Integration of Diffraction Focussing Optics into RAY

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COST STSM, s in cooperation with:

Raytracing routine for transmission zone plates

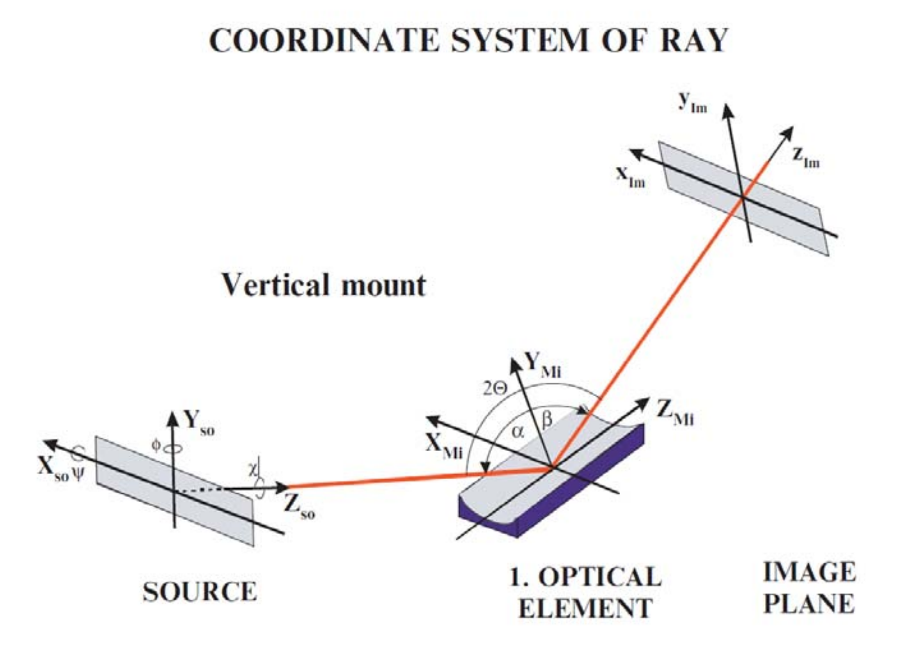
- *BESSY II:* *Franz Schäfers, Alexei Erko, Alexander Firsov*
- *Institute of Physics, Academy of Sciences of the Czech Republic:* *Nikolay Artemiev*

Raytracing routine for reflection zone plates

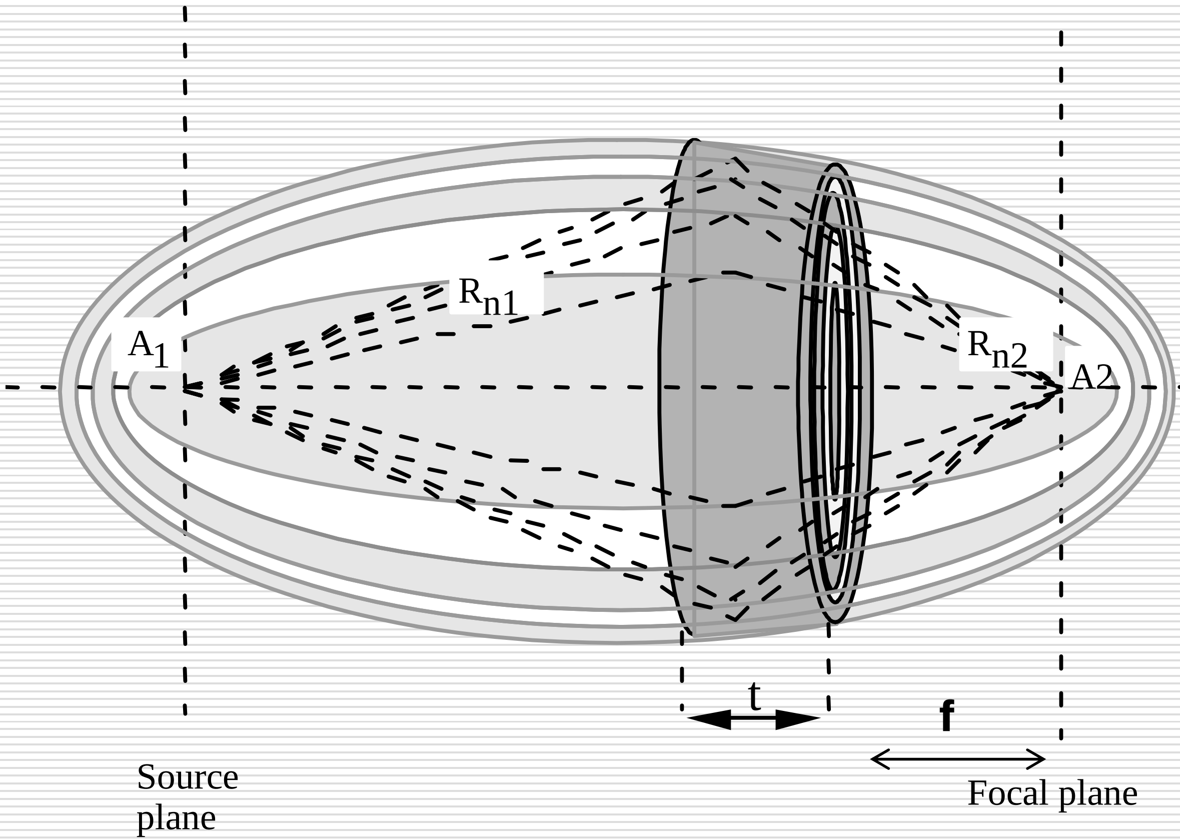
- *Kings College London, U K:* *Shahin Sahraei, Alan G. Michette*

BESSY RAY program (F. Schäfers)

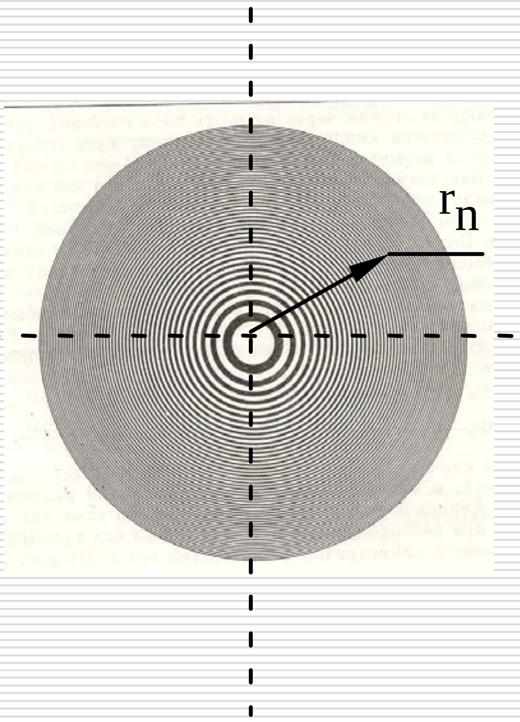
- Simulate Optical systems up to 10 elements
- Beamline design tool
- Geometric Optics
- Sources
  - Point
  - Dipole
  - Undulator
- Optical elements
  - Reflection Mirrors
  - Crystals (graded)
  - Gratings (VLS)
  - Transmission Zone Plates
  - Reflection Zone plates



On-axis zone plates.



Cross-section of On-axes ZP



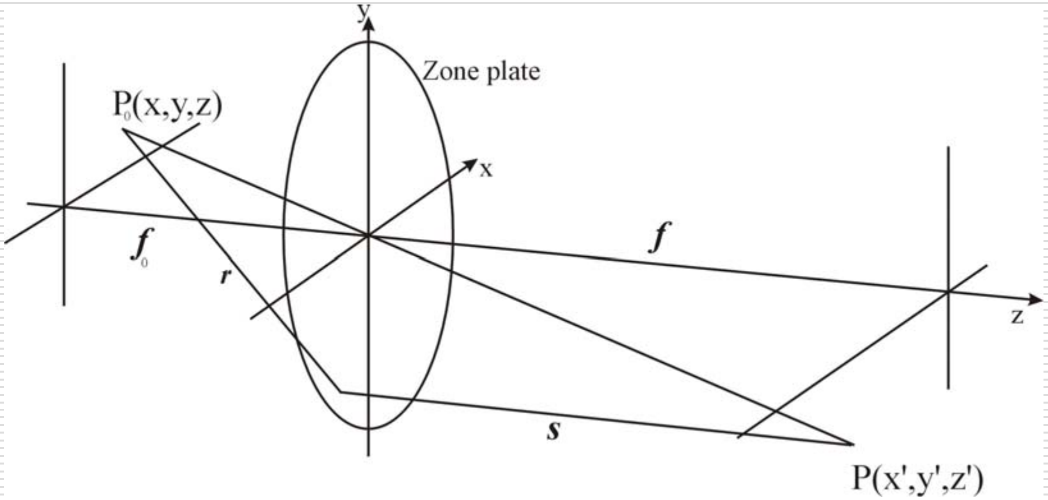
$$r_n = (n\lambda f)^{0.5}$$

Diffraction on a zone plate

*Using the Fresnel – Kirchhoff diffraction integral one may obtain the forms of diffraction patterns. Referring to Figure, this gives the complex disturbance at **P** as*

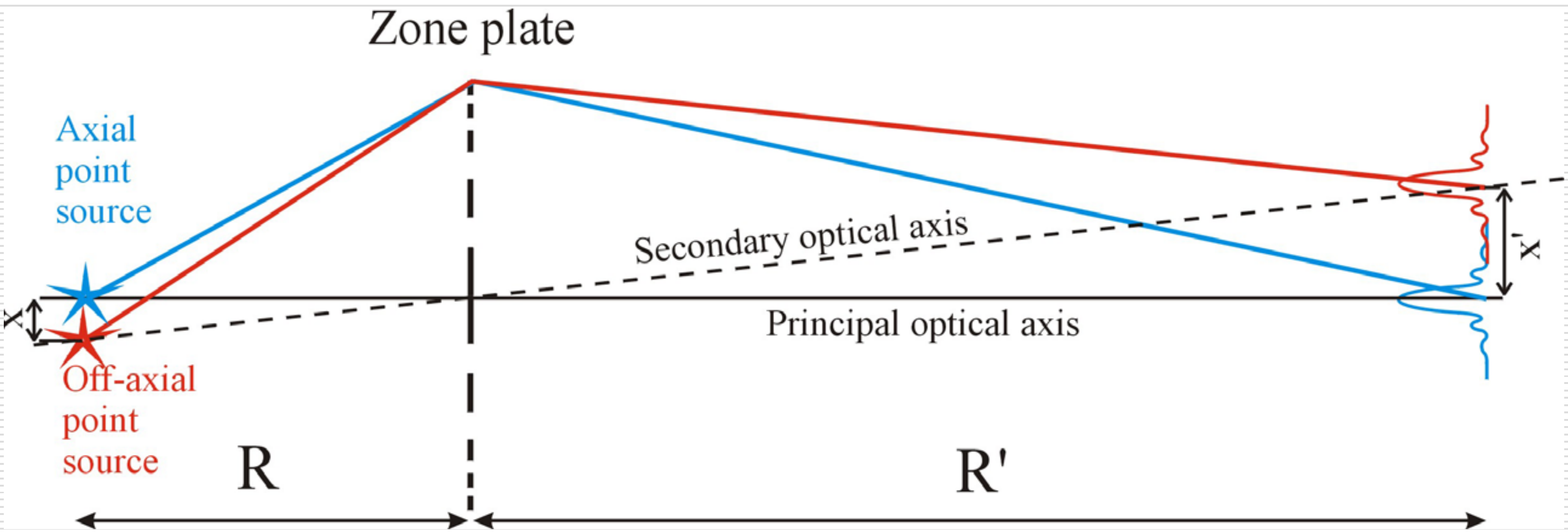
$$U(P) = -(iA/2\lambda)\cdot\iint\frac{\exp[ik(r+s)]}{r\cdot s}(\cos\alpha-\cos\beta)dS$$

The coordinate system used in the calculation of the diffraction pattern of a circular aperture.



