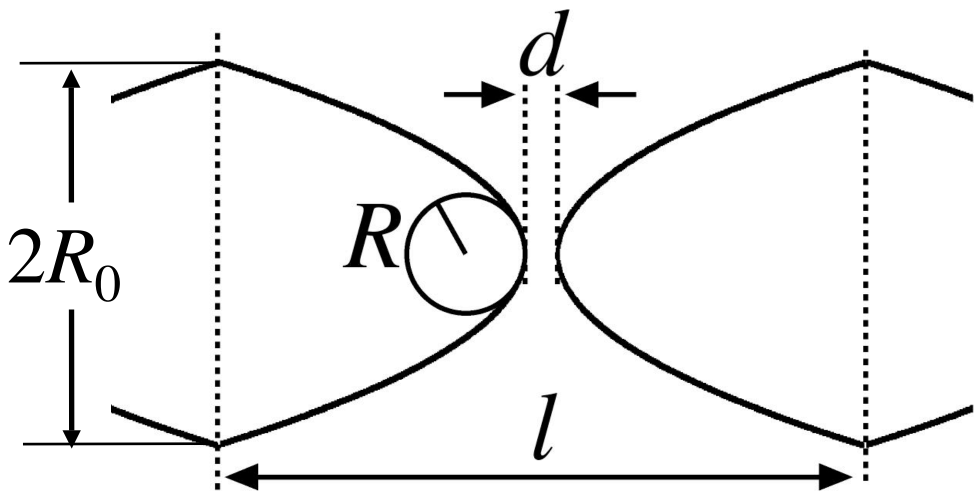
Nanofocusing lenses



Short focal length:

- large demagnification small image
- large numerical aperture small diffraction limit

Single Lens:



$$f_s = \frac{R}{2\delta}, \quad \delta \approx 10^{-6}$$

at 10 keV

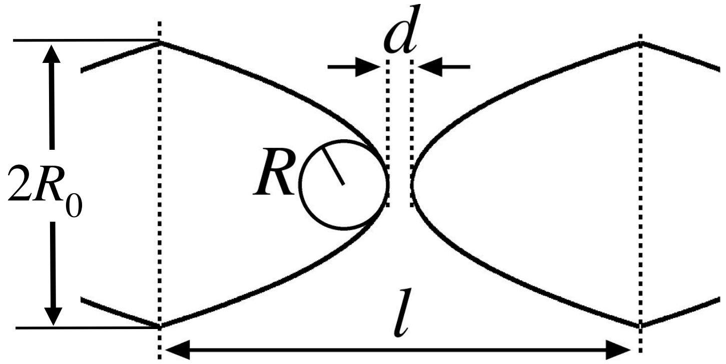
Focal length 10^6 times longer than *R*

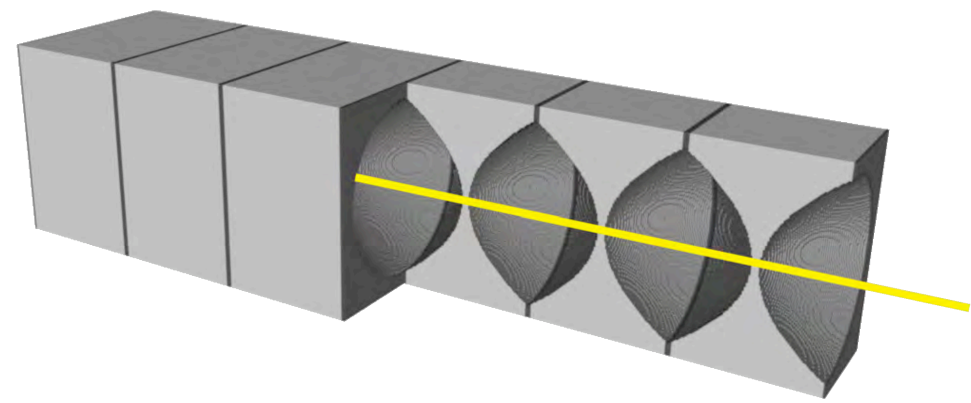
Inside single lens:

- CRL: deviations from straight line: ~ 5 µrad
  thickness *l* = 1 mm: deviation ~ 5 nm
- NFL: deviations from straight line: ~ 10 µrad
  thickness *l* = 85 µm: deviation ~ 1 nm

→ single lens is thin!!

Transmission Through Single Lens





Wave field behind lens:

$$\psi_l = \underbrace{e^{-ik2N\delta\frac{r^2}{2R}}}_{=:1)} \cdot \underbrace{e^{-\mu N\frac{r^2}{2R}}}_{=:2)} \cdot \underbrace{e^{-ikN\delta d}}_{=:3)} \cdot \underbrace{e^{-\frac{\mu N}{2}d}}_{=:4)} \cdot \underbrace{e^{-ikNl}}_{=:5)} \cdot \psi_0$$

1) curvature of wave front
2) Gaussian attenuation of amplitude
3) constant phase shift by lens material of material between apices of parabolas
4) constant attenuation of material between apices
5) phase shift through free propagation

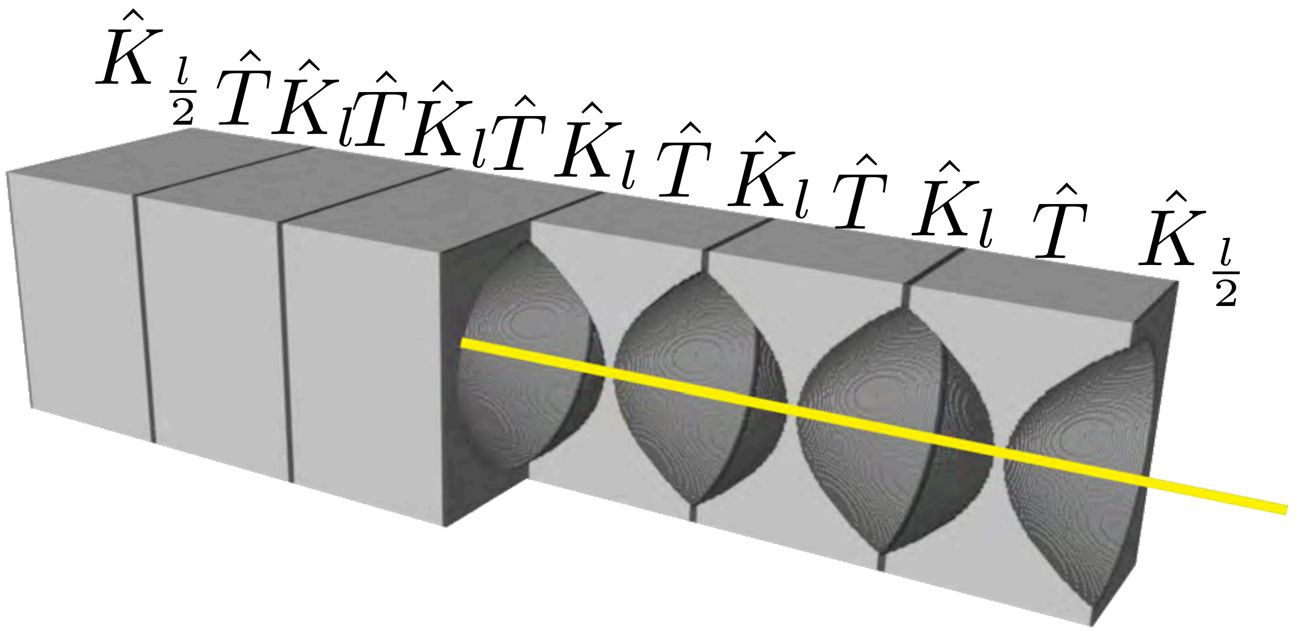
Refractive X-Ray Lens: Wave Optical Picture

Stack of individual lenses:

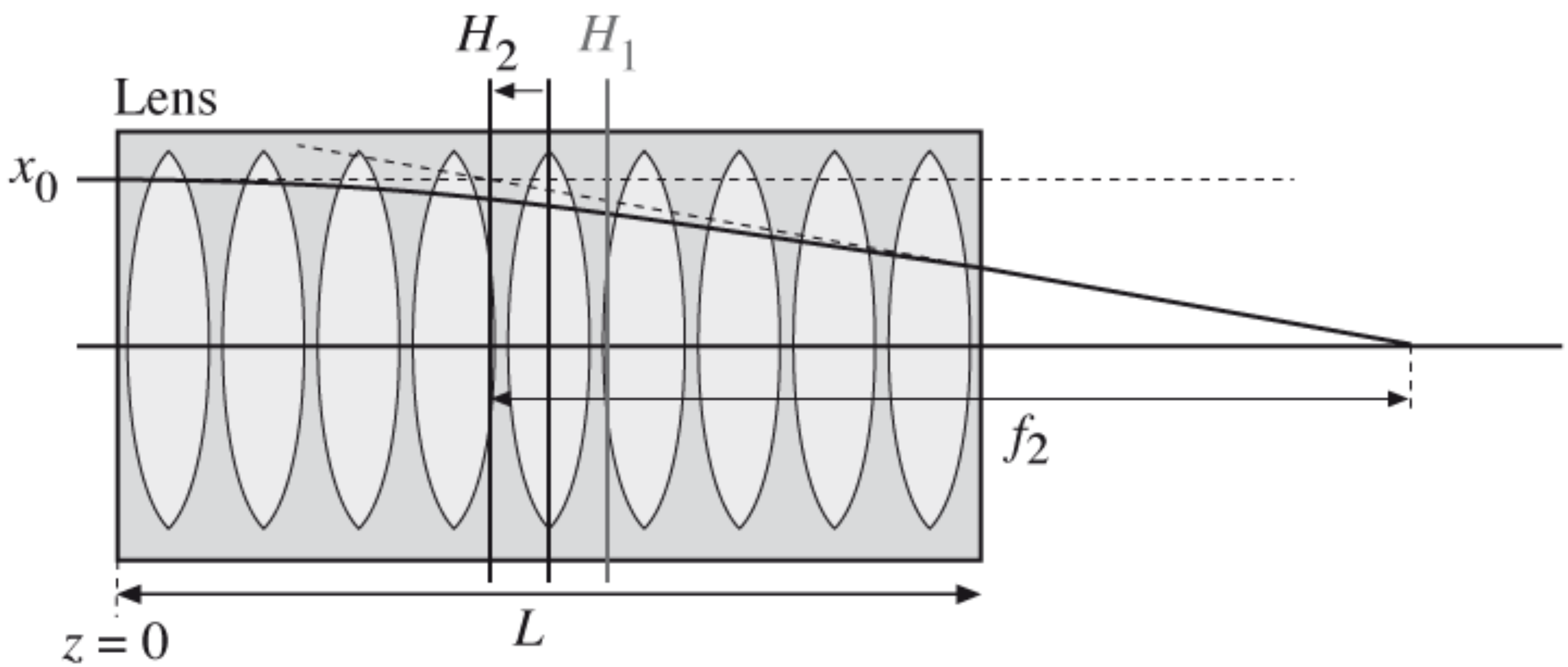
⟶ alternating transmission and propagation

$$\hat{T}_{\text{lens}} = \hat{K}_{\frac{l}{2}} \prod_{i=2}^{N} \left(\hat{T}\hat{K}_l\right) \hat{T}\hat{K}_{\frac{l}{2}}$$

Ordered product of transmission and propagation operators



Thick Refractive X-Ray Lens



$$\omega = \sqrt{\frac{1}{f_e l}}$$

$$f_2 = \frac{r_0}{r'(L)} = \frac{1}{\omega \sin(\omega L)}$$

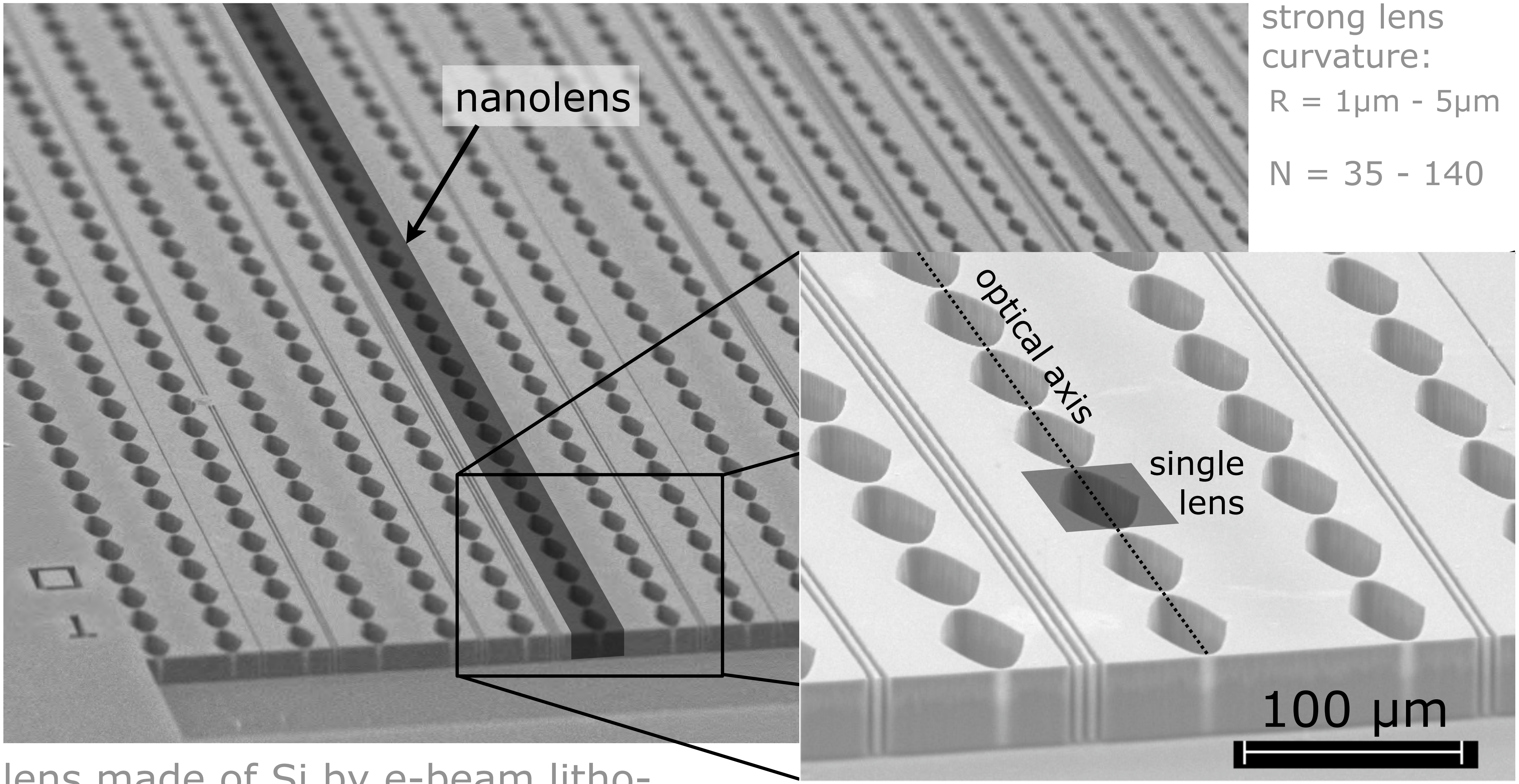
$$r(z) = r_0 \cdot \cos(\omega z),$$

$$r'(z) = -r_0 \omega \sin(\omega z)$$

$$H_2 = \frac{L}{2} - \frac{1 - \cos(\omega L)}{\omega \sin(\omega L)}$$

Schroer, professorial dissertation (2003)
V. Kohn, J. Exp. Theo. Phys. **97**, 204 (2003)

Nanofocusing Lenses (NFLs)



strong lens curvature:

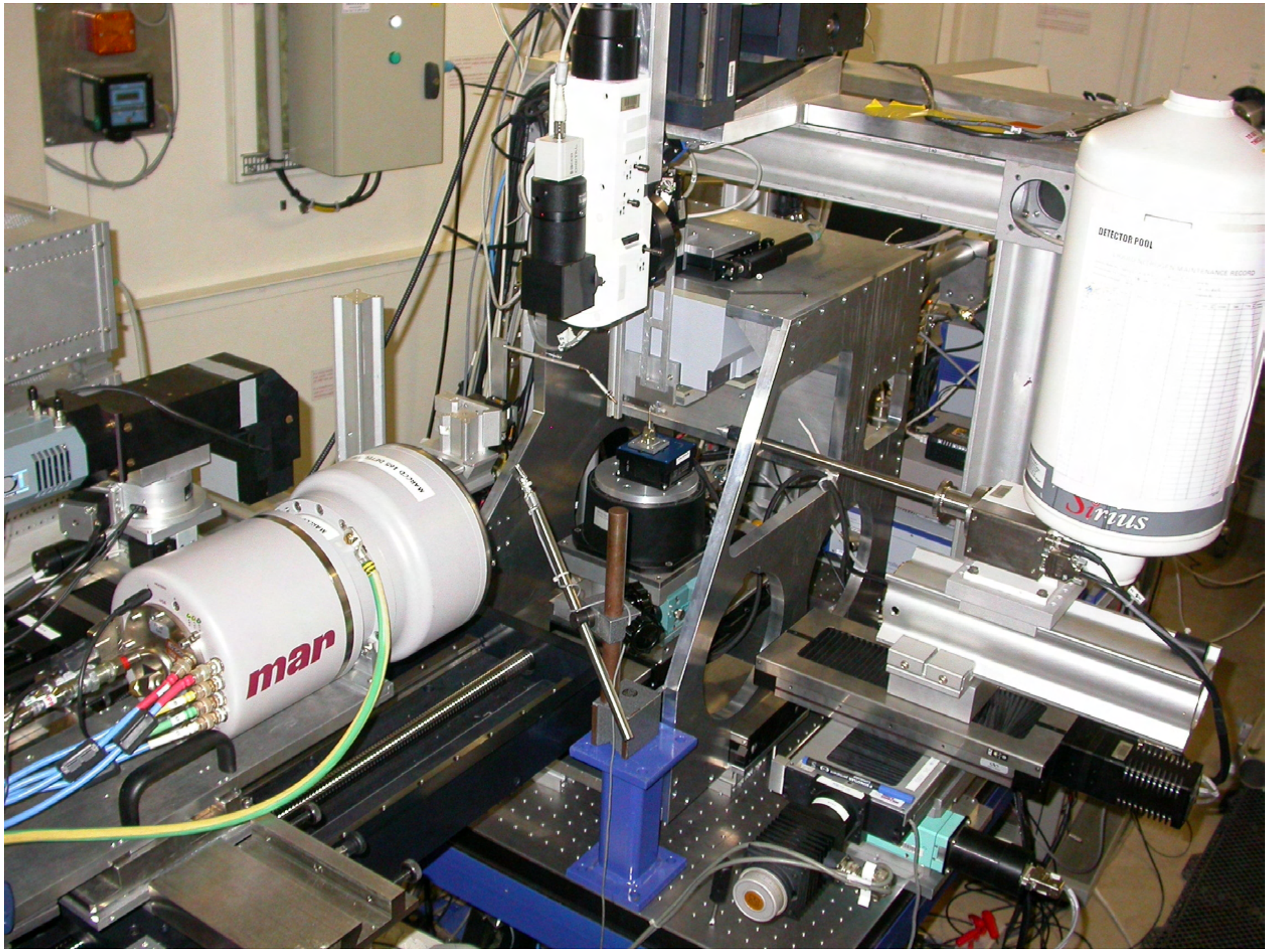
R = 1µm - 5µm

N = 35 - 140

lens made of Si by e-beam litho-graphy and deep reactive ion etching!