Diffraction – raytracing transmission

Transmission from wave description to Ray description: the use of analytical solutions



INTEGRAL DIFFRACTION EFFICIENCIES

=

ray propagation probabilities

Main analytical equations

J. Kirz formulas:

$$E_m = [1/(\pi^2 m^2)]*[1 + \exp(-2\chi\Delta\phi) - 2\cos(\Delta\phi) - \exp(-\chi\Delta\phi)];$$

The maximum of the function E_m

$$\sin(\Delta\phi_{opt}) + \chi\,[(\cos(\Delta\phi_{opt})\ \exp(-\chi\Delta\phi_{opt})] = 0;$$

$\Delta\phi_{opt}$ is the optimal phase shift in zone plate material.

$$t_{opt} = \Delta\phi_{opt} / (2\pi\delta); \qquad \chi = \delta/\beta$$

zero order diffraction E_0 and absorbed intensity E_{abs}:

$$E_0 = 0.25\,[1 + \exp(-2\chi\Delta\phi) + 2\cos(\Delta\phi)\exp(-\chi\Delta\phi)];$$

$$E_{abs} = 0.5\,[1 - \exp(-2\chi\Delta\phi)].$$

Ray propagation probabilities.

$$E_{lost} = E_{abs} + \sum_{m=-\infty}^{m=-1} E_m + \sum_{m=5}^{m=\infty} E_m$$

m = 1;3;5

$$E_m = I_m / I_{in} = [1/(\pi^2 m^2)]*[1 + \exp(-2\chi\Delta\phi) - 2\cos(\Delta\phi) - \exp(-\chi\Delta\phi)];$$

Diffraction – limited resolution model

DIFFRACTION LIMITED RESOLUTION

=

ray propagation probabilities

The solution of the Fresnel Kirchhoff diffraction integral can be found in a form of the Bessel function of first order with an argument

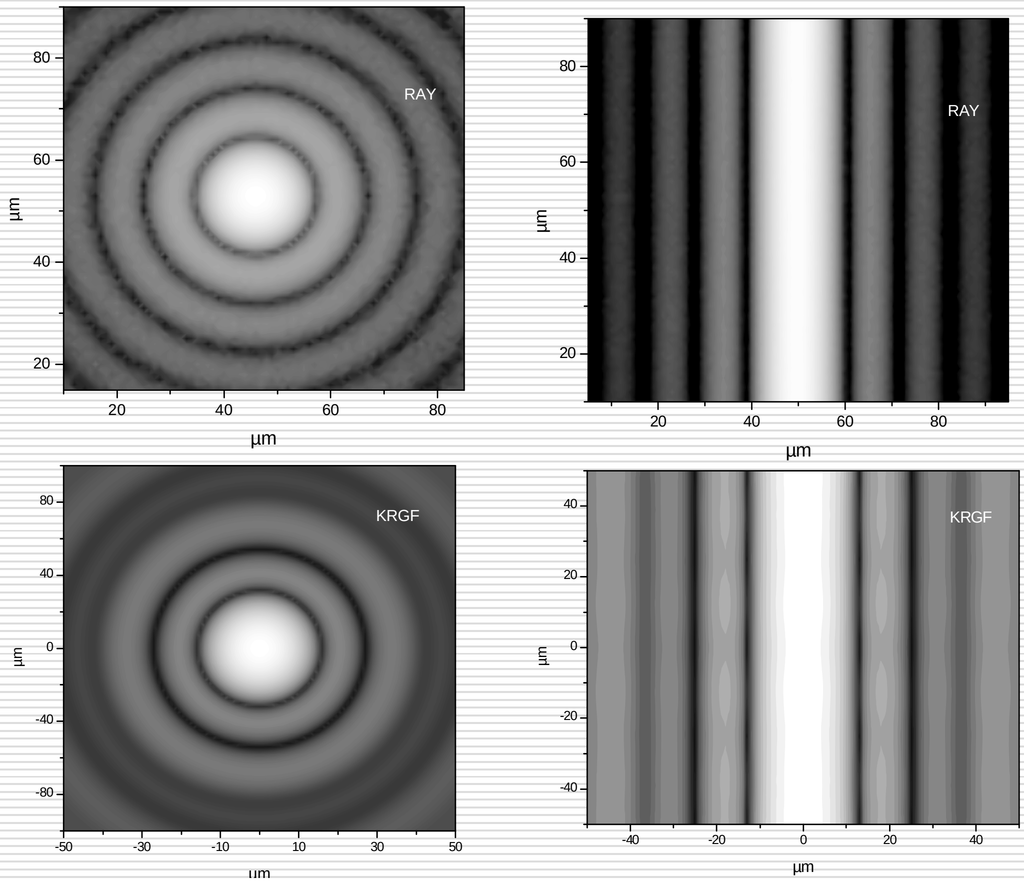
$$\nu_m = rN\, k\, (r'/F_m);$$

where ***r´*** the radial distance between the optical axis and an arbitrary point in the image plane. In our case ***r´ = x´***.

the radial intensity distribution at the focus of a zone plate is well described by an Airy pattern analogous to a perfect thin lens:

$$E_{m'}(\nu_m) \sim [2J_1(\nu_m)/\nu_m]^2$$

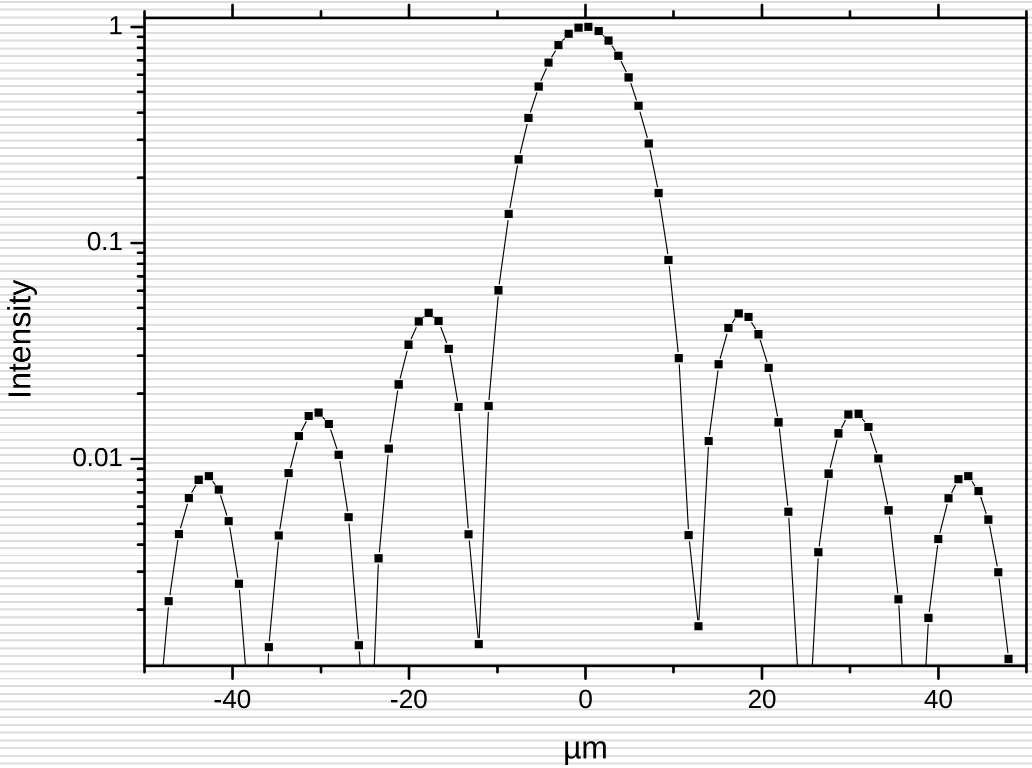
TEST OF THE COMPUTER CODE



A focal plane of circular (a) and linear (b) zone plates calculated using programs RAY (Up) and KRGF (bottom).

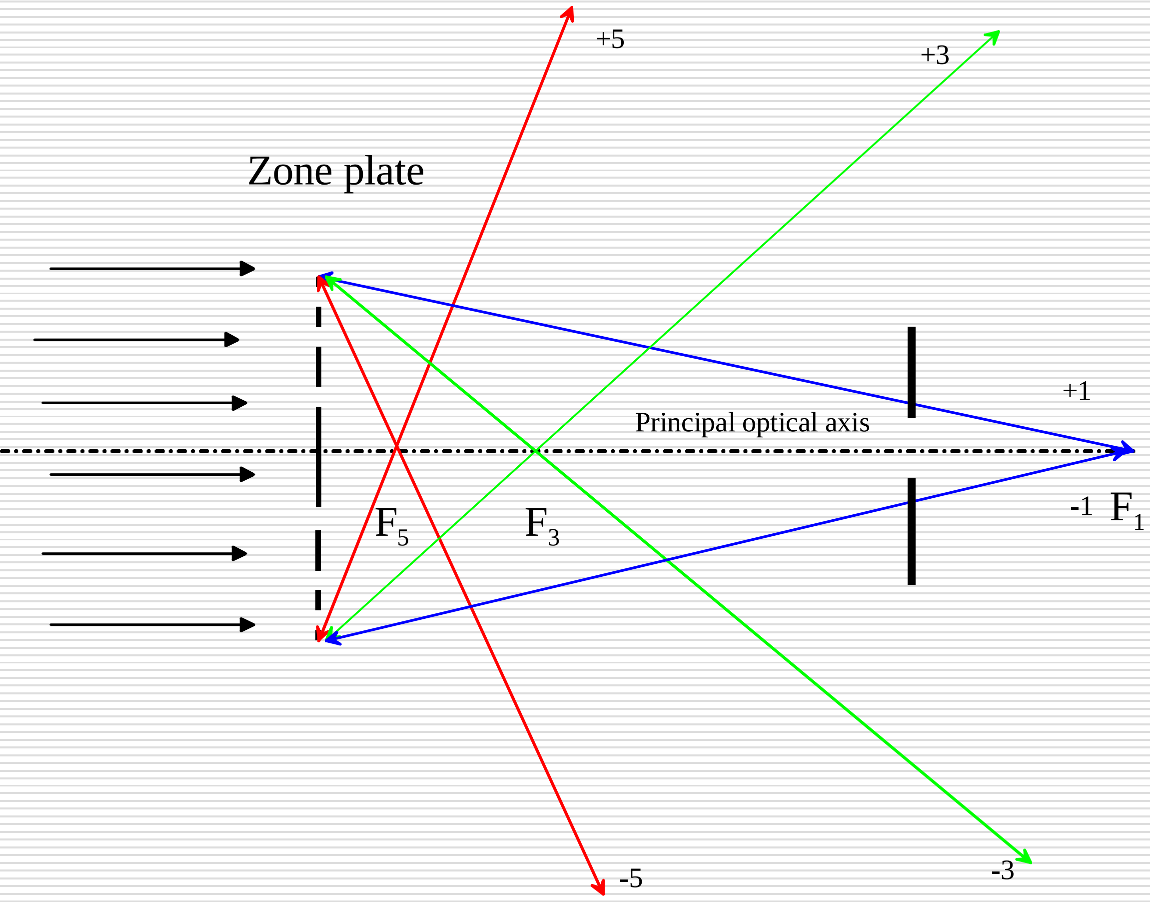
Zone plate type	First order focal length F_1	Aperture	R1 / R2
Linear	1000 mm	1 mm x 1 mm	2000 mm / 2000 mm
Circular	1000 mm	Ø 1 mm	2000 mm / 2000 mm