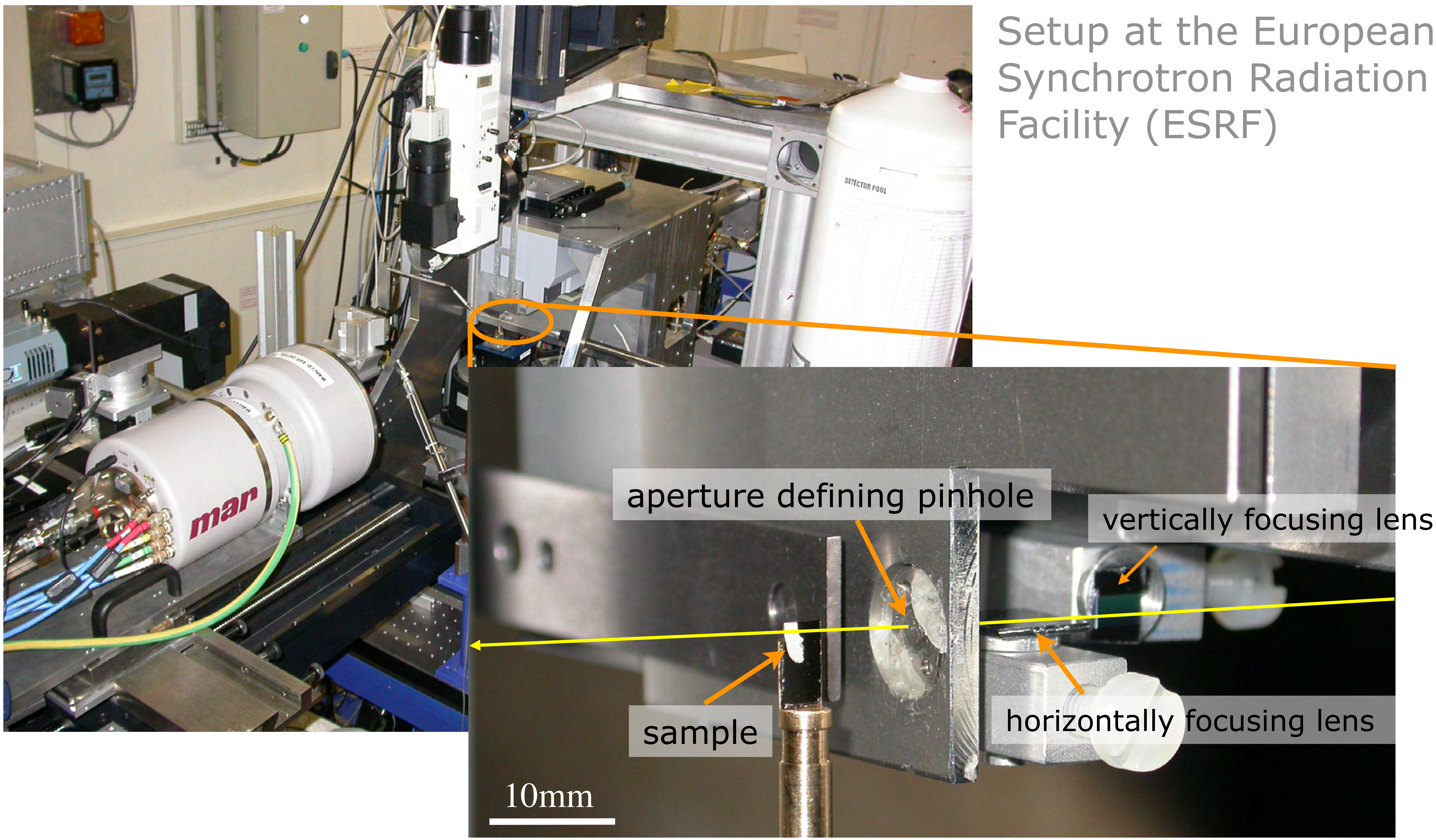
APL 82, 1485 (2003)

Crossed Nanofocusing Lenses



Setup at the European Synchrotron Radiation Facility (ESRF)

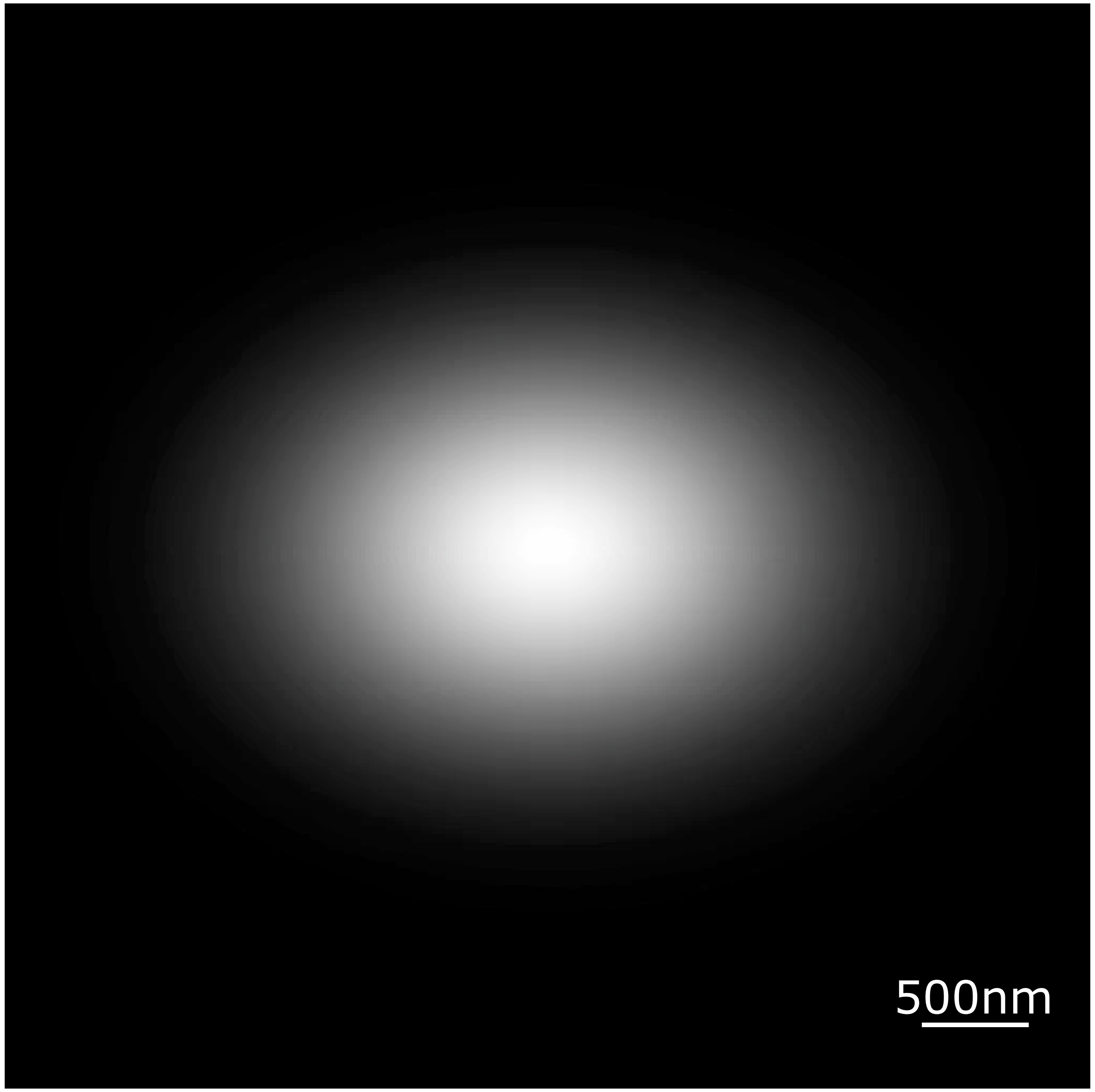
Crossed Nanofocusing Lenses



Setup at the European Synchrotron Radiation Facility (ESRF)

Ideal Parabolic NFL

Gaussian aperture:



Parabolic lens shape:

Gaussian transmission

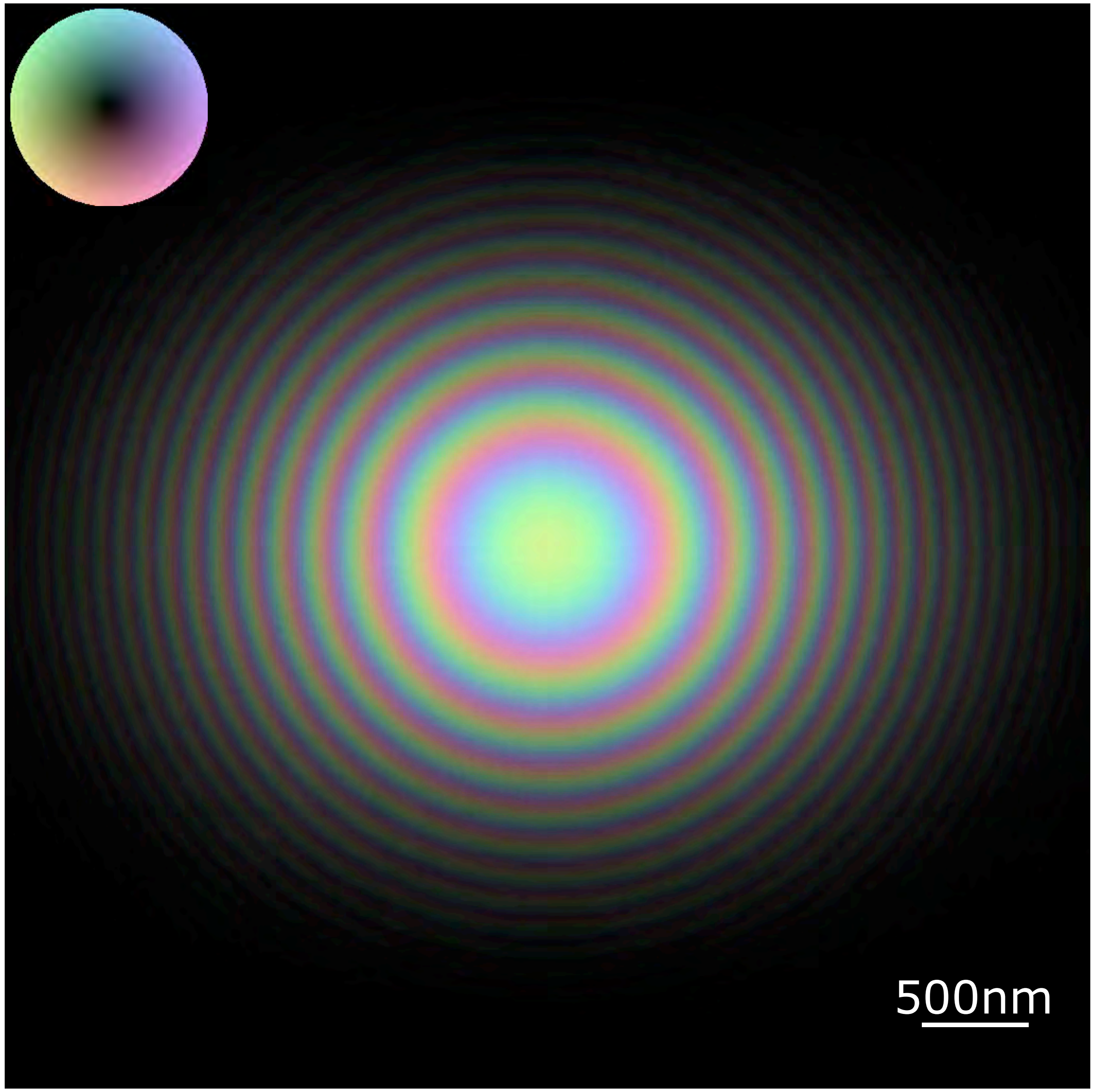
horiz. f = 13.2 mm
vert. f = 22.7 mm

$$NA \propto \frac{1}{\sqrt{f}}$$

NA in horiz. direction bigger than in vert. direction

Ideal Parabolic NFL

Gaussian amplitude:



X-ray microscopy with Gaussian beam:

For a given microbeam:

Focus size depends on contrast mechanism:

- fluorescence: intensity
- diffraction: amplitude

focus for diffraction is $\sqrt{2}$ times bigger than for fluorescence

(phase color coded)

Coherence in Focused Beam

Coherent diffraction imaging:

Lateral coherence length must exceed

- sample size or
- beam size

Mutual intensity function

$$J(r, r') = \langle E(r,t) \cdot E^*(r',t) \rangle_t$$

for monochromatic beam

for

- Gaussian chaotic source (approximation)
- propagation to lens (van Cittert-Zernike)
- transmission through lens
- propagation to focus

Mutual Intensity in Focus

$$J(r,r') = A \cdot e^{-\frac{r^2+r'^2}{2\cdot\sigma_b^2}} \cdot e^{-\frac{(r-r')^2}{2\cdot\sigma_{\mathrm{coh}}^2}}$$

$$\sigma_b = \sqrt{2\sigma_{b_{\mathrm{geo}}}^2 + 2\sigma_t^2}$$

$$\sigma_{\mathrm{coh}} = 2\sigma_t\sqrt{1 + \frac{\sigma_t^2}{\sigma_{b_{\mathrm{geo}}}^2}}$$

↓ FWHM

Focus size (amplitude)

$$b_{\mathrm{ampl}} = \sqrt{2b_{\mathrm{geo}}^2 + 2d_t^2}$$

↓ FWHM

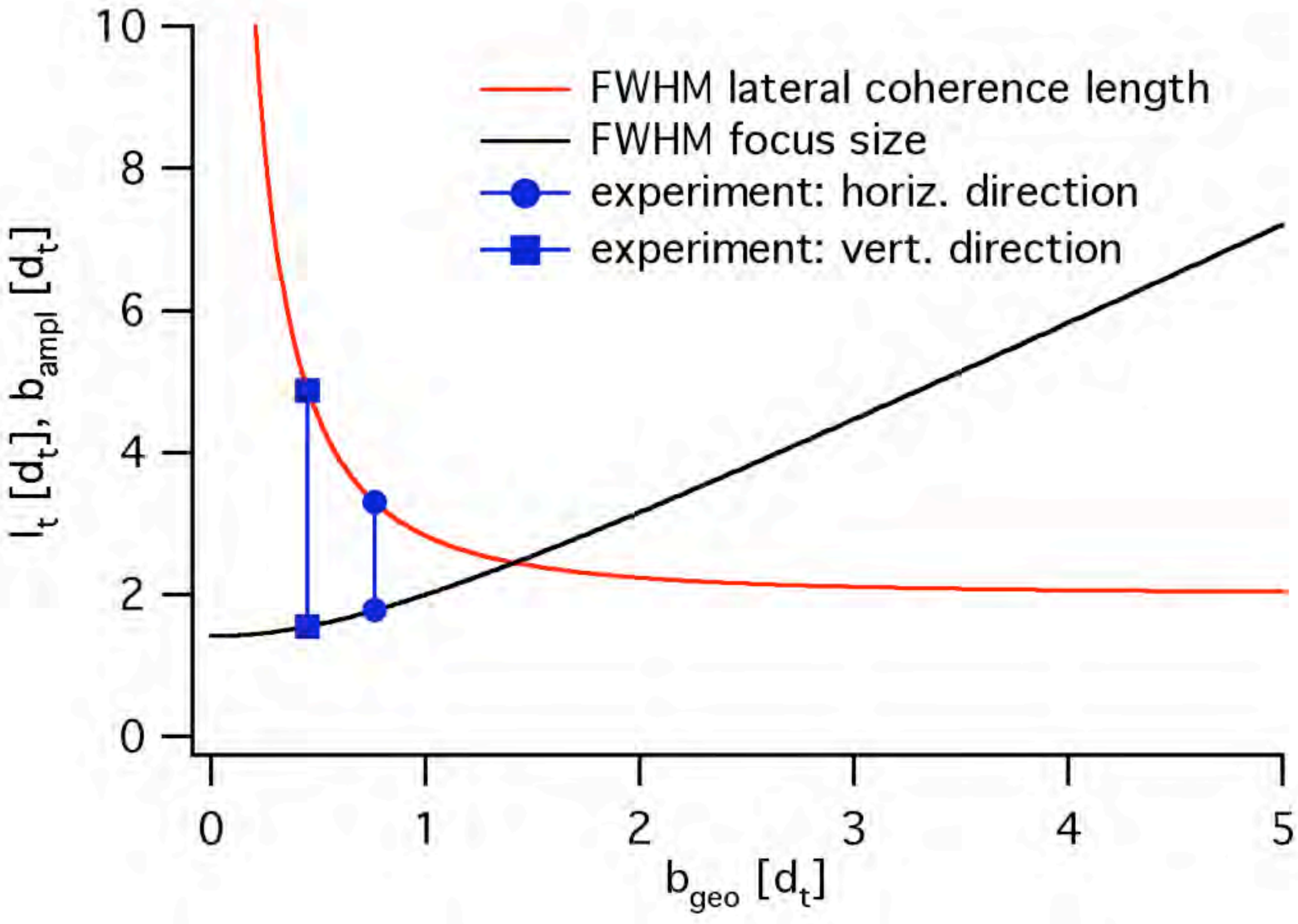
lateral coherence length in focus

$$l_t = 2d_t\sqrt{1 + \frac{d_t^2}{b_{\mathrm{geo}}^2}}$$

geometic image of source → b_{geo}^2

Airy disc size → d_t^2

Coherence in Focus



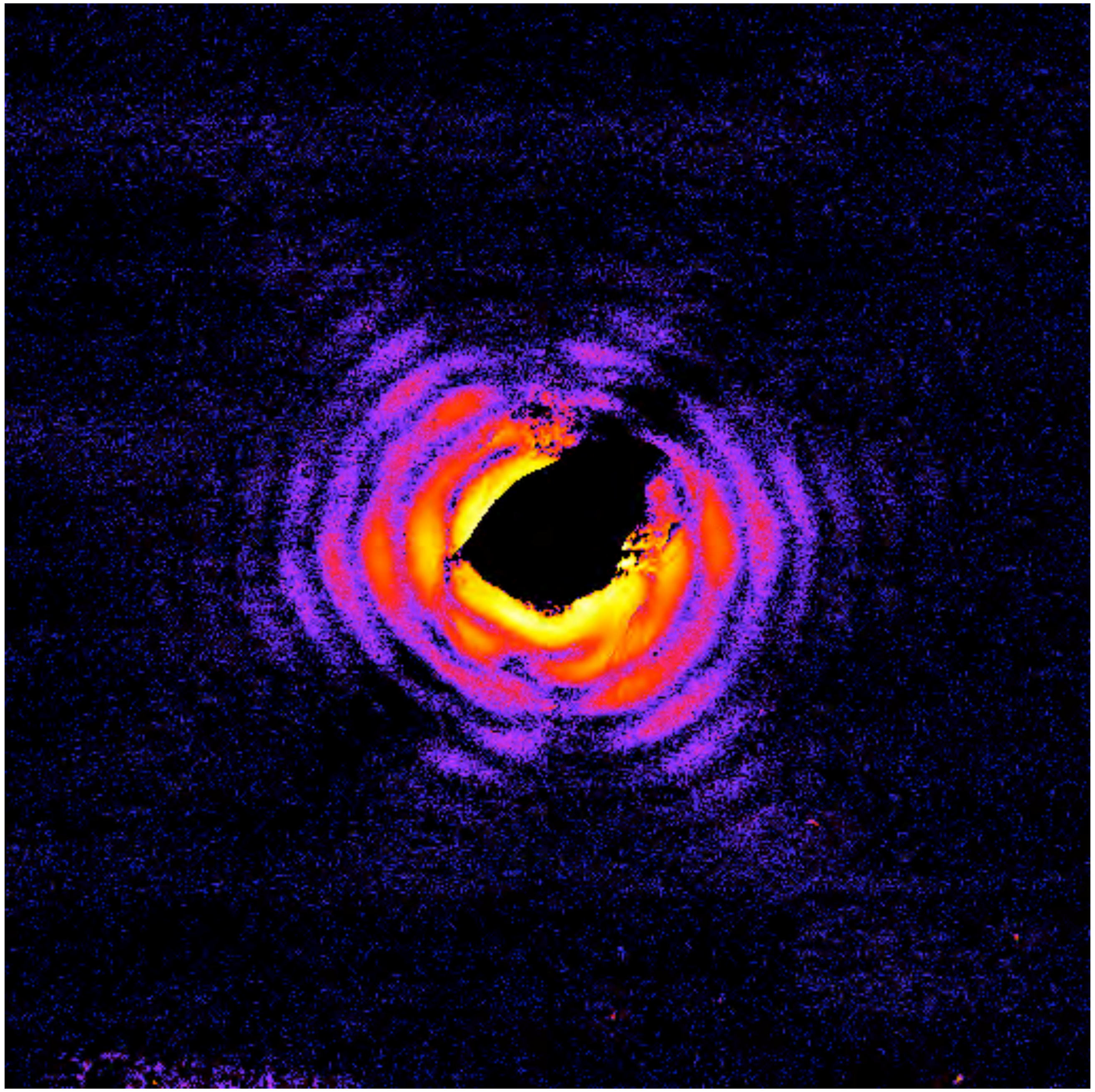
Focus size (amplitude):

$$b_{\mathrm{ampl}} = \sqrt{2b_{\mathrm{geo}}^2 + 2d_t^2}$$

lateral coherence length:

$$l_t = 2d_t\sqrt{1 + \frac{d_t^2}{b_{\mathrm{geo}}^2}}$$

Diffraction Pattern of Gold Nanoparticle



sample-detector distance:

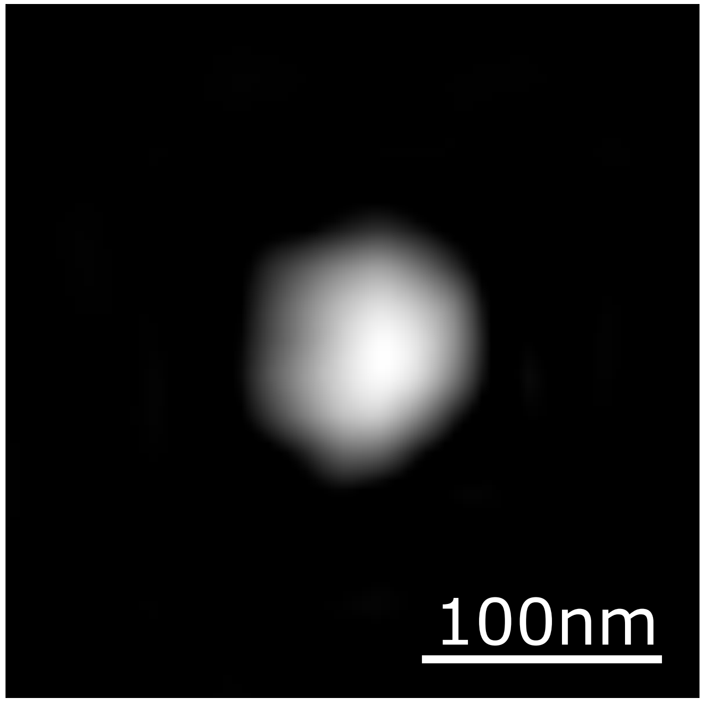
1250 mm (in air)

detector: FReLoN 4M

50µm pixel size

exposure time: 10 x 60 s

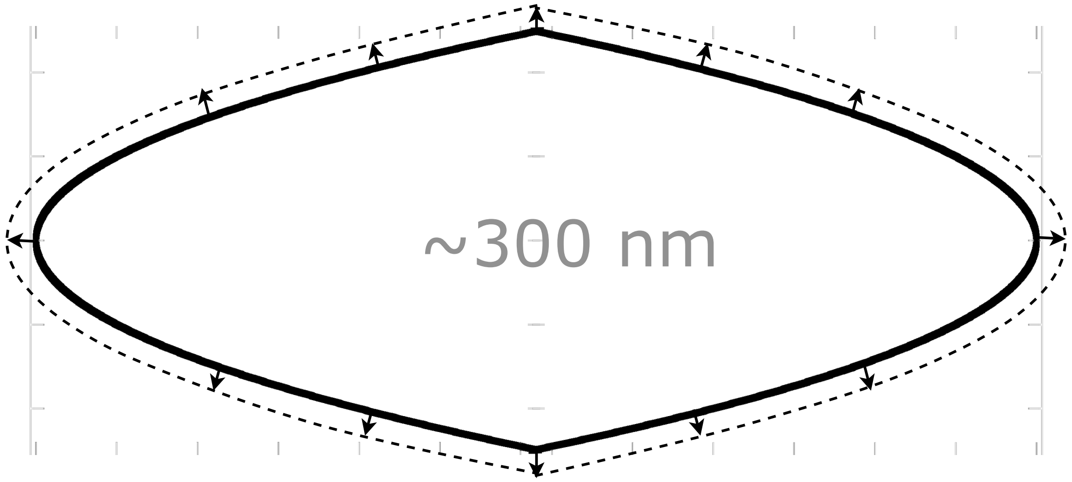
Reconstruction:



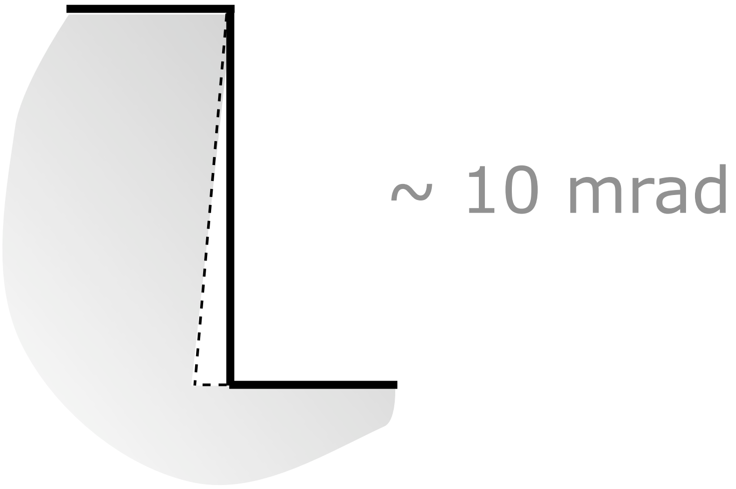
PRL **101**, 090801 (2008)

So Far: No Ideal Lens...

Shape errors:
Underetching & proximity effect:

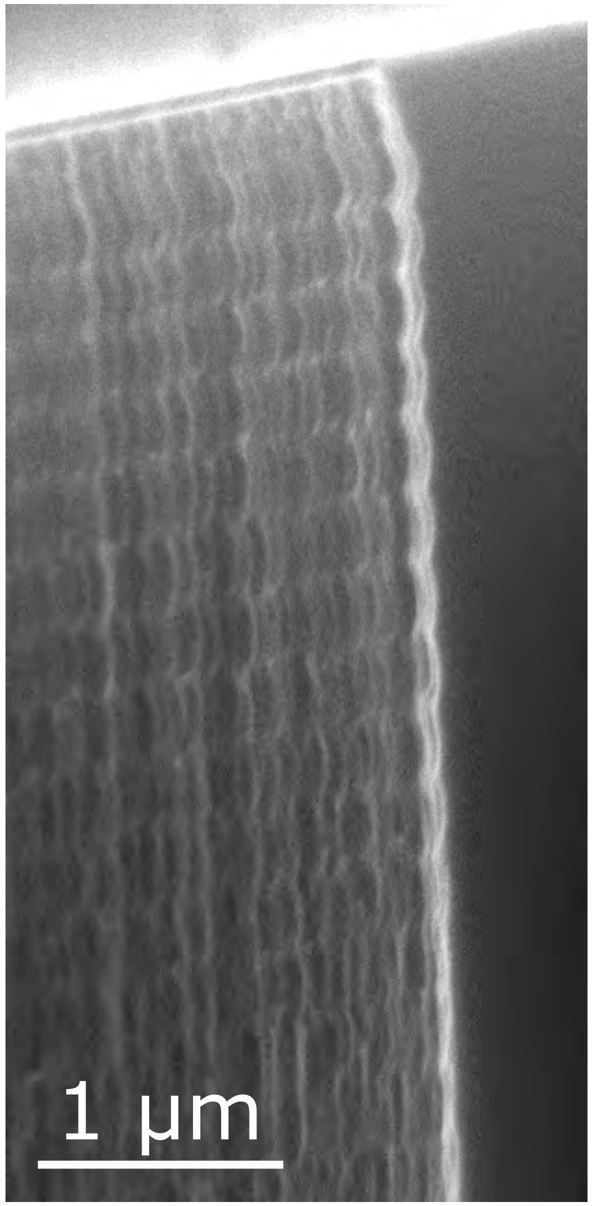


deviation from parabola

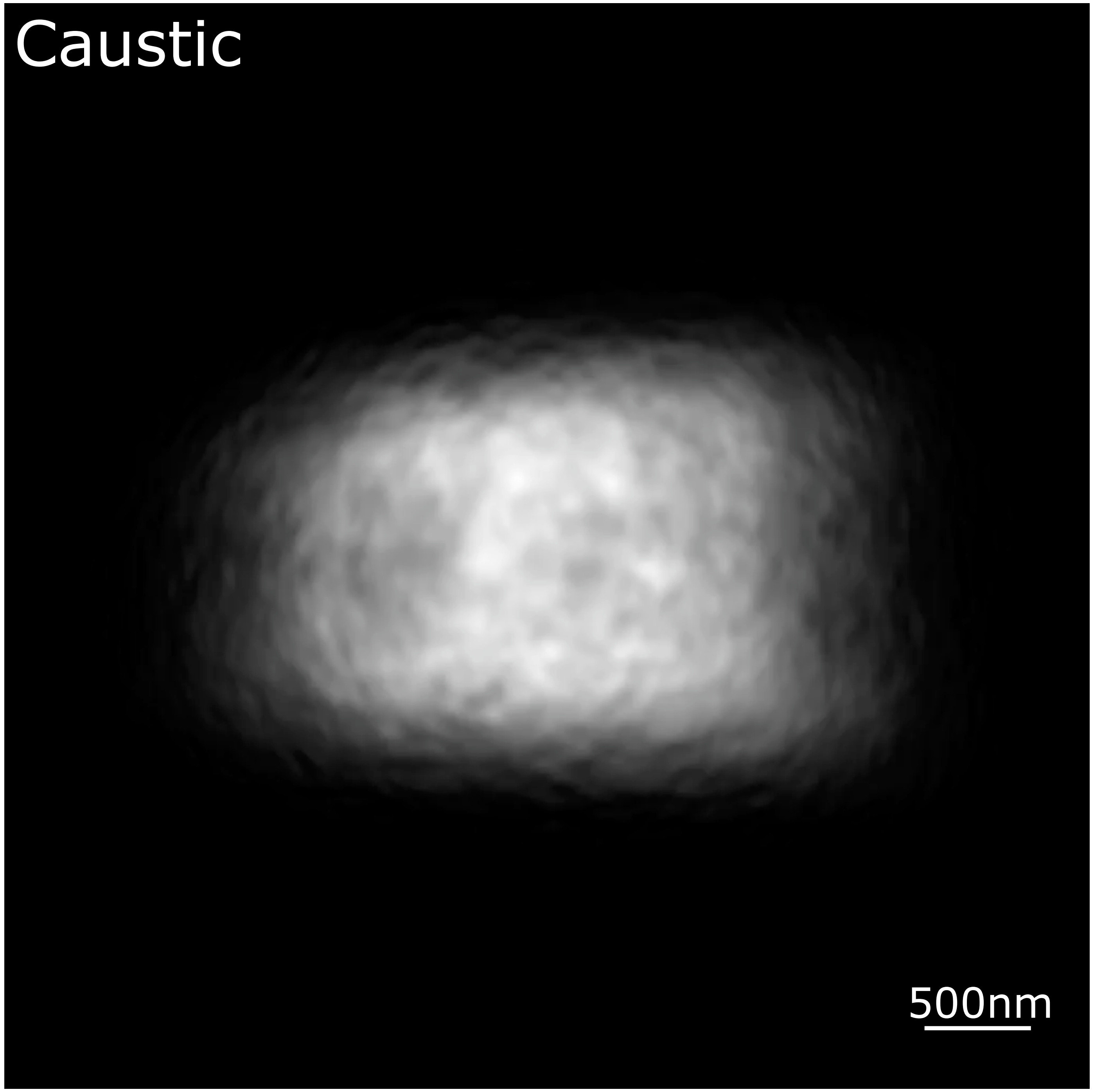


tilted side wall

Roughness:



Numerical Model of Nanoprobe

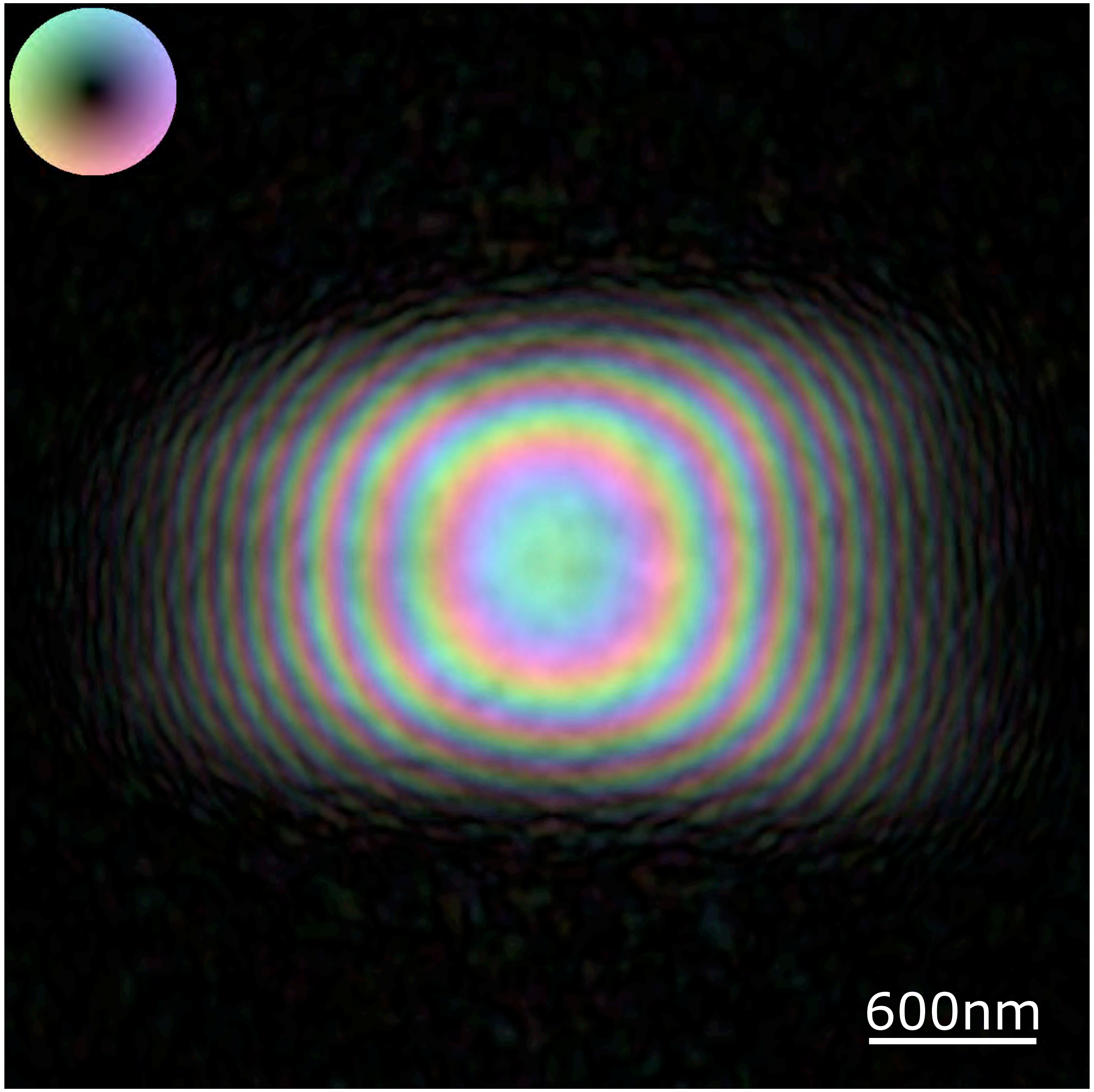


Includes:

- underetching
- tilted side walls
- roughness
- periodic structures

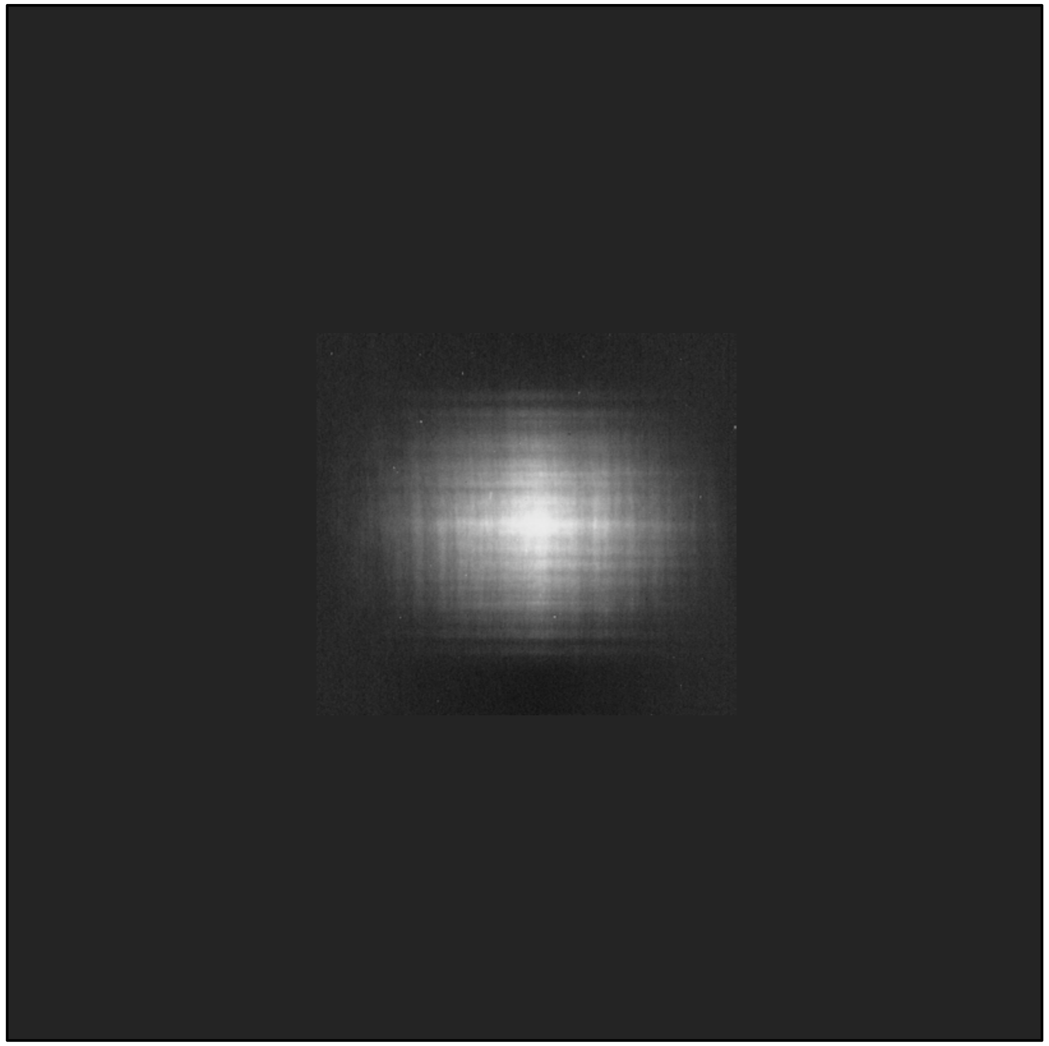
Parameters deduced from beam shape in far field.

Complex Amplitude in Focused Beam

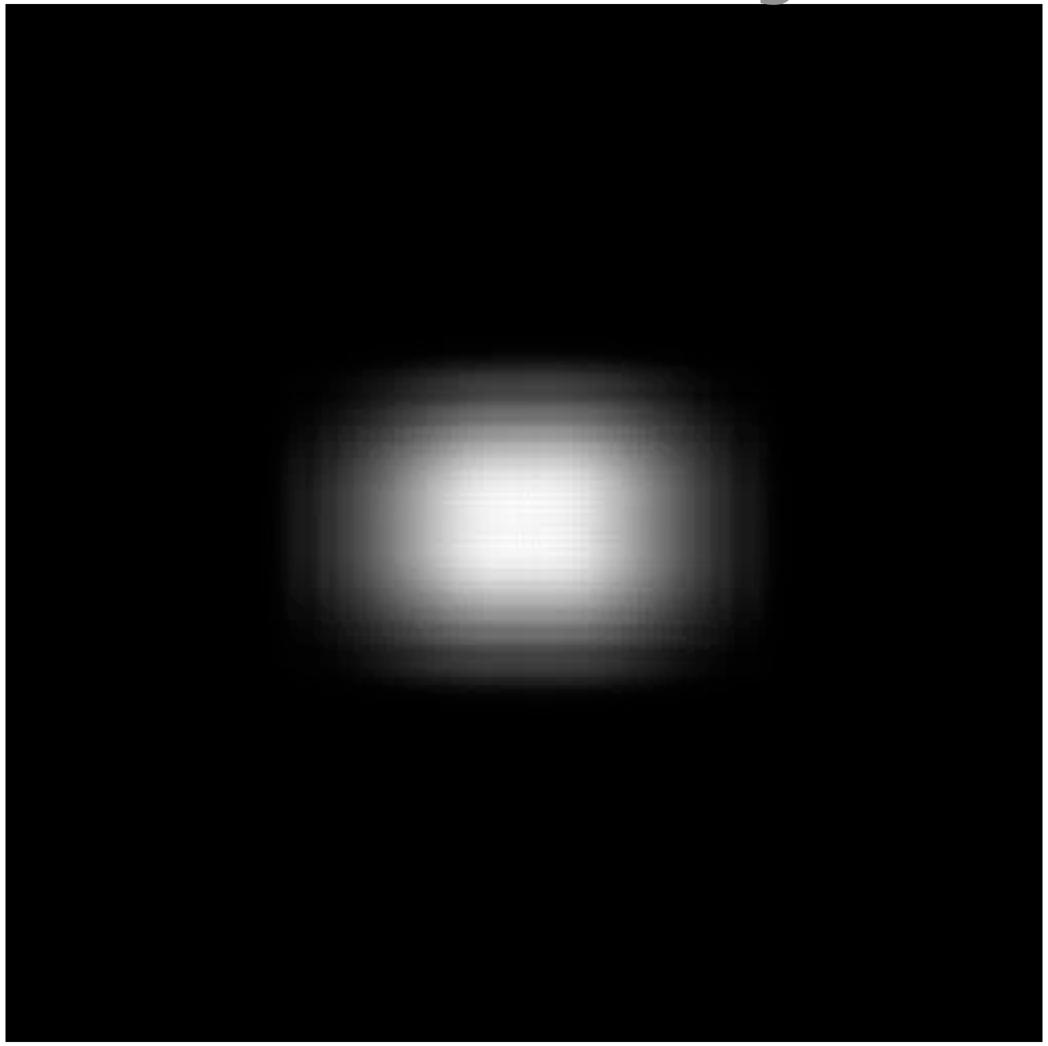


Wave Front: Focusing with Aberrations

Measured farfield

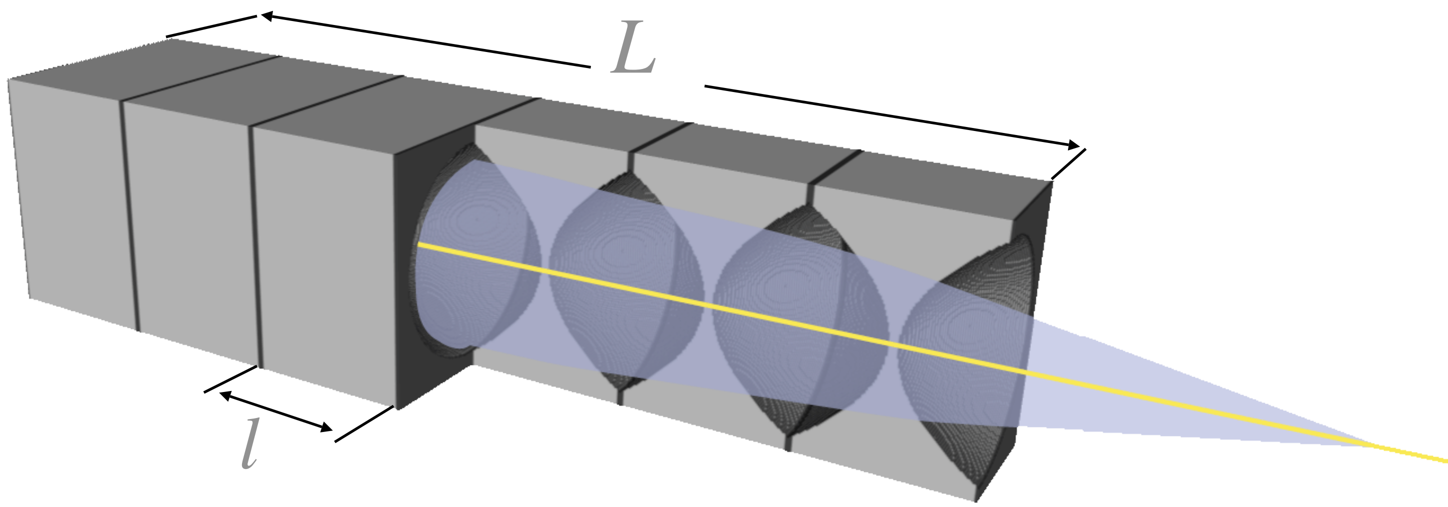


Numerical modeling



Effective Aperture and Diffraction Limit

Nanofocusing lens:



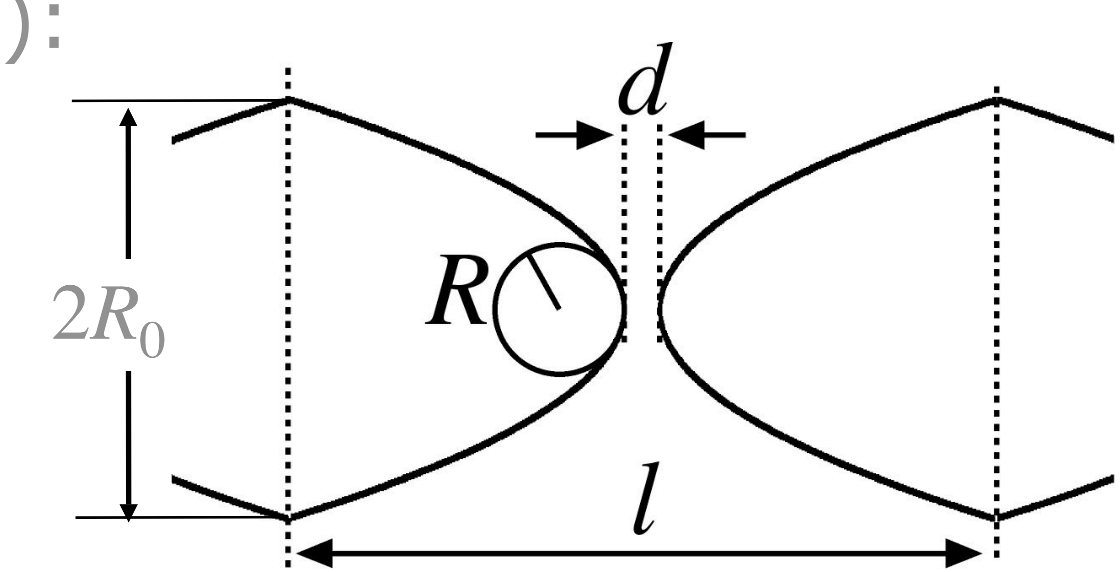
$$f_{min} = \sqrt{f_0 L} = \sqrt{\frac{Rl}{2\delta}}$$

with $f_0 = \frac{R}{2N\delta}$

lens short (attenuation negligible):

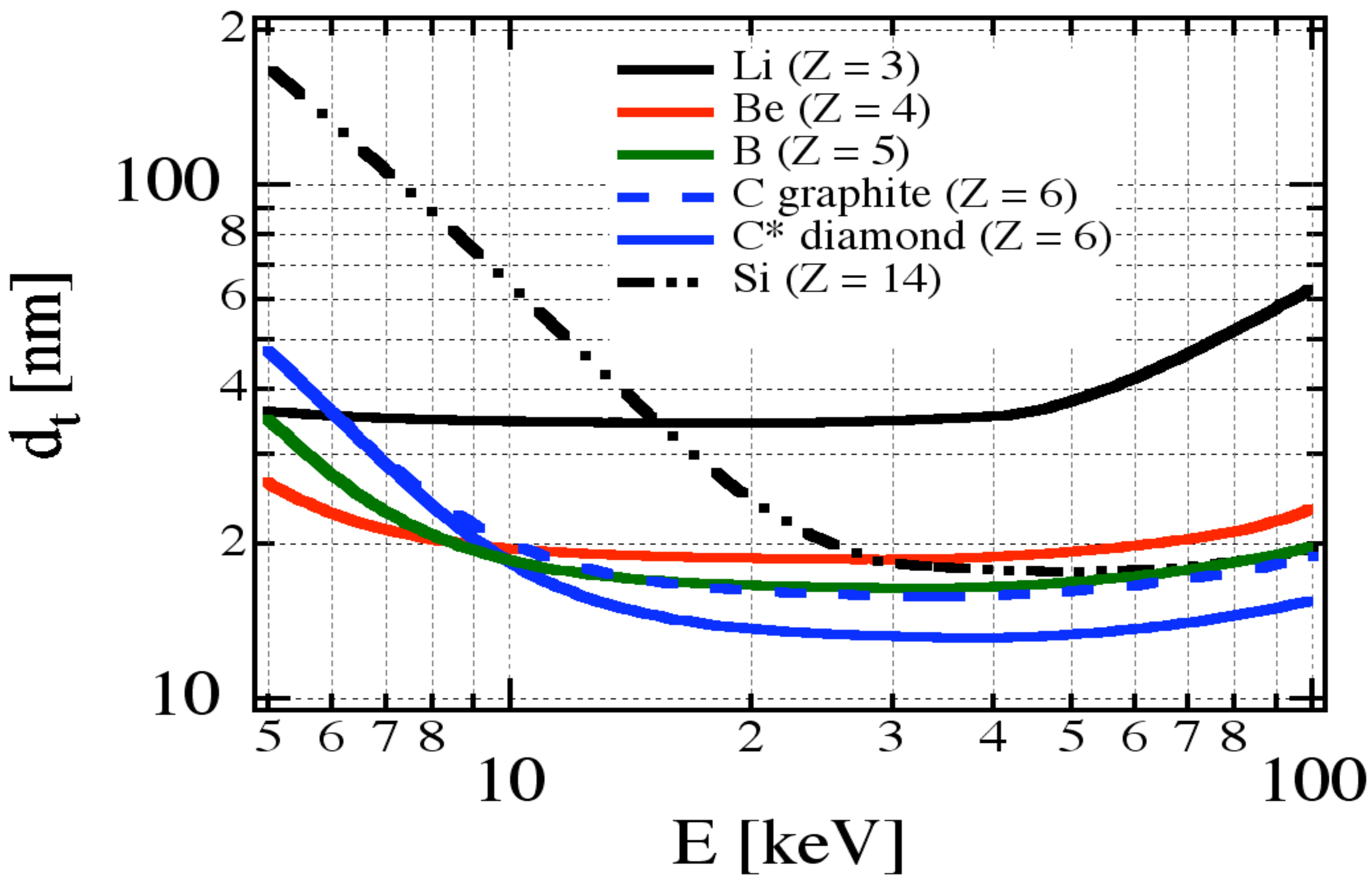
$$D_{eff} < 2R_0 \approx 2\sqrt{Rl}$$

$$NA = \frac{D_{eff}}{2f_{min}} \leq \frac{2\sqrt{Rl}}{2\sqrt{\frac{Rl}{2\delta}}} = \sqrt{2\delta}$$



Effective Aperture and Diffraction Limit

Diffraction limit:



N = 100
$l \geq 0.084$
R = 0.5 - 50µm

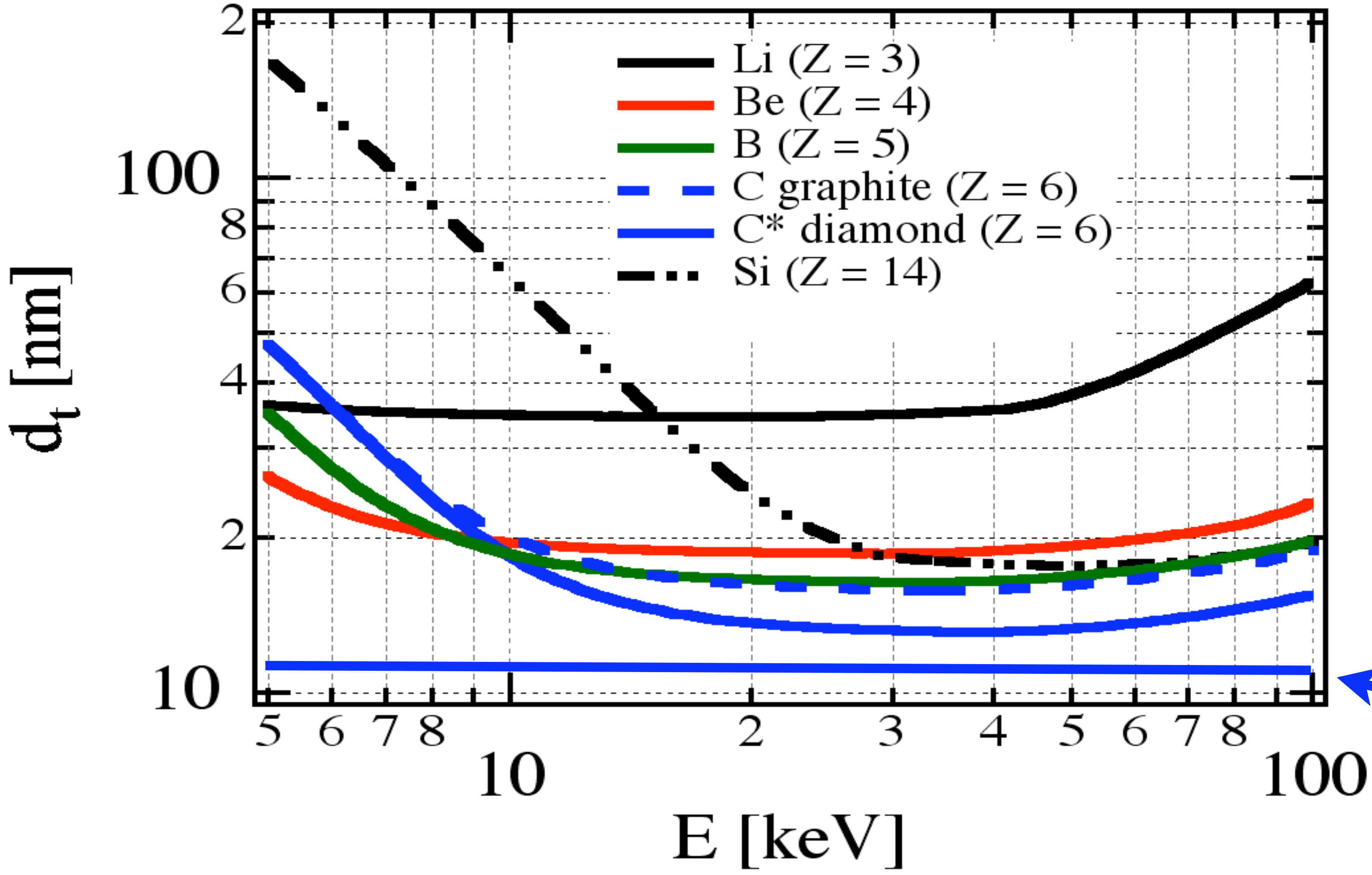
bounded by

$$0.75 \frac{\lambda}{2\sqrt{2\delta}} \propto \text{const.}$$

Best materials: high density and low *Z*

Effective Aperture and Diffraction Limit

Diffraction limit:



limit for diamond

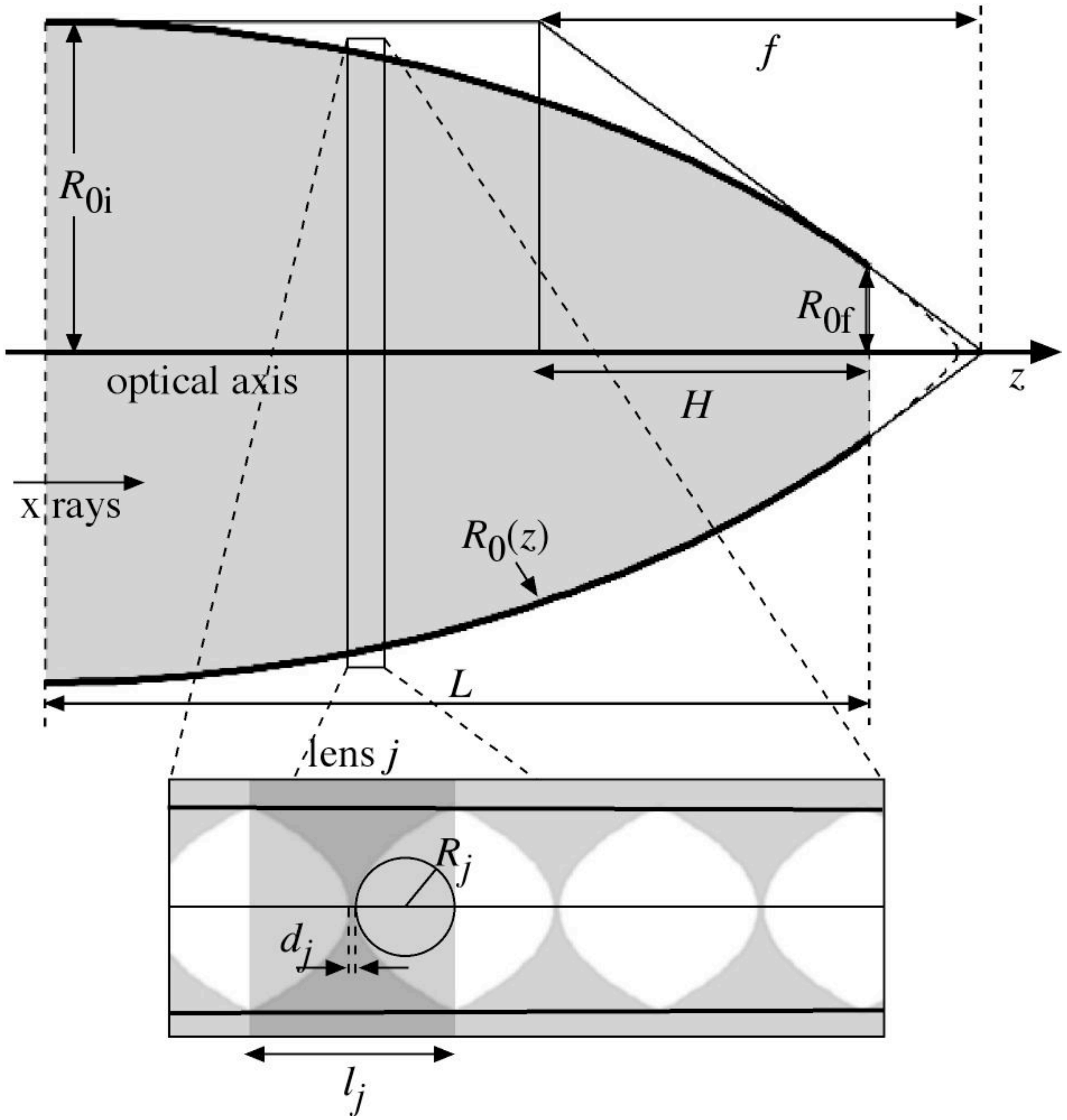
N = 100
l ≥ 0.084
R = 0.5 - 50μm

bounded by

$$0.75\frac{\lambda}{2\sqrt{2\delta}} \propto \text{const.}$$

Best materials: high density and low *Z*

Adiabatically Focusing Lenses



Adapt aperture to converging beam

↓

increase refractive power per unit length towards exit of lens

↓

increase numerical aperture

$$NA > \sqrt{2\delta}$$

↓

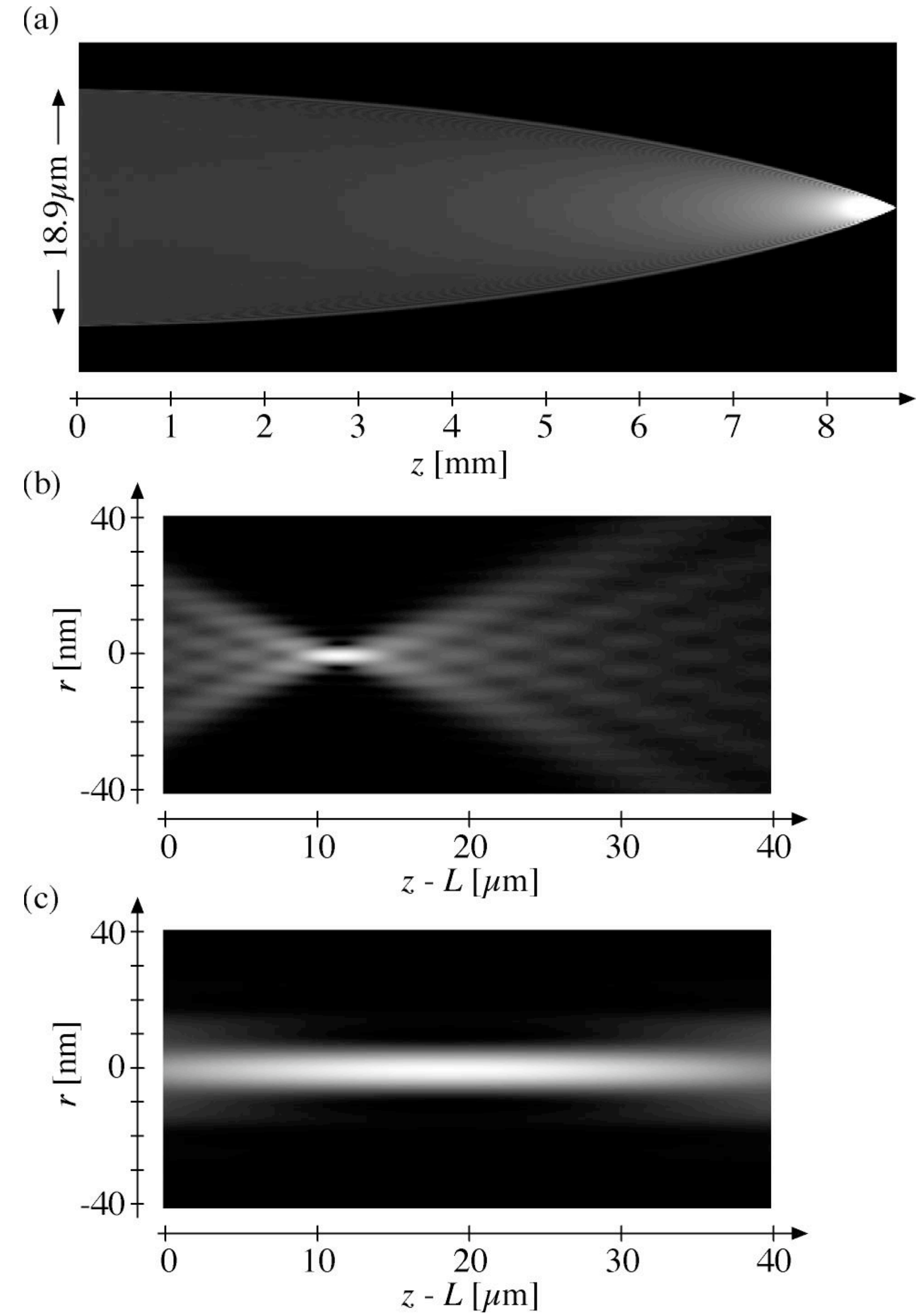
reduce diffraction limit (down to < 5 nm for C*)

Very demanding in terms of nano-fabrication: optimize NFLs first!

PRL **94**, 054802 (2005)

Example AFL

contracting wave field inside lens



Diamond lens:

low atomic number *Z* and high density ρ

N = 1166 individual lenses
entrance aperture: 18.9μm
exit aperture: 100nm
f = 2.3mm

diffraction limit: 4.7nm

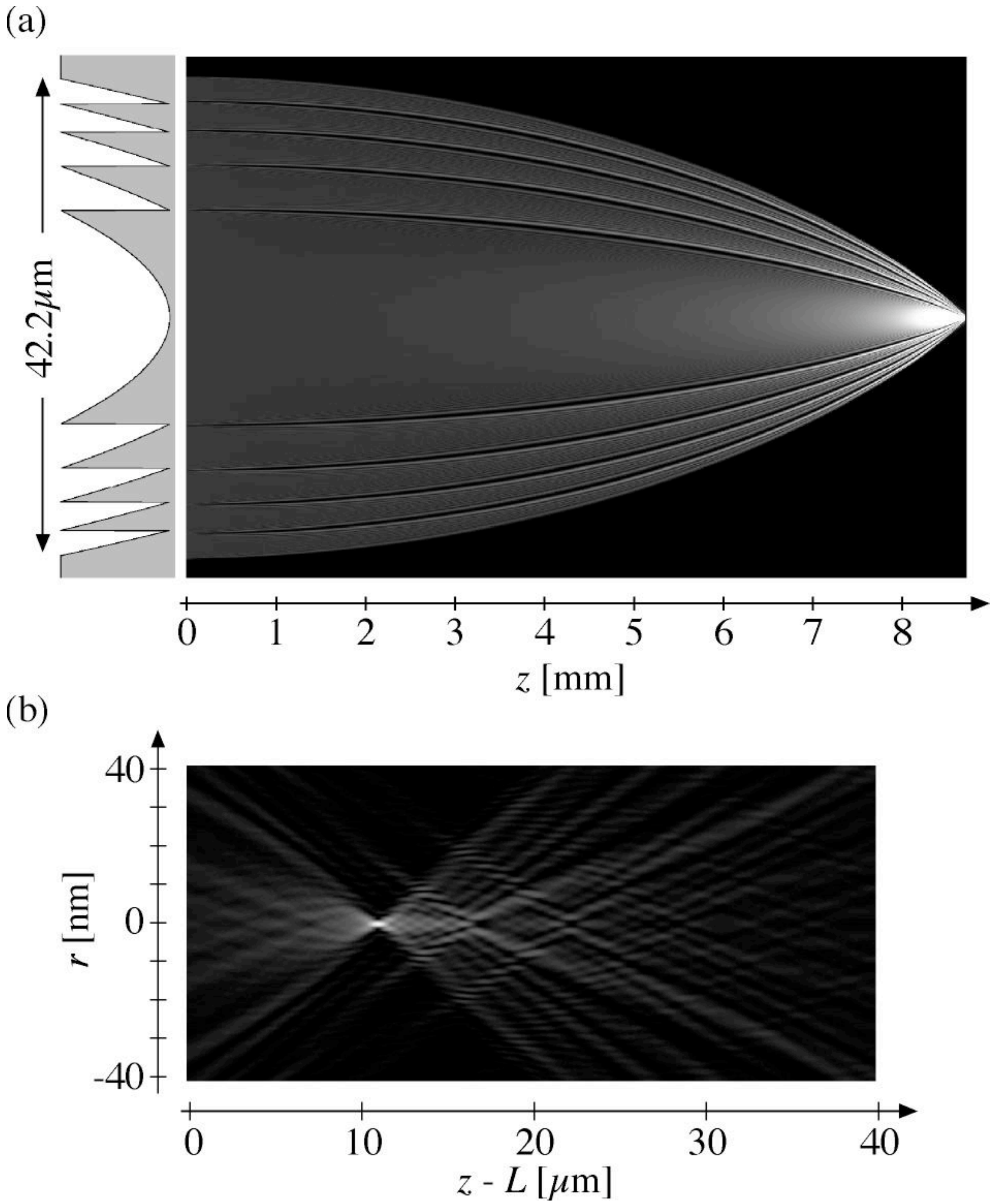
compare to NFL:
same aperture

diffraction limit: 14.2nm

AFL: Attenuation limits aperture

Workaround:

kinoform lens shape,
segment size follows
converging beam:

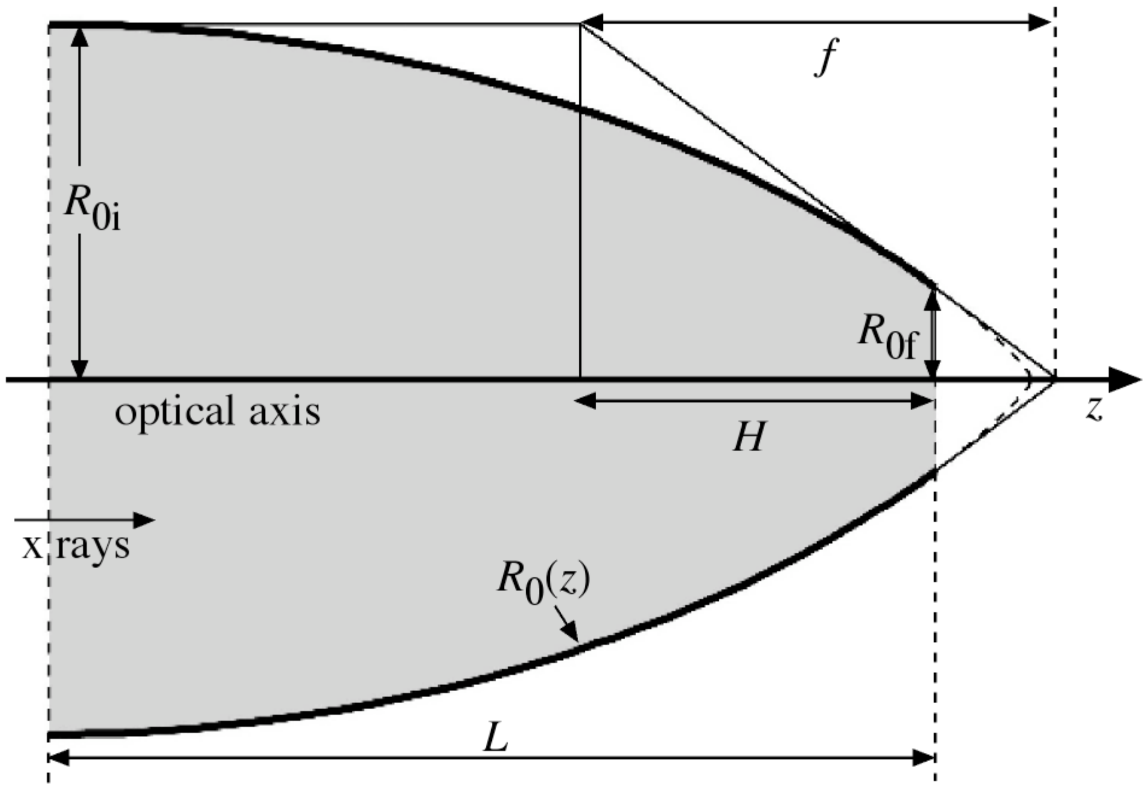


diffraction limit: 2.2nm

This is no hard limit, but
is difficult to implement
in practice.