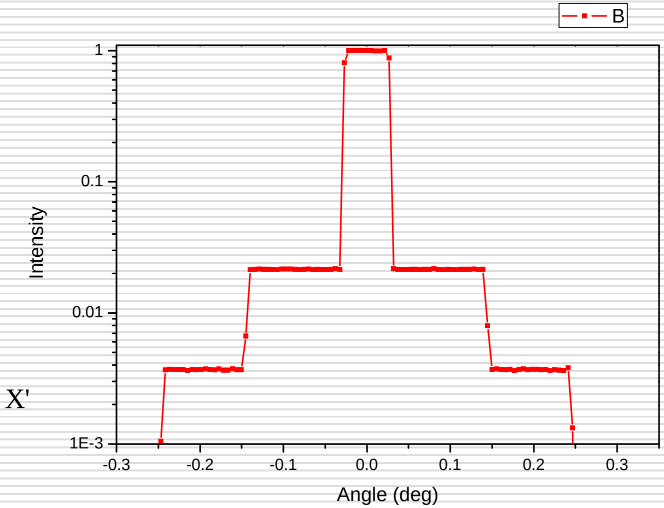
Diffraction limited resolution

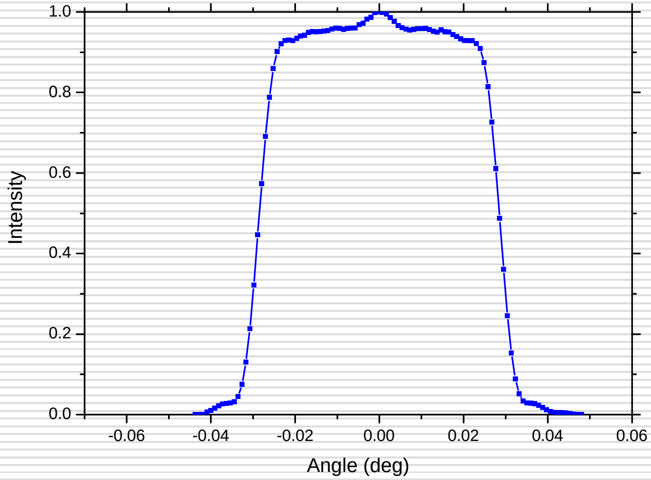


Intensity profile in the focal plane of the zone plate calculated by the RAY. 100 000 000 rays.

Spatial frequency spectra







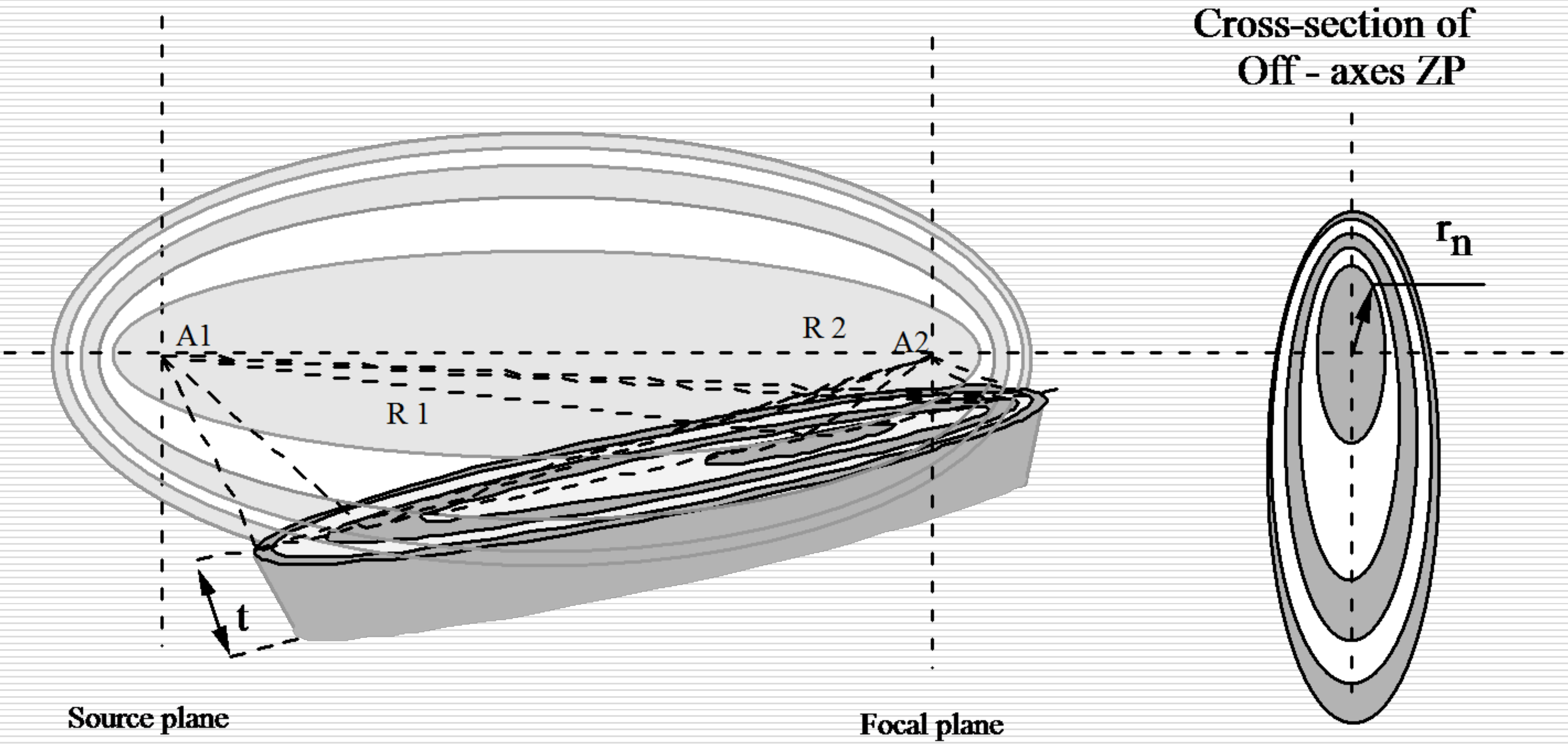
(STSM)

Ray-tracing Routine for Reflection Zone Plates

Shahin Sahraei, Alan Michette, Alexei Erko, Franz Shäfers

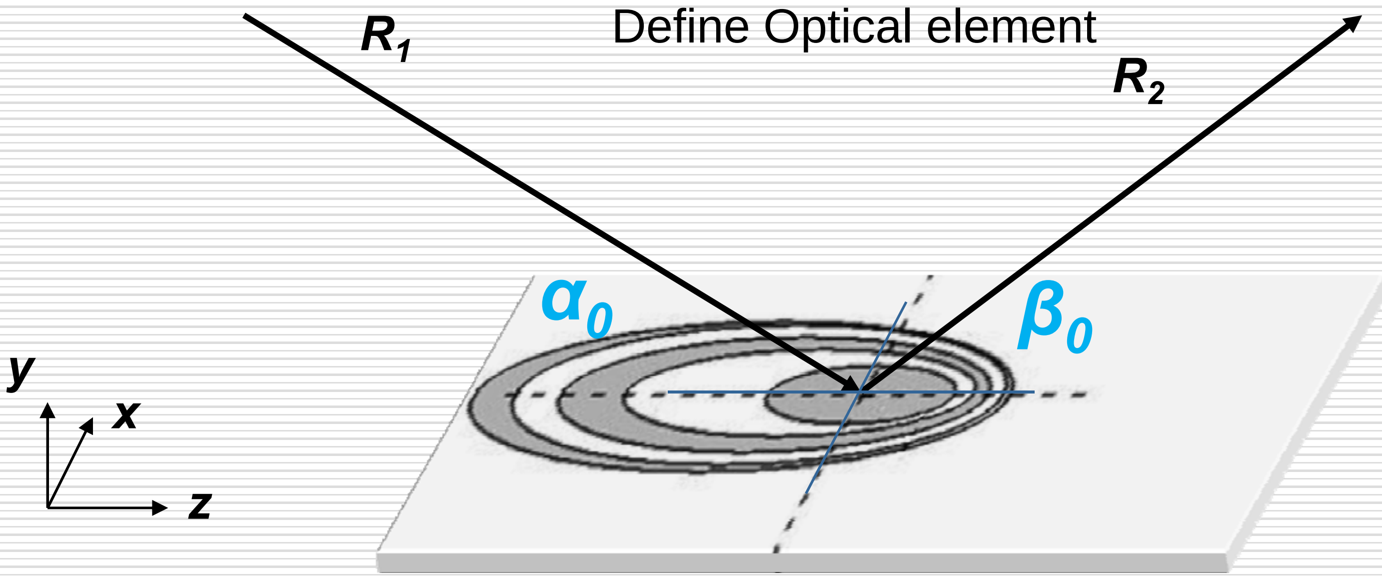
King's College London
BESSY GmbH

Elliptical Reflection (Bragg-Fresnel) zone plate



Optical element definition

Figure from Shahin Shahraei

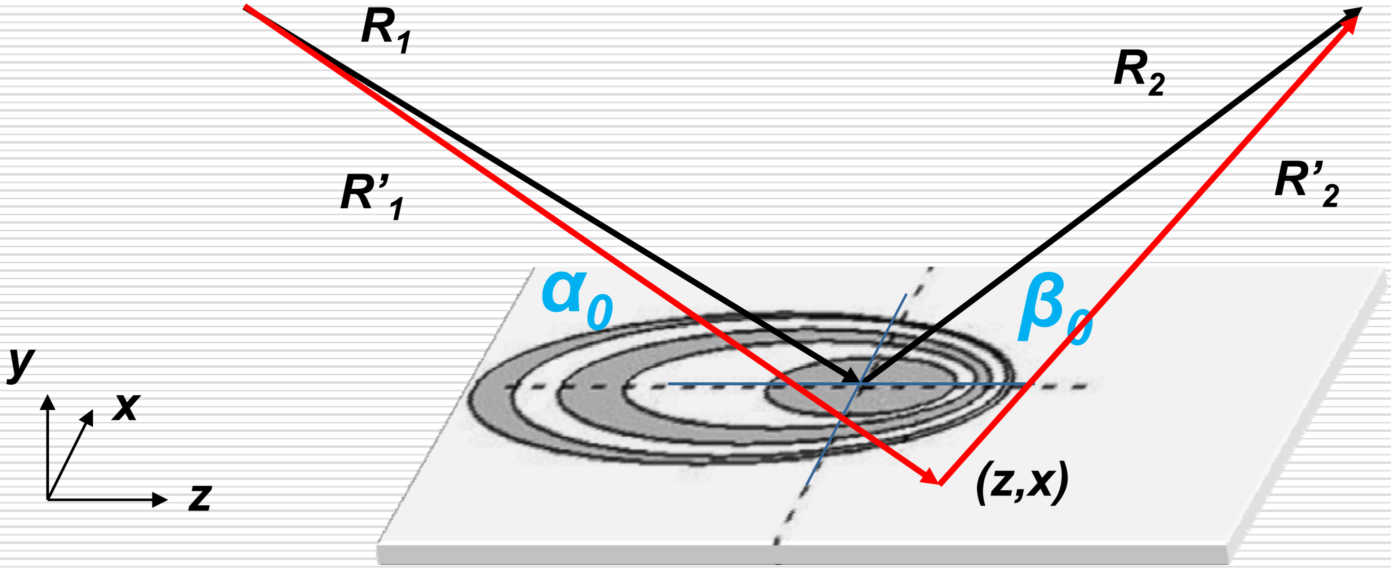


Parameters to define RZP

- Entrance arm length
- Exit arm length
- Grazing angle $\beta_0 = \alpha_0$

RAY parameters definition

Figure from Shahin Shahraei



RZP plane

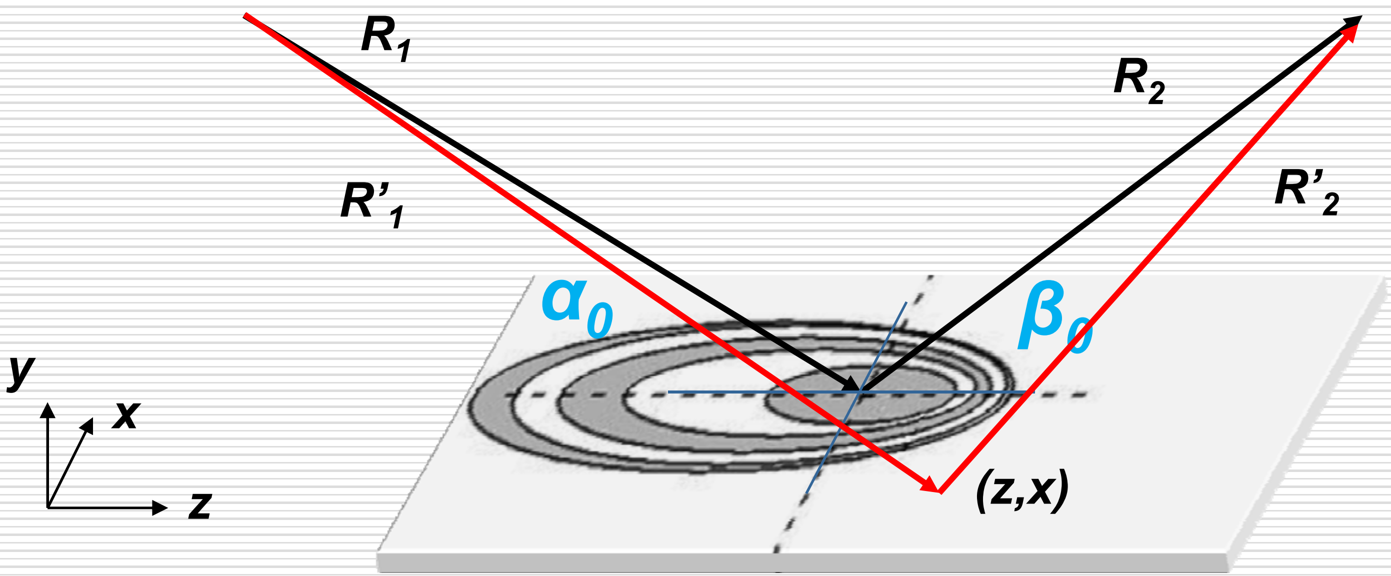
R' from user parameters

$$R'^2_1 = \left(R_2 \cos(\alpha_0) + z\right)^2 + x^2 + \left(R_2 \sin(\alpha_0)\right)^2$$

$$R'^2_2 = \left(R_2 \cos(\alpha_0) - z\right)^2 + x^2 + \left(R_2 \sin(\alpha_0)\right)^2$$

Vector model definition

Figure from Shahin Shahraei



RZP plane

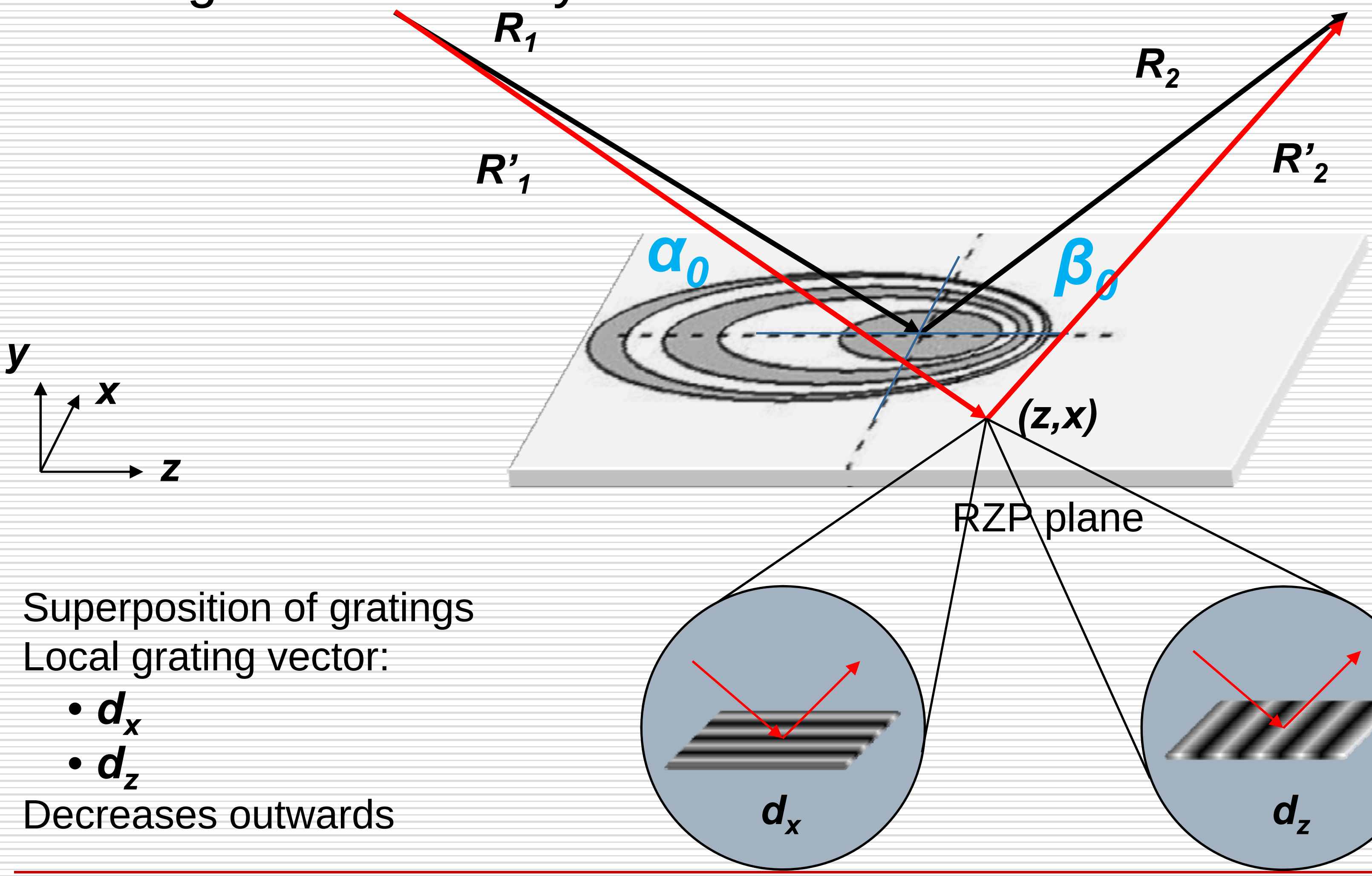
Direction cosines

Incident $\cos\alpha_z = \dfrac{R_1\cos(\alpha_0) + z}{R'_1}$ $\cos\alpha_x = \dfrac{x}{R'_1}$ $\cos\alpha_y = \dfrac{R_1\sin(\alpha_0)}{R'_1}$

Diffracted $\cos\beta_z = \dfrac{R_2\cos(\alpha_0) - z}{R'_2}$ $\cos\beta_x = \dfrac{x}{R'_2}$ $\cos\beta_y = \dfrac{R_2\sin(\alpha_0)}{R'_2}$

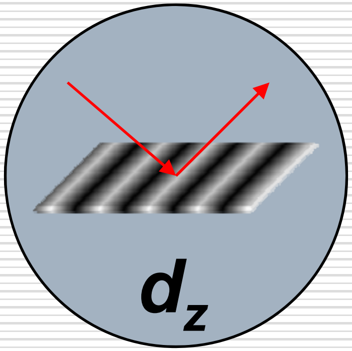
Main calculation principle

Grating subrutine by Michel Neviere

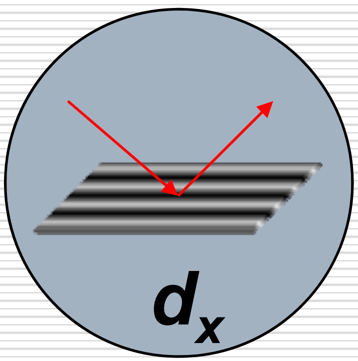


- Superposition of gratings
- Local grating vector:
  - d_x
  - d_z
- Decreases outwards

Superposed gratings vector parameter



$$DZ = \frac{1}{d_z} = \frac{1}{m\lambda}\left(\frac{R_1\cos(\alpha_0)+z}{R'_1} - \frac{R_2\cos(\alpha_0)-z}{R'_2}\right)$$



$$DX = \frac{1}{d_x} = \frac{1}{m\lambda}\left(\frac{x}{R'_1} + \frac{x}{R'_2}\right)$$