Next Step: AFLs Made of Silicon

entrance aperture: $2R_{0i}$ = 20µm
exit aperture: $2R_{0f}$ = 1µm
energy: 10 - 20keV in 500eV steps



properties:

f = 2.7mm
d_t = 12.6nm

as horizontal lens in x-ray nanoprobe (e. g. ID13 ESRF):

L_1 = 47m,
source size: 150µm

horizontal focus: 15.3nm
(17400 x reduction)

Wave Propagation Through FZP

parabolic wave equation:

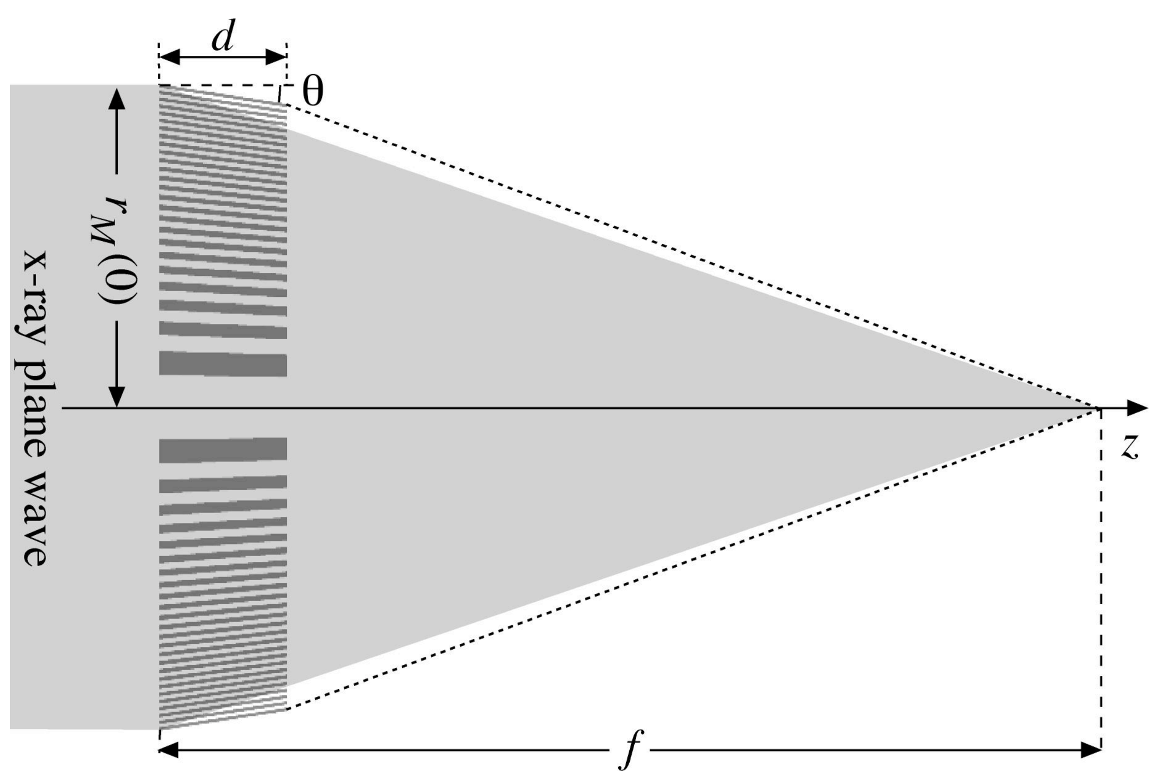
$$2ik\frac{\partial u}{\partial z}+\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+k^2\left(n^2(x,y,z)-1\right)u=0$$

$n(x,y,z)=1-\delta(x,y,z)+i\beta(x,y,z)$ complex potential!

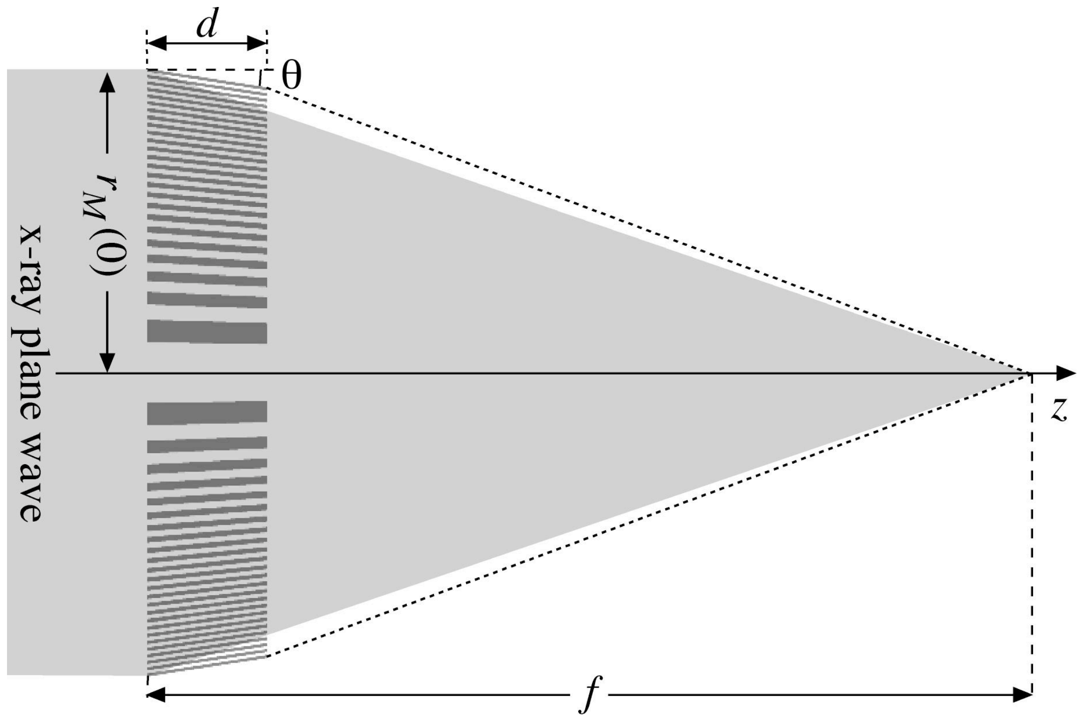
Ni/vac. zone plate

E = 20 keV, $r_M(0)$ = 0.8µm

Δr_M = 1nm



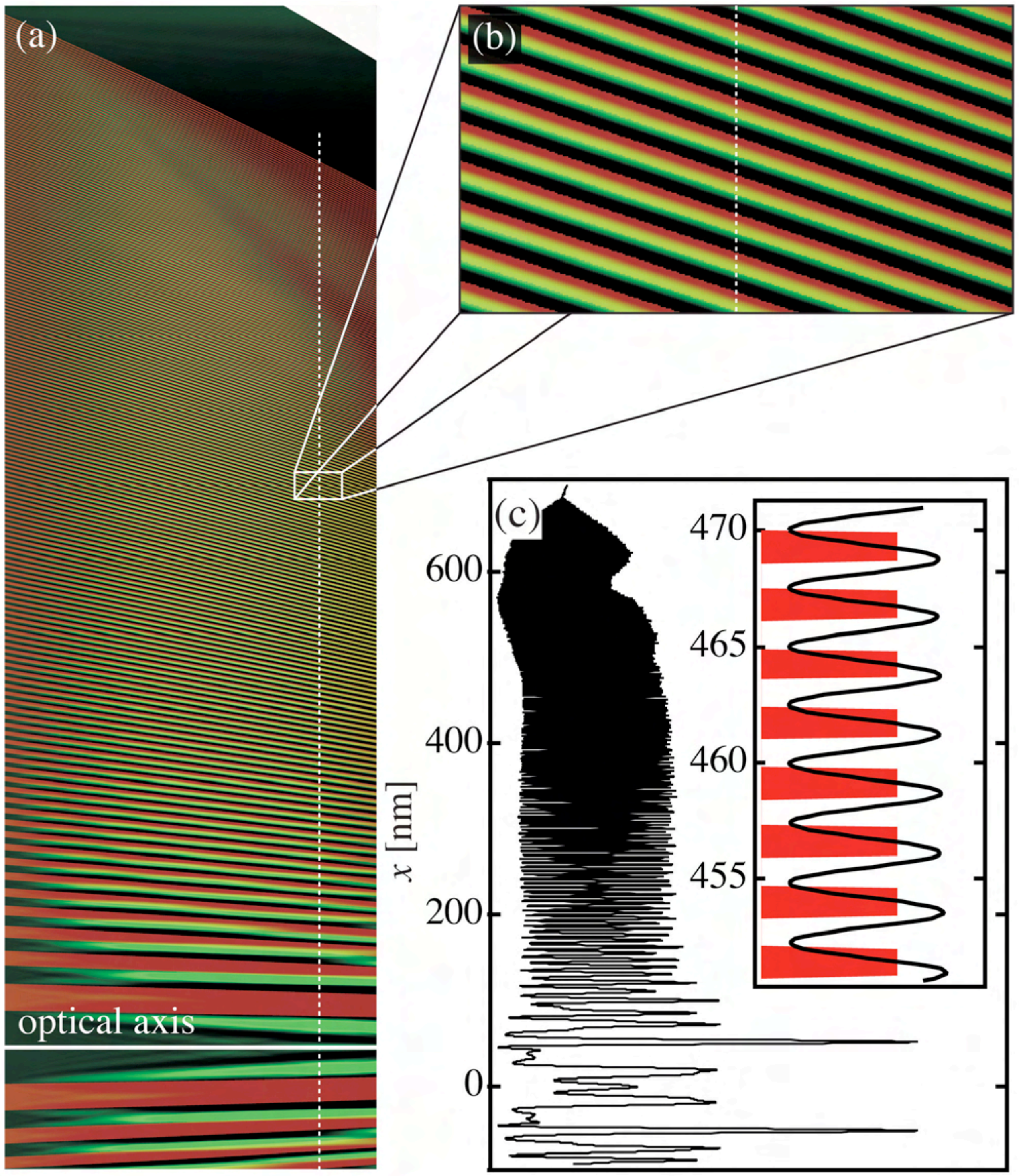
Wave Field Inside FZP



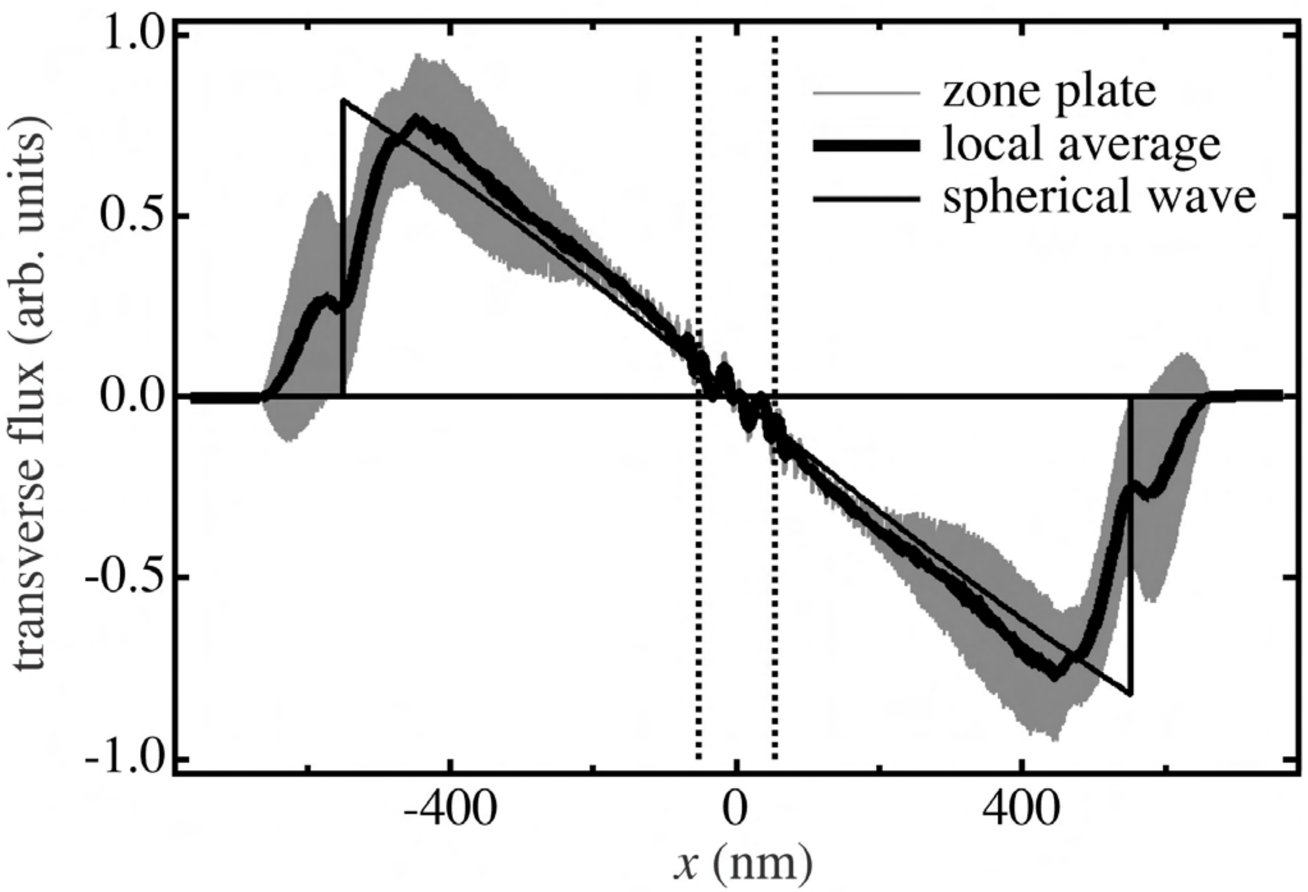
ideal tilted FZP
[Kang, et al., PRL **96,** 127401 (2006)]

incoming plane wave

propagate exit wave field to focus



FZP Focus



transverse flux density:

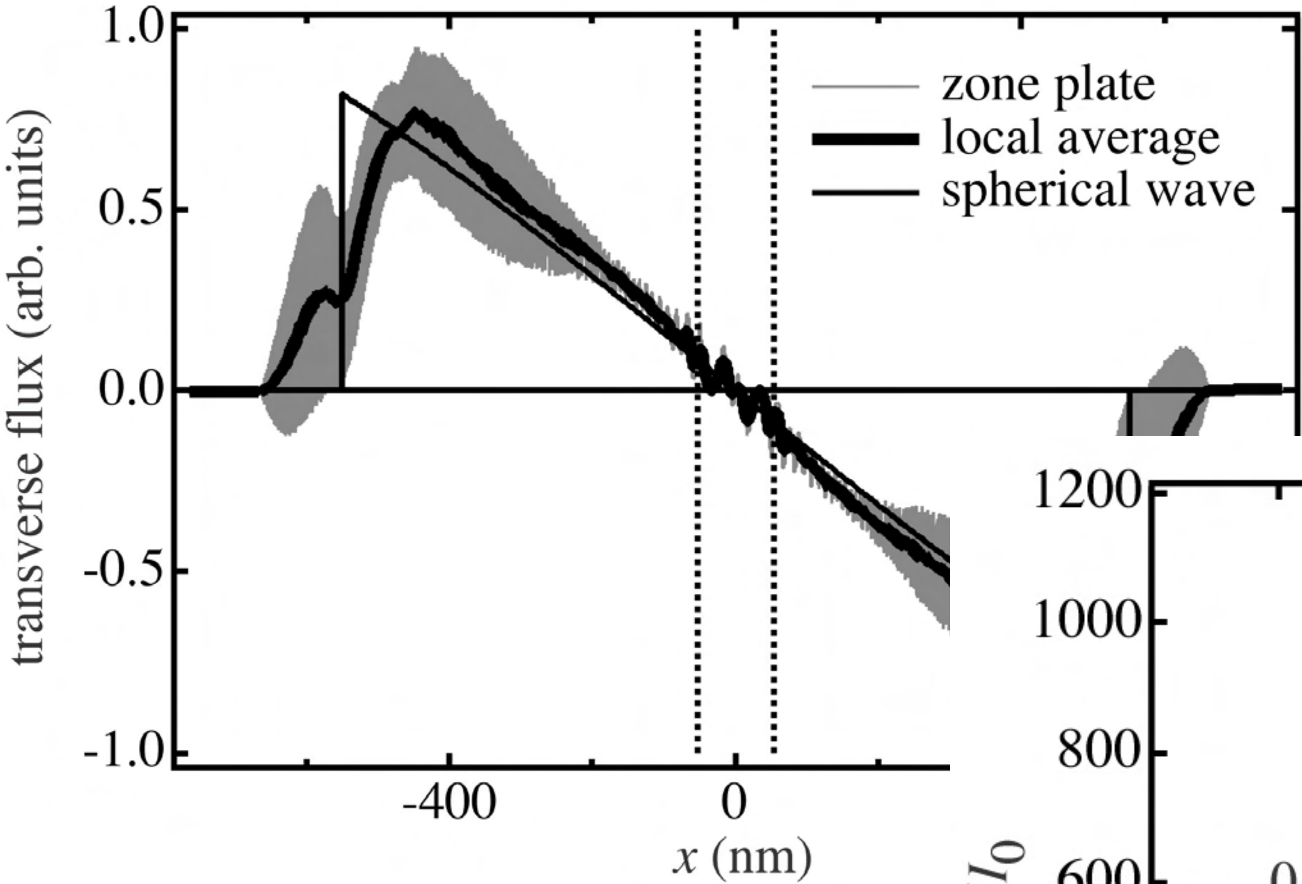
$$J_x(x,z) = \frac{1}{2ik}\left[\langle \psi | \partial_x \psi \rangle - \langle \partial_x \psi | \psi \rangle\right]$$

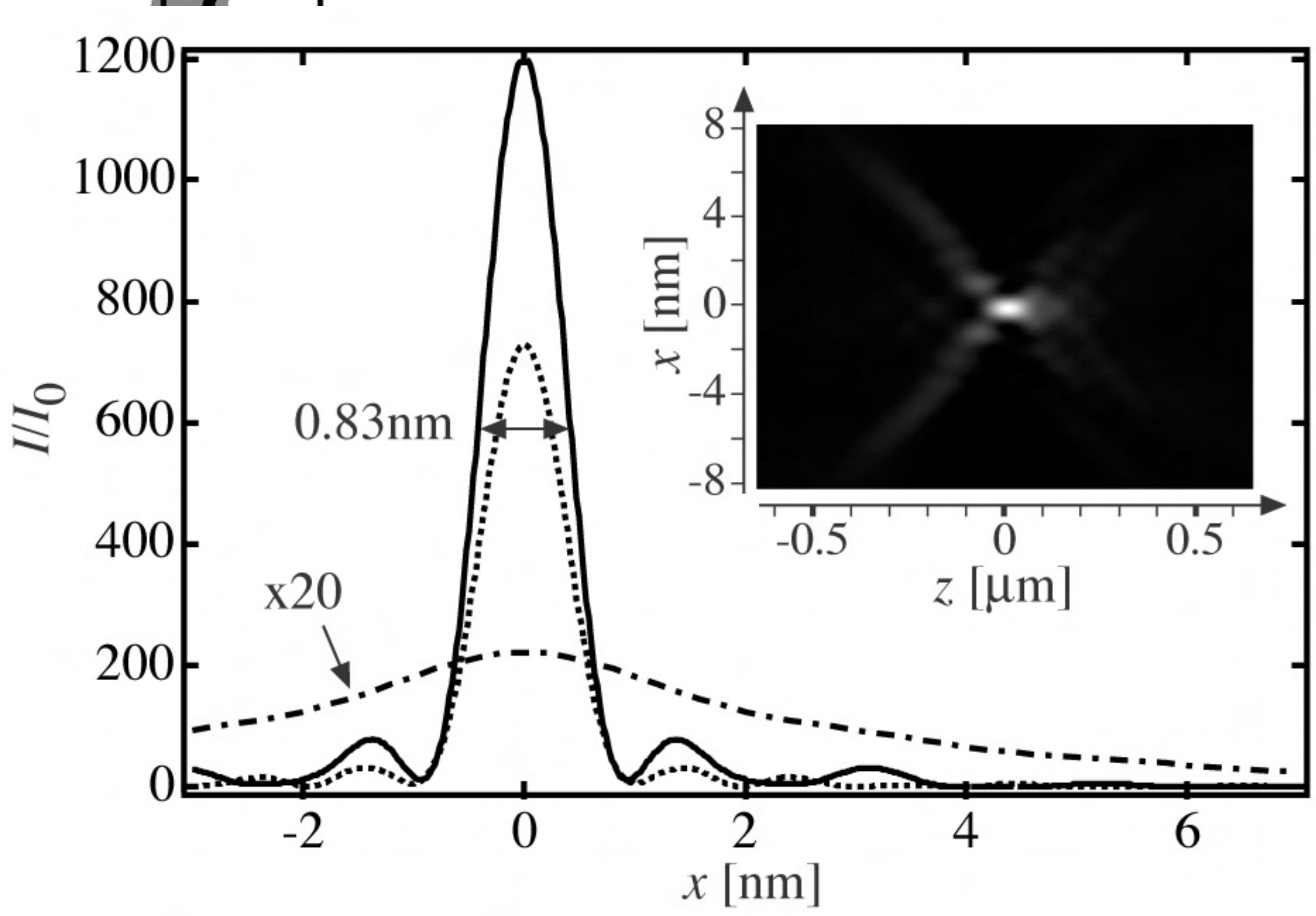
PRB **74**, 033405 (2006)