Determine Line density

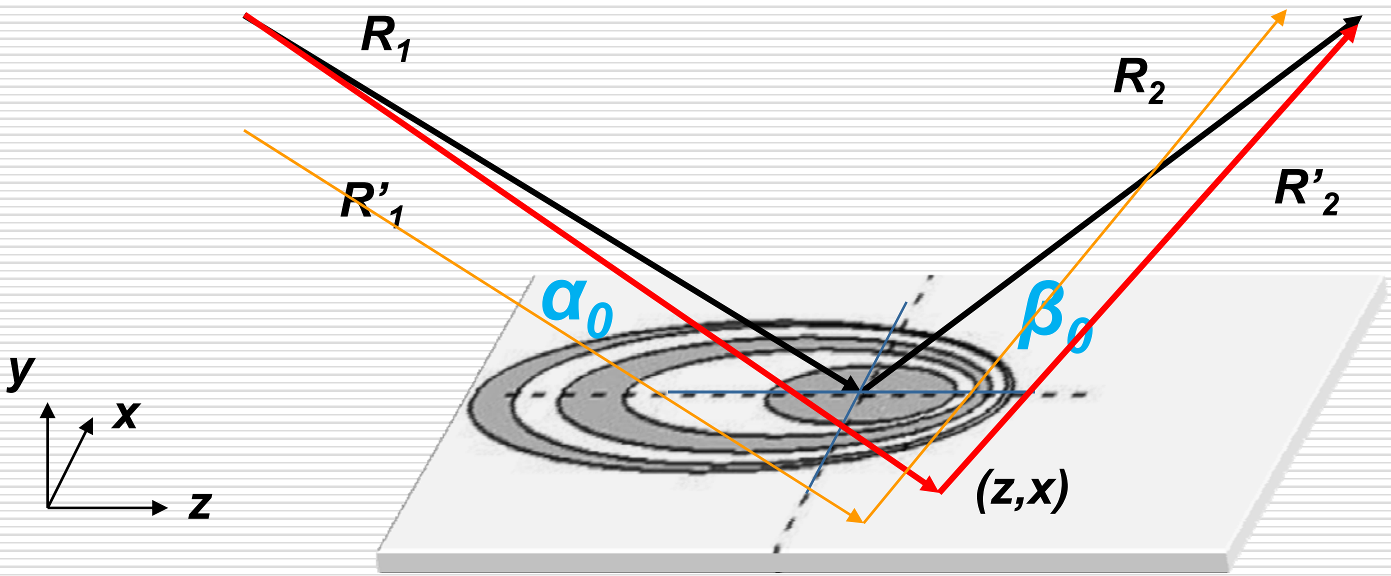
•Direction Cosines

•Design energy

Figure from Shahin Shahraei

Ray subrutin finctions

Figure from Shahin Shahraei



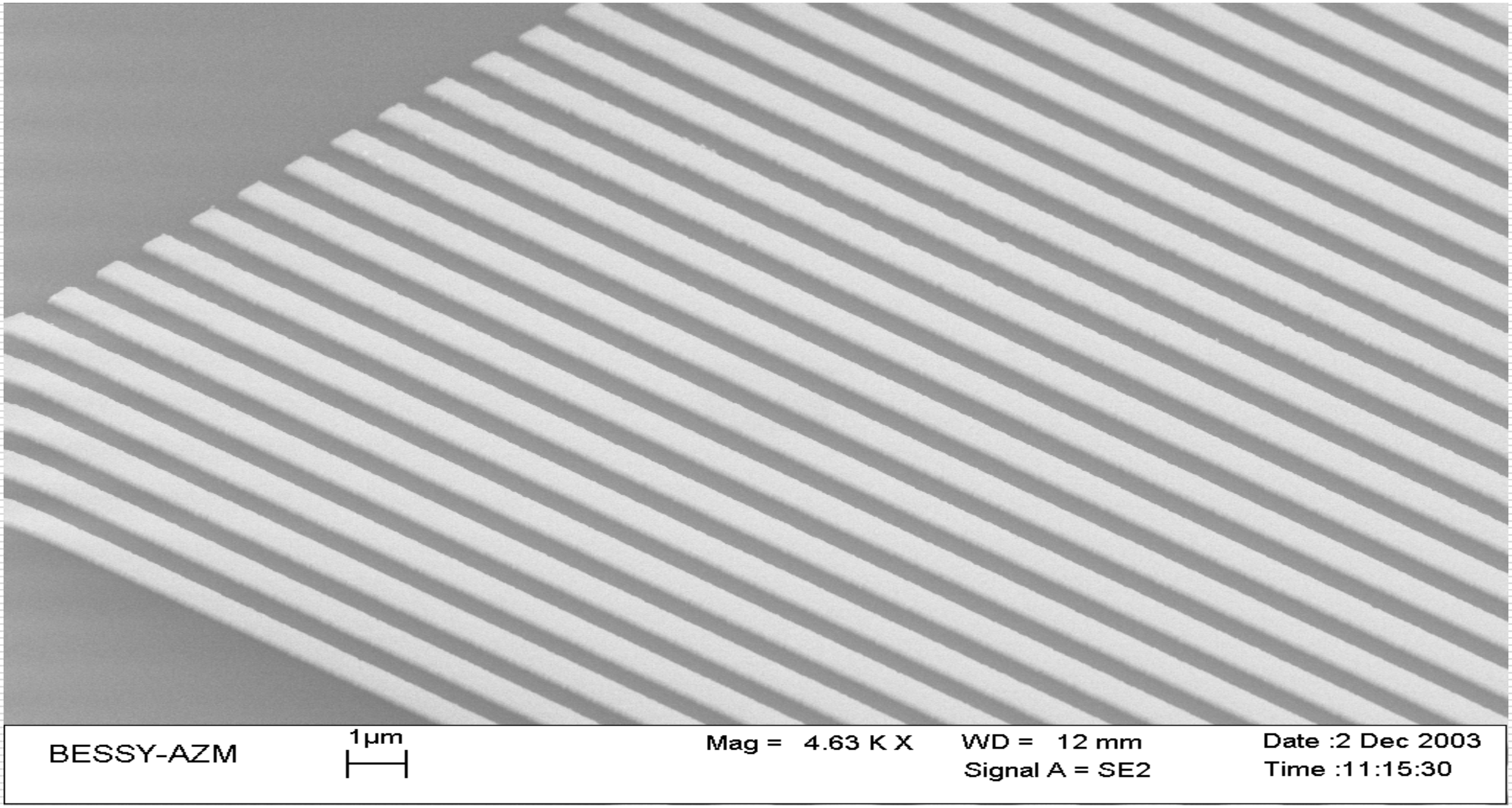
RZP plane

- Randomly generated Ray

  Position within source size

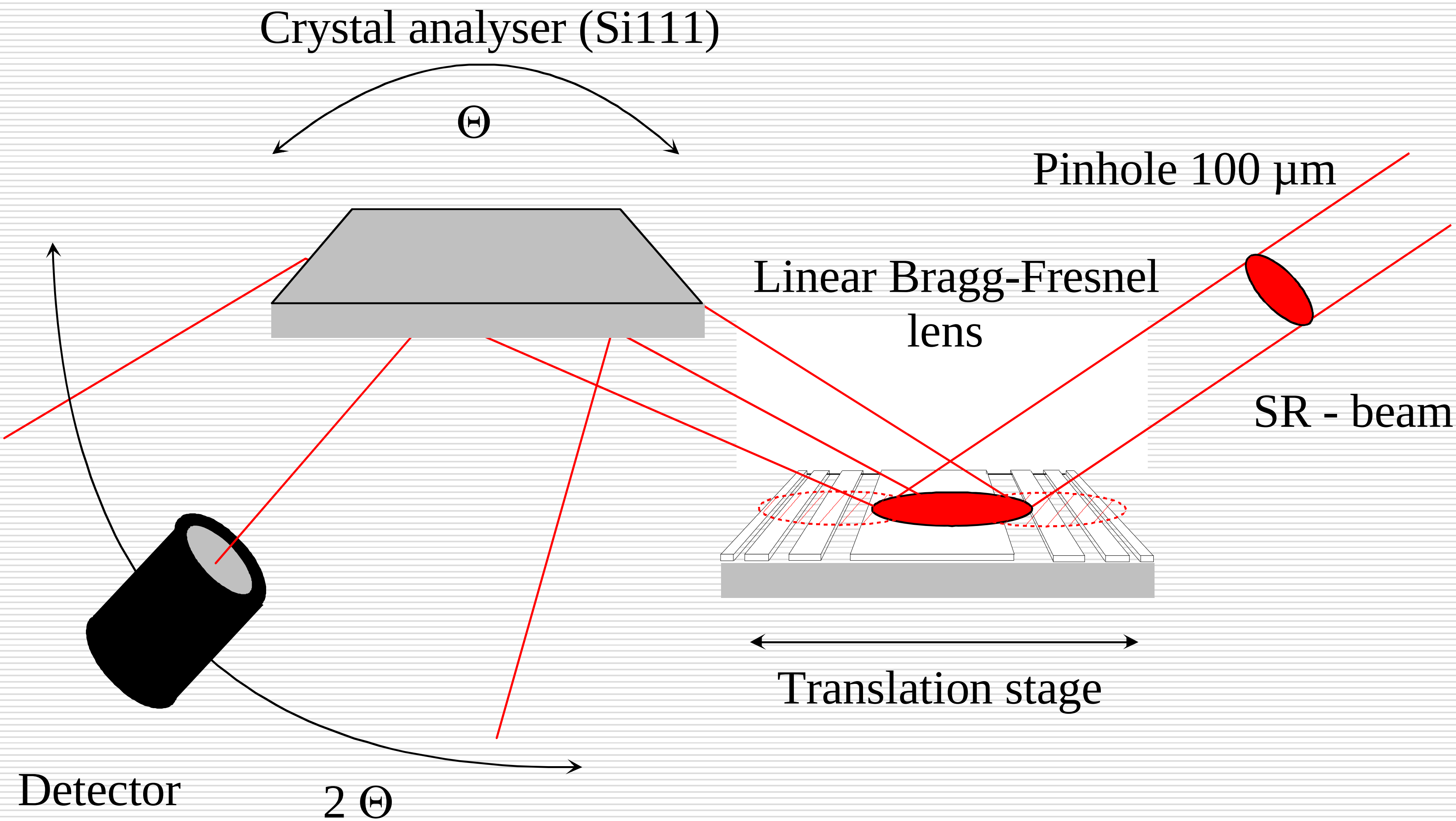
  Direction cosines within divergence
- Calculate DX, DZ at intercept
- Determine direction cosines of diffracted ray from grating subroutine

Ray RZP code application: Bragg-Fresnel Lens

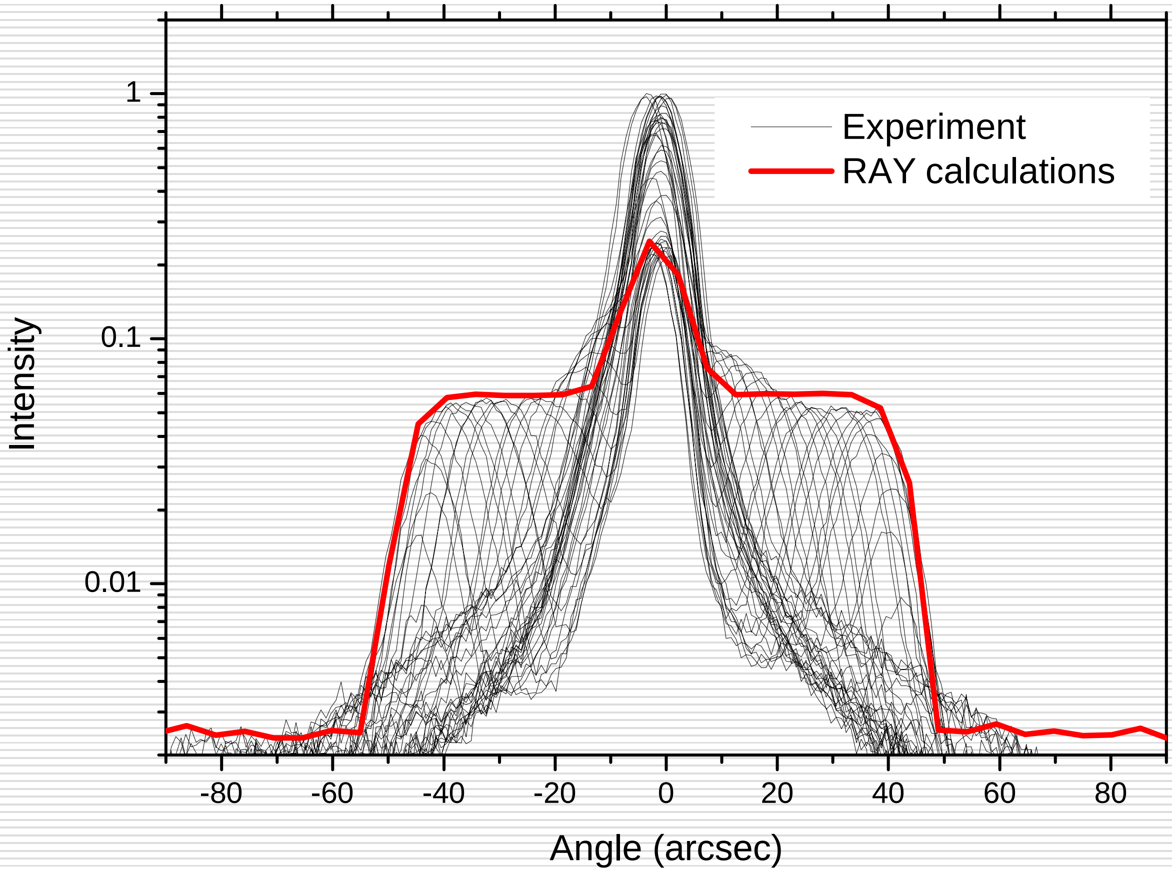


Last zones of the linear BFL on a Si 111 crystal surface (A. Firsov)

Bragg-Fresnel linear lens measurements



Bragg-Fresnel lens Spatial frequency spectra



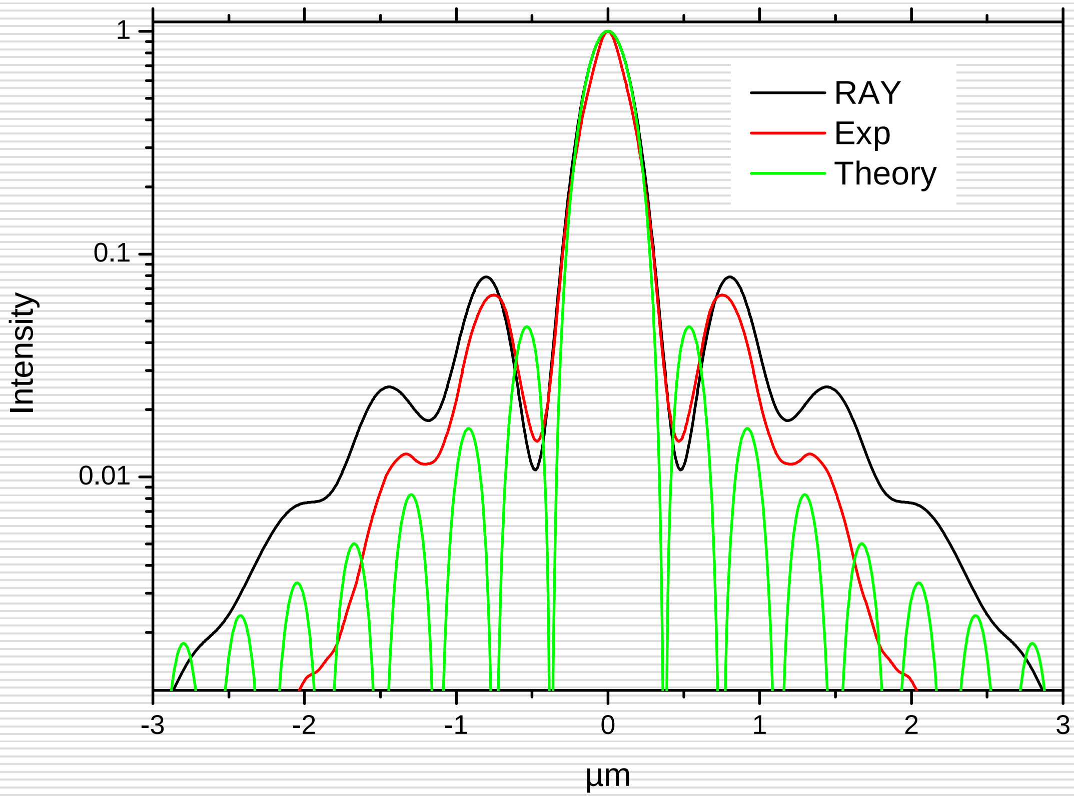
Bragg-Fresnel lens parameters:
Focal distance: 1 m
Minimum zone width: 1.47 µm
Energy : 8500 eV
Bragg angle: 13.45°
Au thickness: 200 nm

Corresponding **normal-incidence zone plate** parameters:

Focal distance: 1 m
Minimum zone width: 0.34 µm
Energy : 8500 eV
Bragg angle: 90°
Au thickness: 1350 nm

Beam divergence: 4.5 arc sec

Calculations and measurements of a spatial resolution



Fourier transformation of the spatial frequency spectrum.

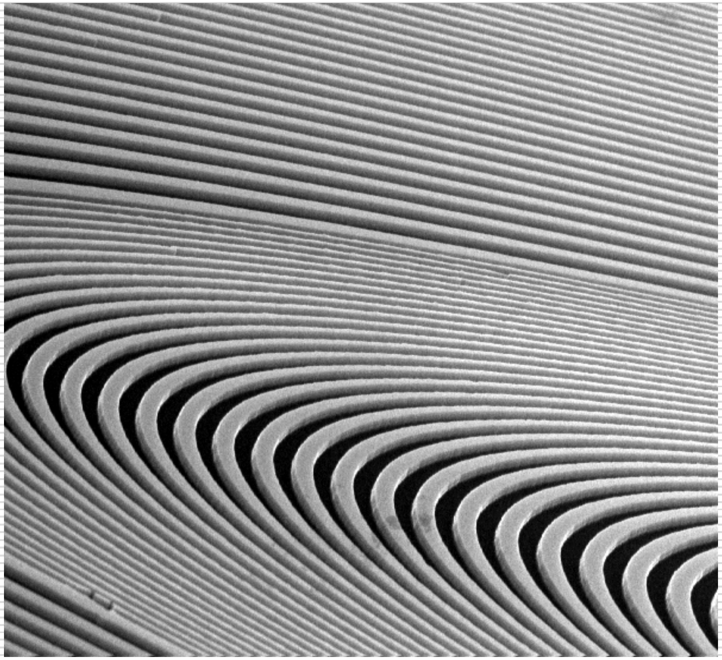
Experimental measurements and Ray model with beam divergence of 4.5”

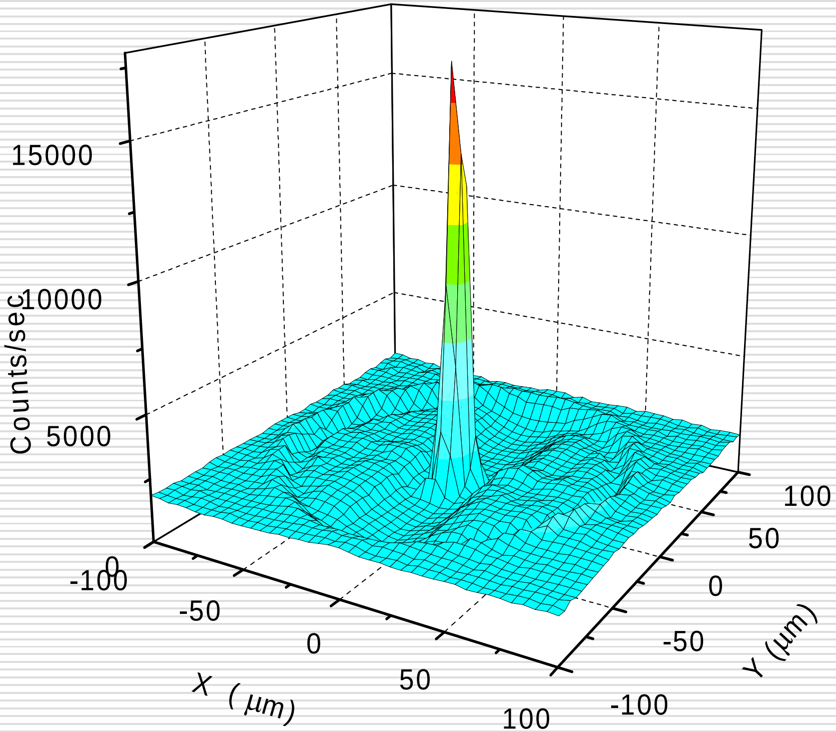
FWHM = 0.38 µm

Minimum zone 1.47 µm

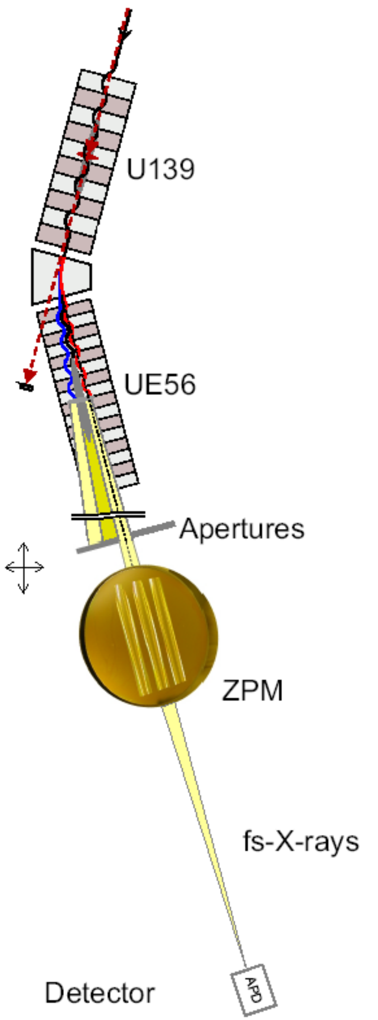
Synthetic holograms. Bragg-Fresnel optics.