FZP Focus

transverse flux density:

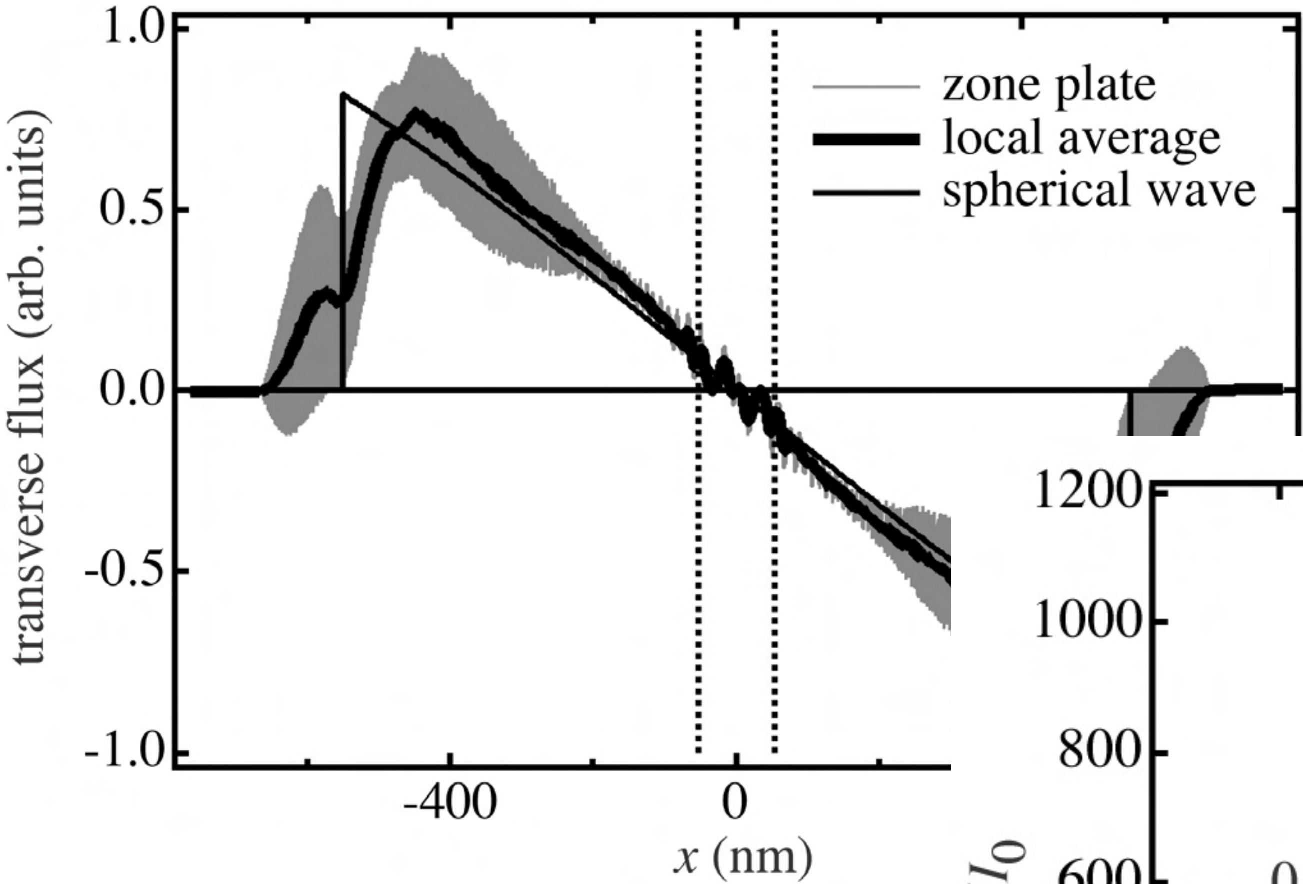
$$J_x(x,z) = \frac{1}{2ik}\left[\langle\psi|\partial_x\psi\rangle - \langle\partial_x\psi|\psi\rangle\right]$$





PRB **74**, 033405 (2006)

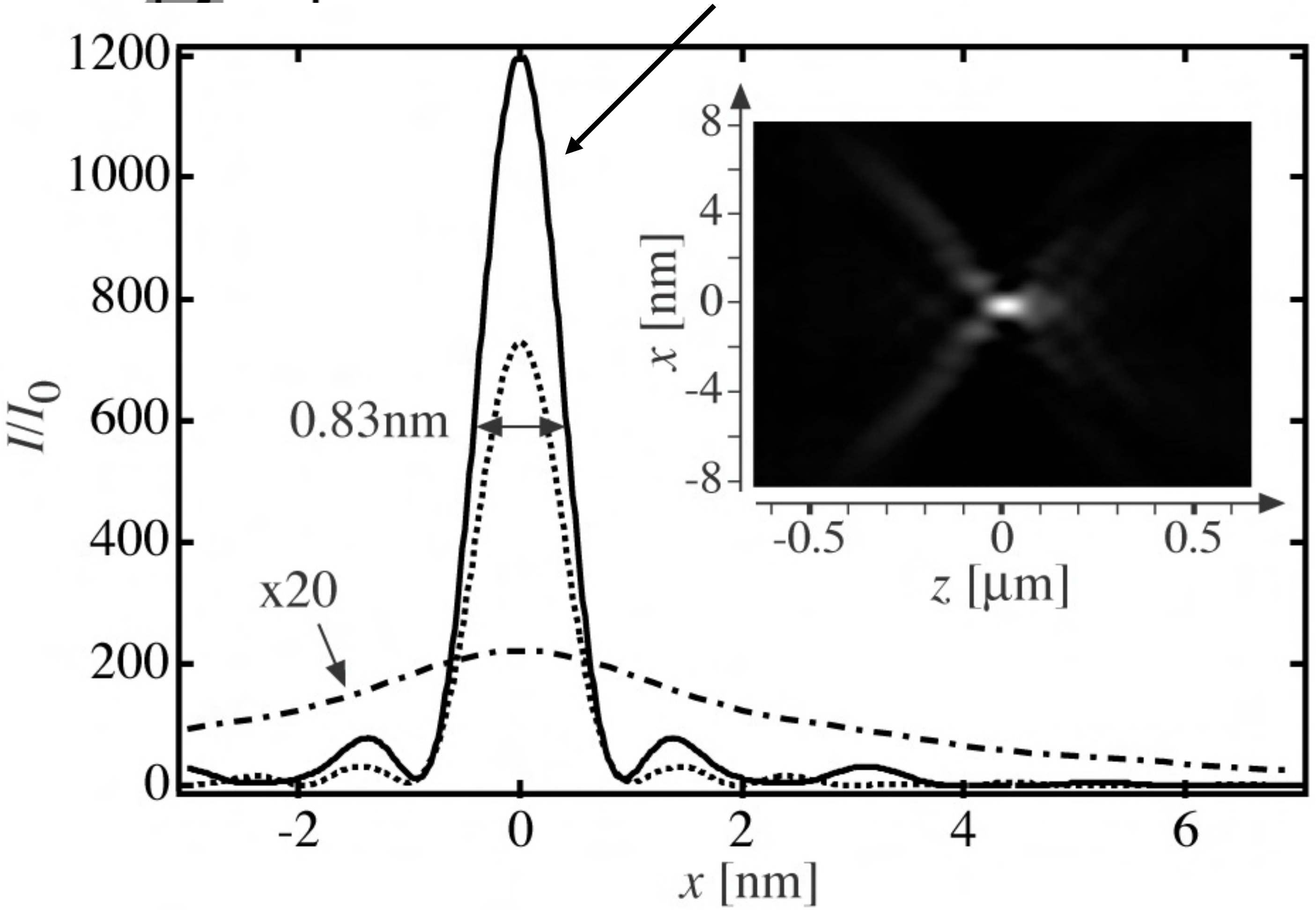
FZP Focus



transverse flux density:

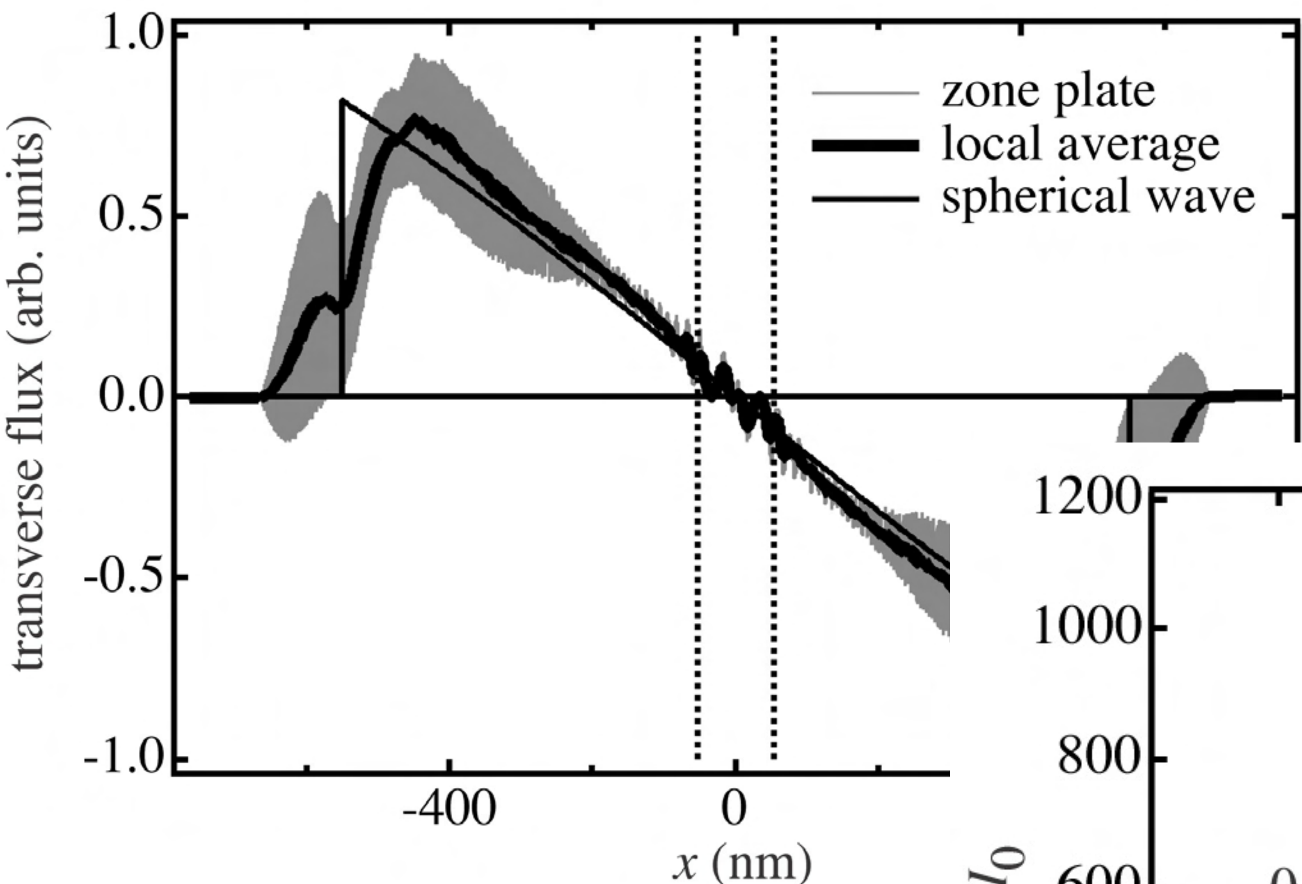
$$J_x(x,z) = \frac{1}{2ik}\left[\langle\psi|\partial_x\psi\rangle - \langle\partial_x\psi|\psi\rangle\right]$$

tilted FZP



PRB **74**, 033405 (2006)

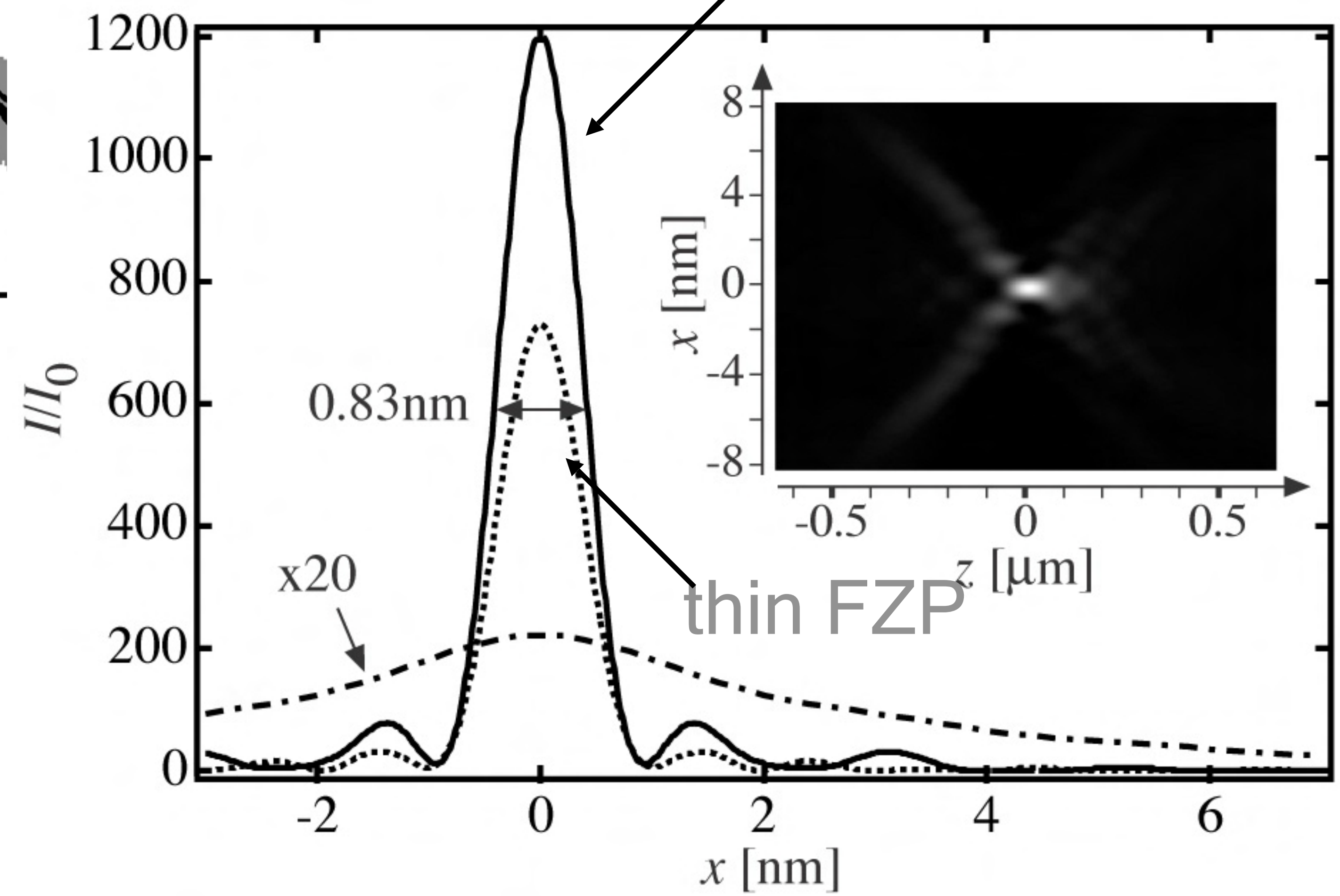
FZP Focus



transverse flux density:

$$J_x(x,z) = \frac{1}{2ik}\left[\langle\psi|\partial_x\psi\rangle - \langle\partial_x\psi|\psi\rangle\right]$$