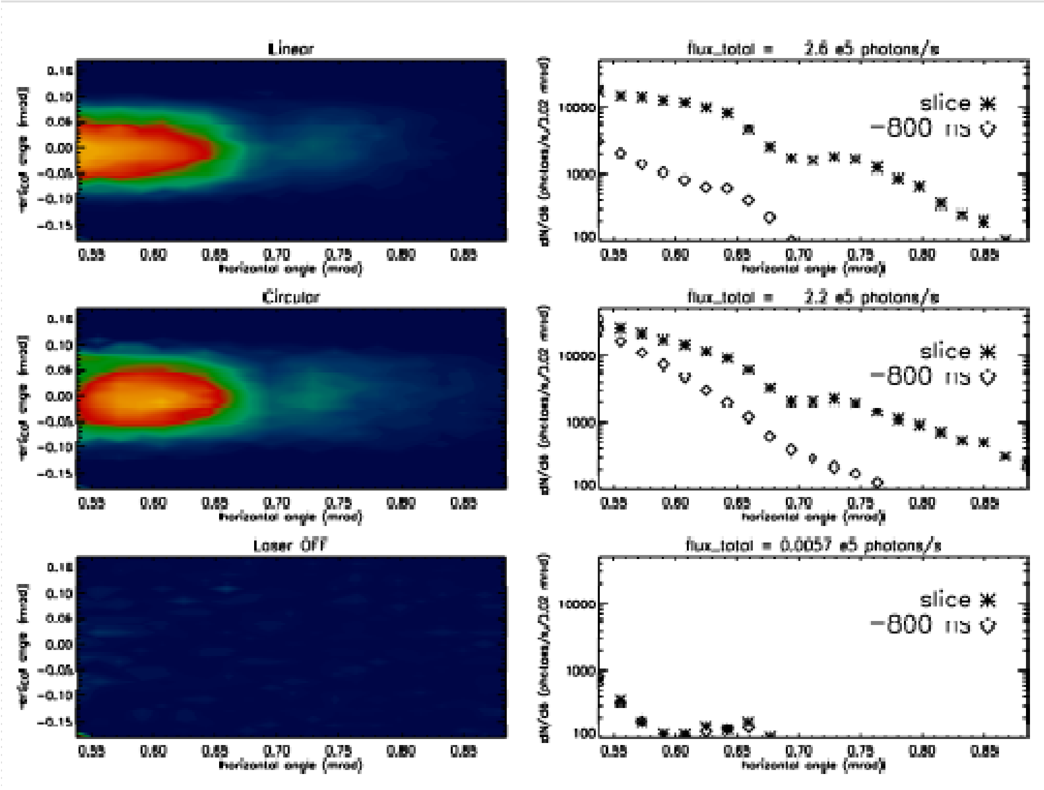
Elliptical Bragg-Fresnel Lens based on Si (111) with extended first and third diffraction orders. Dimensions: 3000μ by 484μ; last zone size – 0.3μ).

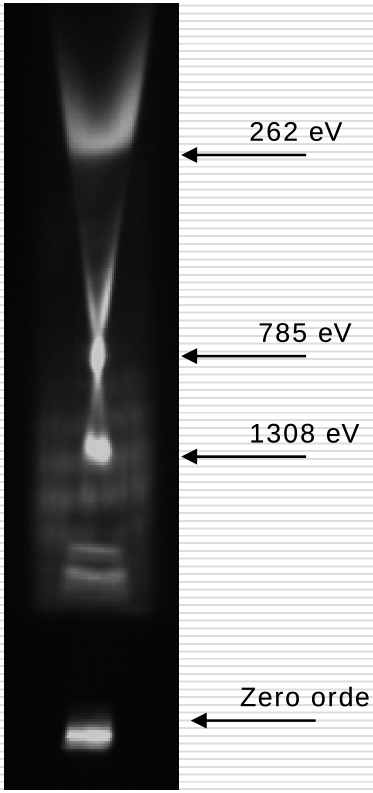




Reflection Zone Plates map sliced photons





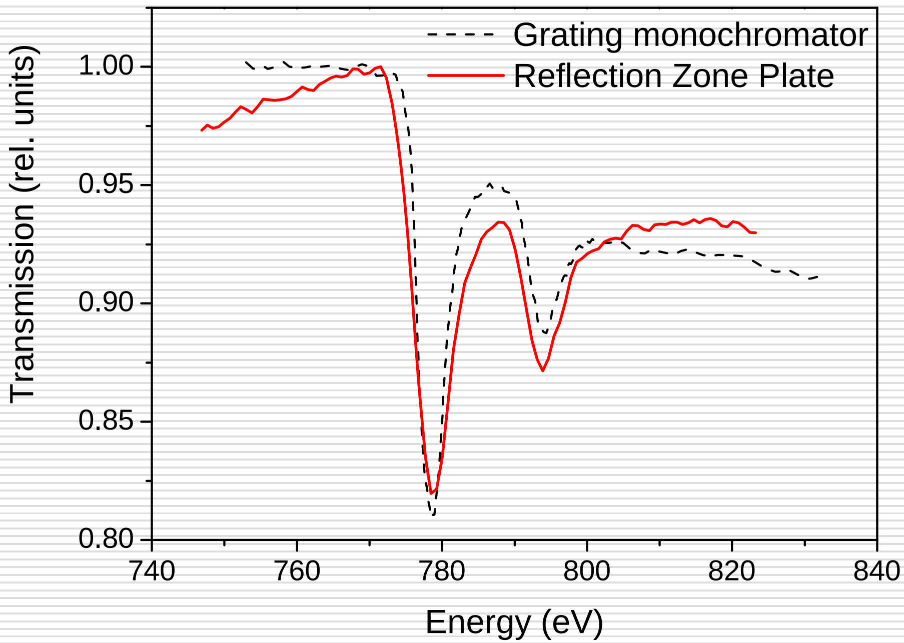


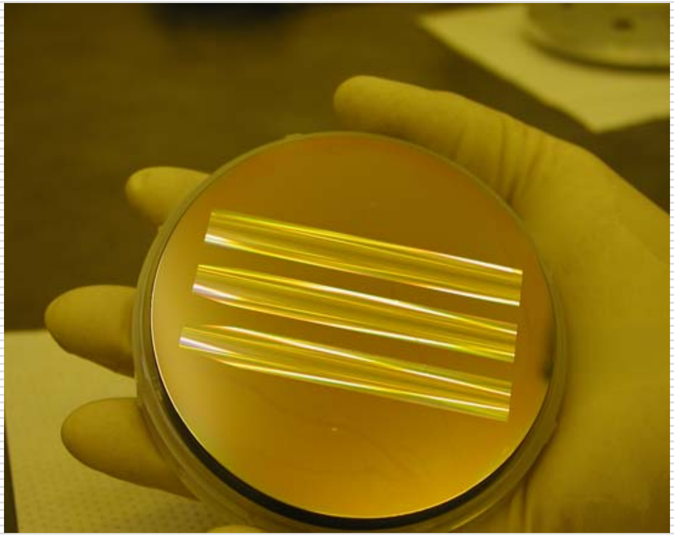
Beamline optics focal spot: **~ 300 µm (H) x 25 µm (V)**
Energy dispersion in focal plane: **~ 40 eV / mm**
Total beamline optics transmittance: **~ 6.5%**
Time resolution of beamline optics: **~ 30 fsec**

Reflection Zone Plates for fs XAS

Combination on the same optical element the reflection, focusing and dispersion.

- Extremely high radiation stability:	**> 10 GW / mm²**
- Time resolution:	**< 30 fsec**
- Integral efficiency:	**> 10%**
- Energy dispersion in focal plane:	**~ 40 eV / mm**

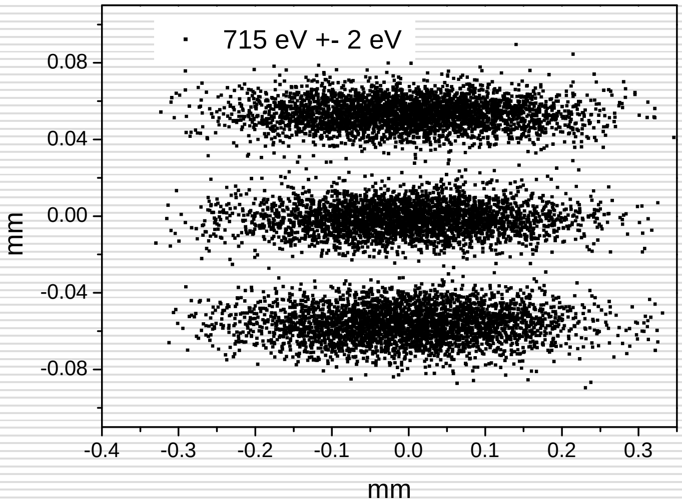


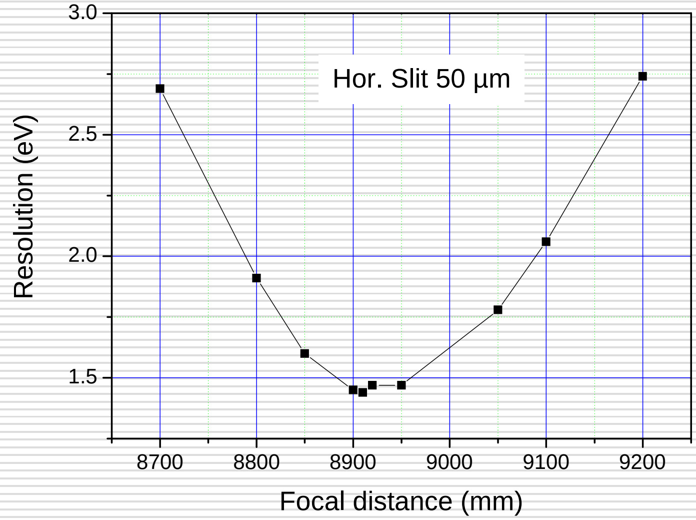


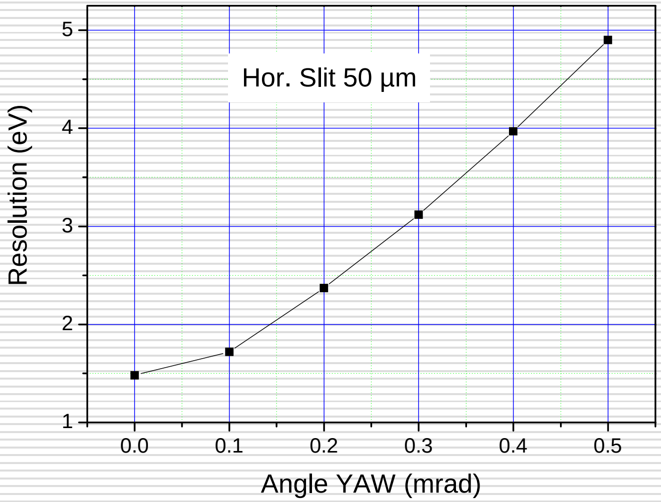
Gold reflection off-axis zone plates on a Si substrate: 715 eV, 785 eV, 861 eV. Focal distance: 902 cm. Outer zone: 1 µm. Aperture: 80 mm x 10 mm