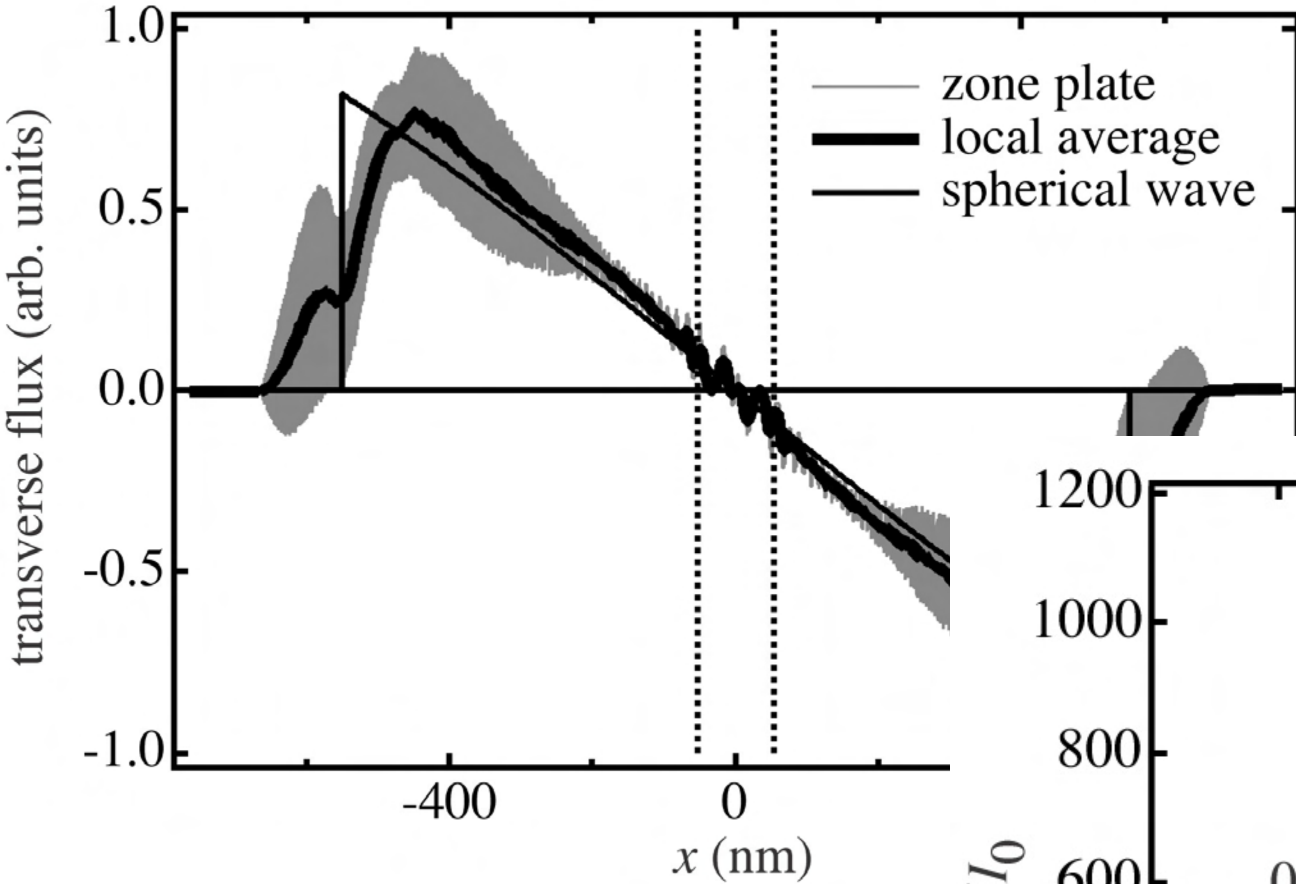
tilted FZP



thin FZP

PRB **74**, 033405 (2006)

FZP Focus

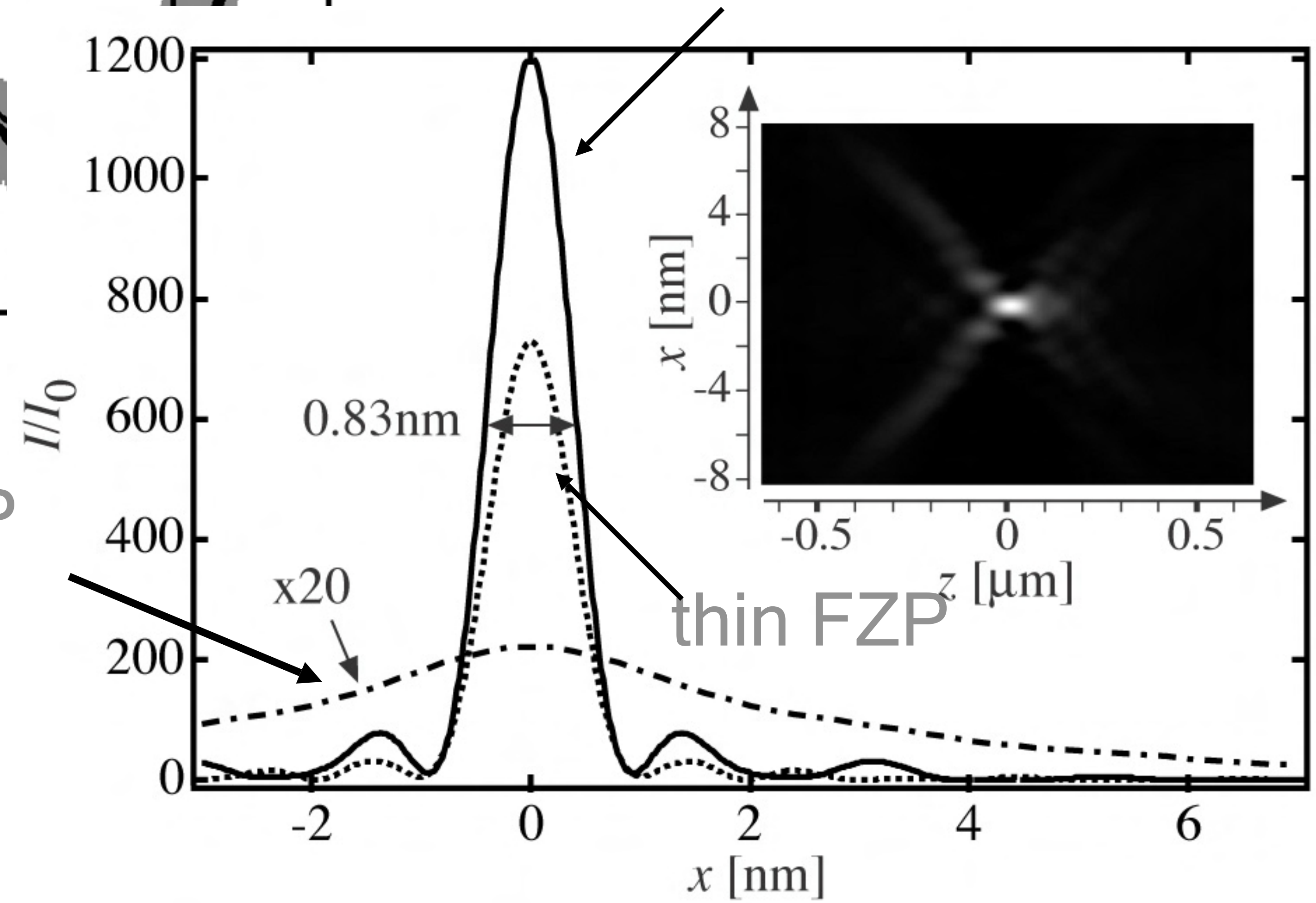


transverse flux density:

$$J_x(x,z) = \frac{1}{2ik}\left[\langle\psi|\partial_x\psi\rangle - \langle\partial_x\psi|\psi\rangle\right]$$

tilted FZP

untilted FZP



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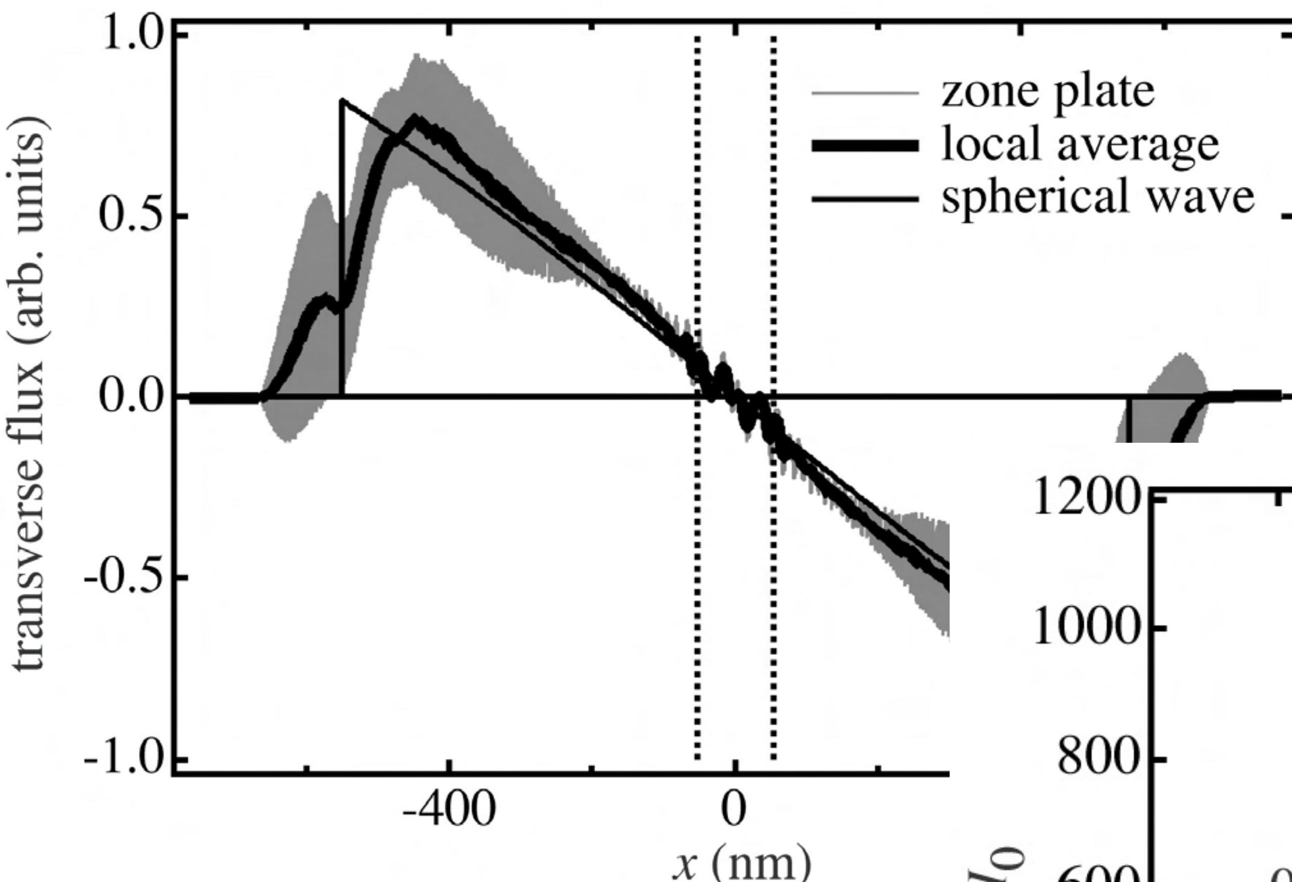
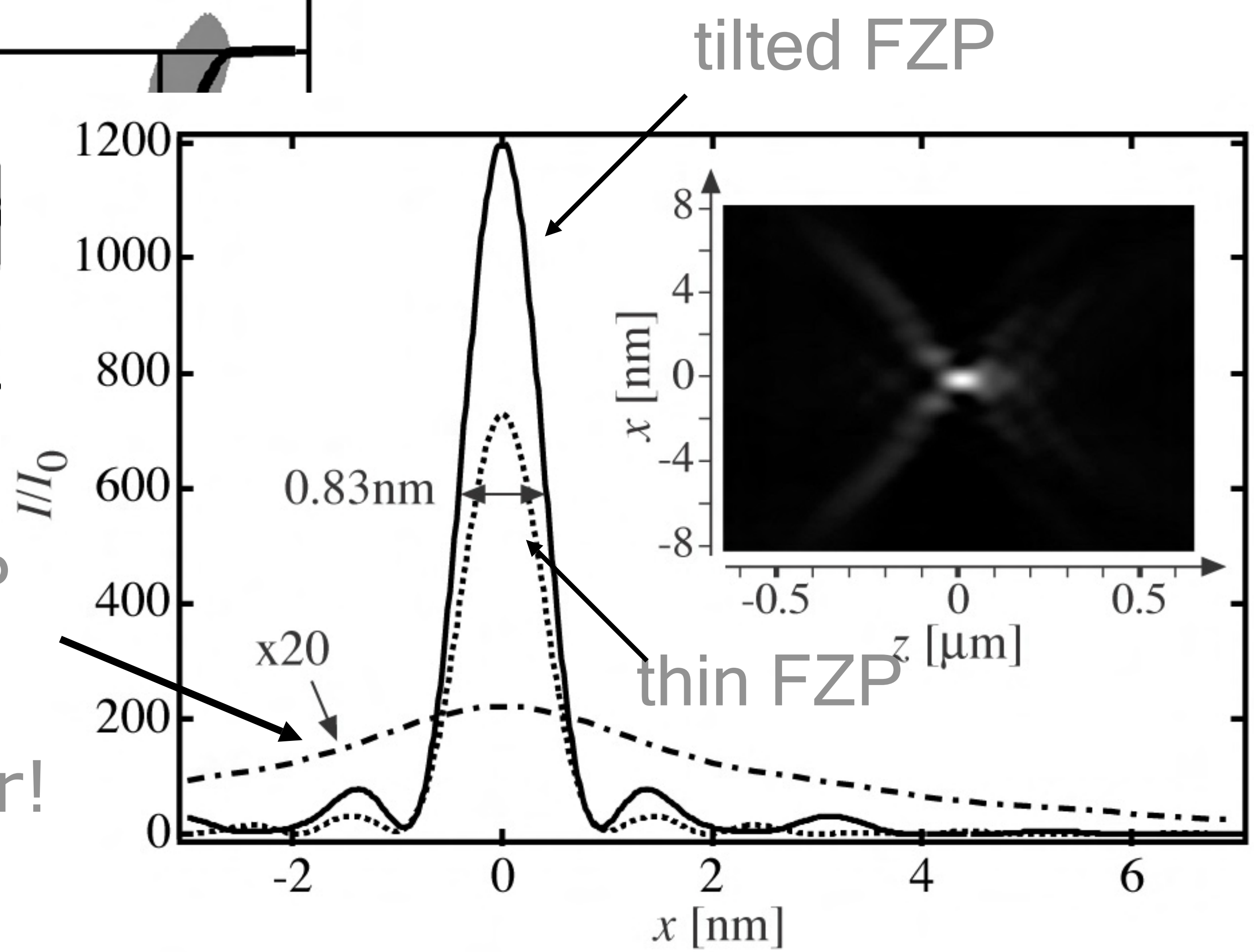
FZP Focus



transverse flux density:

$$J_x(x,z) = \frac{1}{2ik}\left[\langle \psi | \partial_x \psi \rangle - \langle \partial_x \psi | \psi \rangle\right]$$



Limit: atomicity of matter!

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FZP: Summary

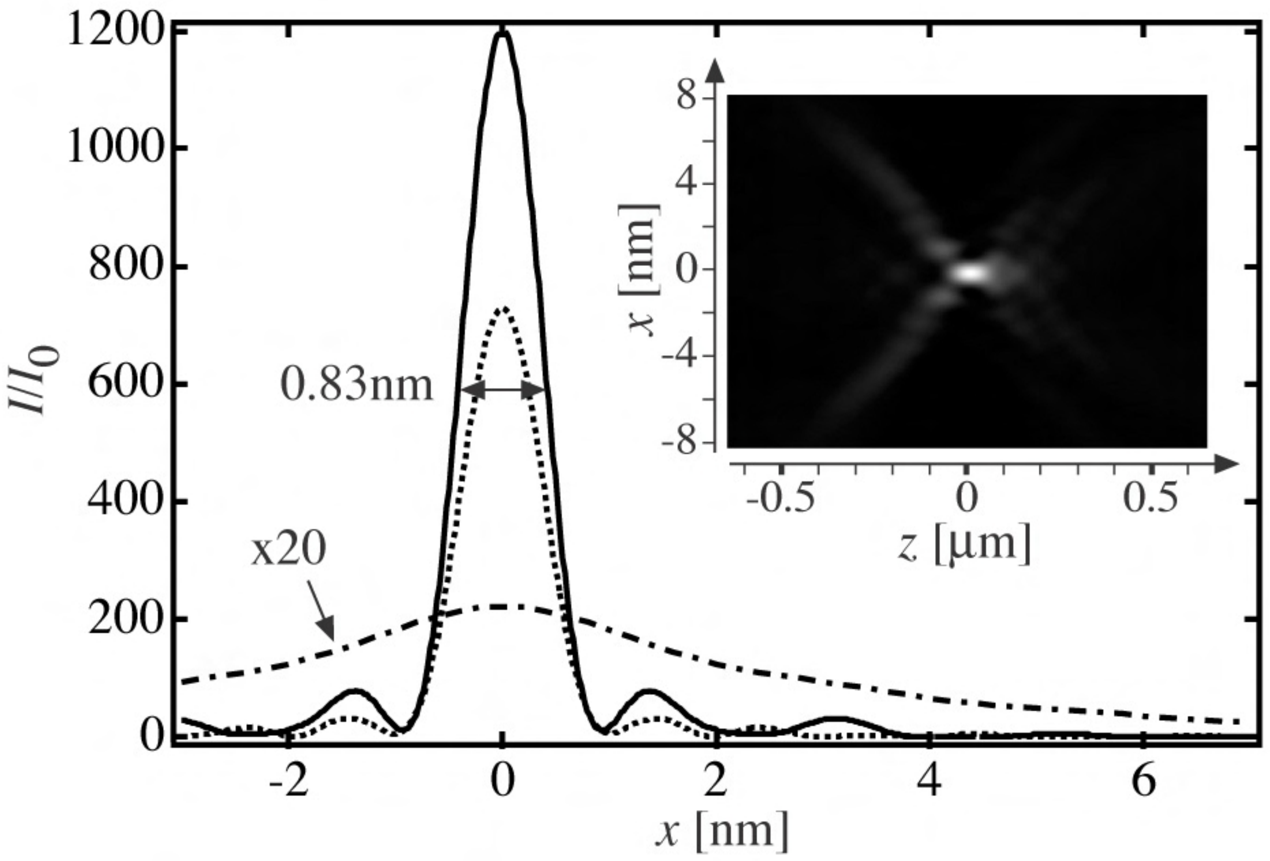
no limit as long as matter is homogeneous

multilayers have been shown to behave homogeneously down to below 2 nm d-spacing (1 nm layers)

high efficiency, since only one diffraction order is excited!

atomicity will limit zone placement!

other optics may be calculated similarly!



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Conclusion

Nanofocusing lenses:

- *NA* limited by critical angle: $NA \leq \sqrt{2\delta}$
  (Refractive power to unit length fixed by fixed size of aperture and density of low *Z* material.)

Adiabatically focusing lenses:

- hard x-ray beam size down to 5 nm seems feasible.
- limiting factors: attenuation of lens material and smallest feature size.
- adiabatic kinoform lenses could reduce focus size (~ 2nm).

Thick tilted FZP:

- limit of focus given by atomicity of matter.
- < 1nm focusing conceivable.