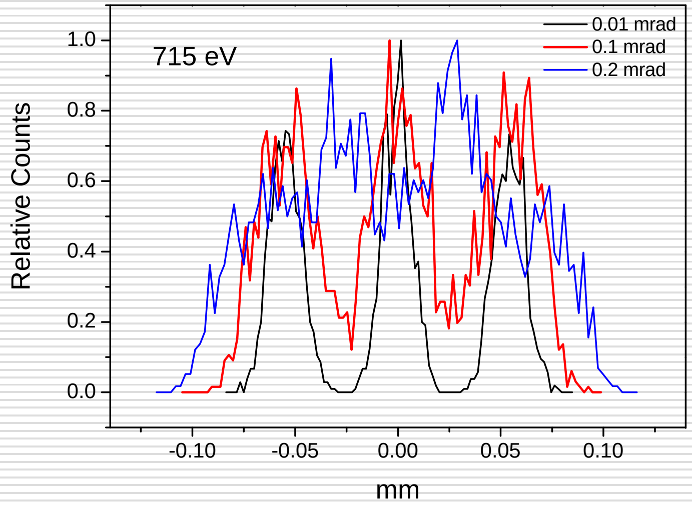
Lenses groove depth is 14 nm.

RAY RZP code application: fs RZP focal plane

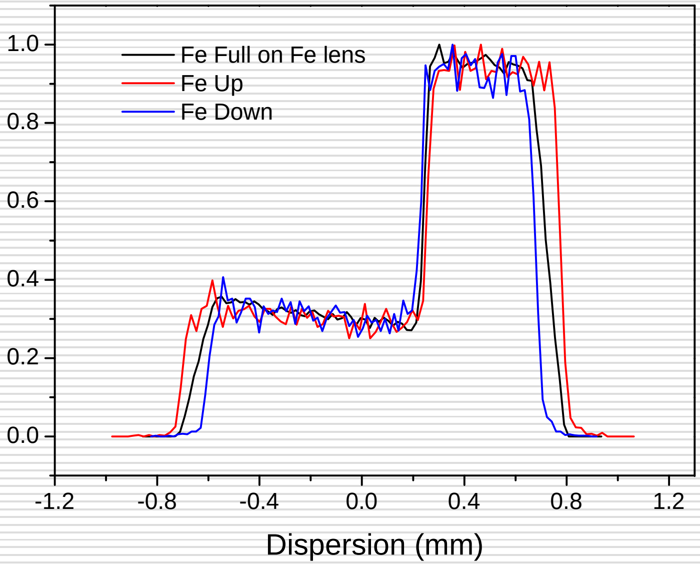




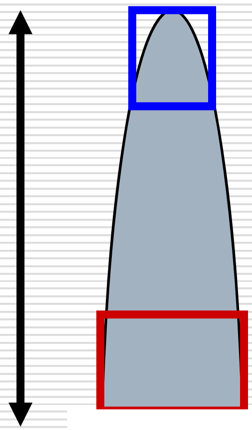




RAY code application: Absorption spectra on Fe and Co

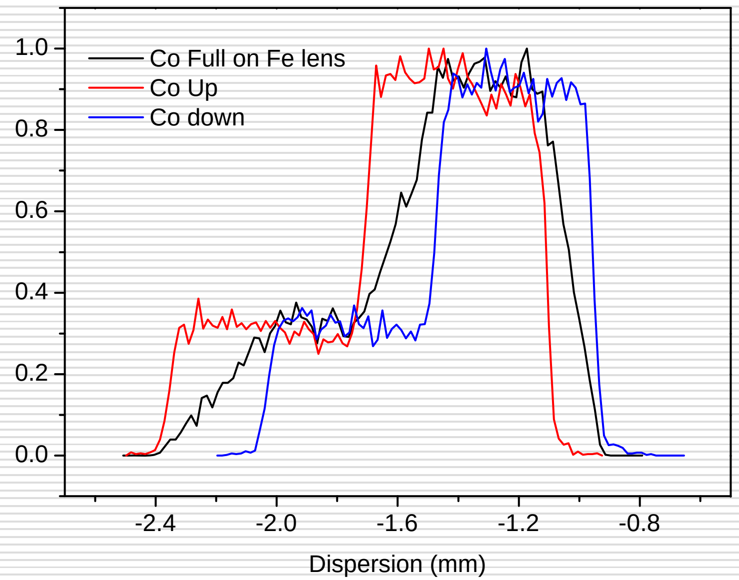


Absorption L α spectra of the Fe on a Fe-designed RZP

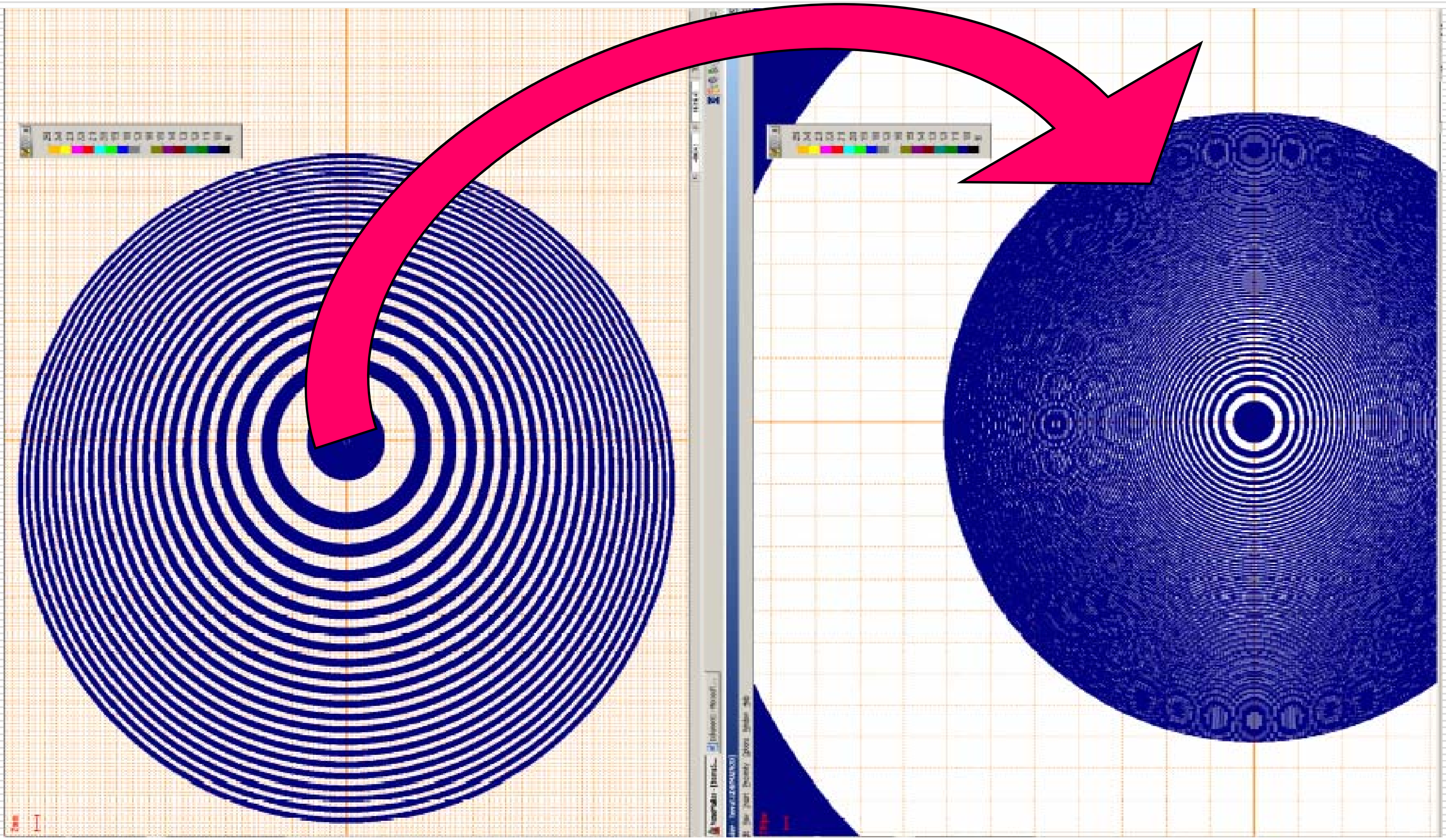


Different irradiated areas on a zone plate

Absorption L α spectra of the Co on a Fe-designed RZP

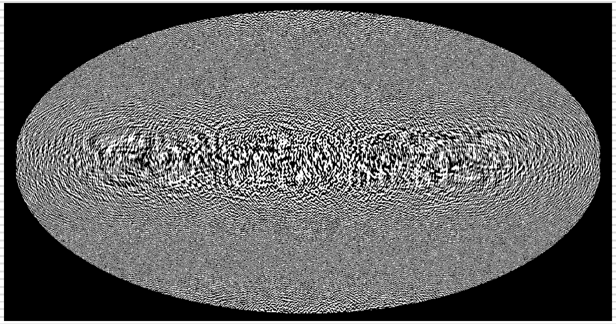


Lens for Terahertz radiation. Wavelength is 200 µm, focus distance is 10 cm.

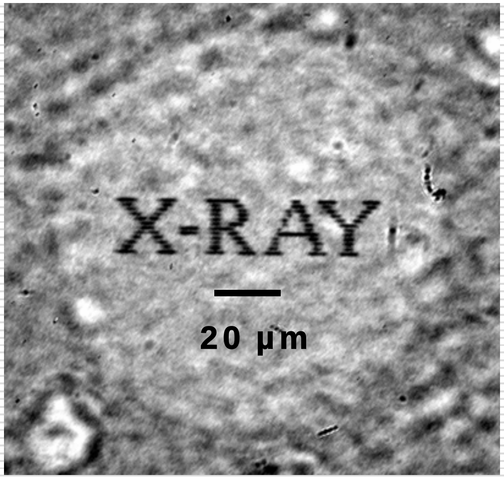


Synthetic holograms. Reconstruction.

Computer-generated hologram



Reconstructed image



Computer-generated "virtual" image

Thank you!