HELMHOLTZ
ZENTRUM BERLIN
für Materialien und Energie

```
######     ###     ##    ##
##   ##   ## ##     ##   ##
##   ##  ##   ##     ## ##
######  ##     ##     ###
## ##  #########      ##
##  ## ##      ##     ##
##   ####      ##     ##
```

The BESSY RAYTRACE PROGRAM

to calculate (not only)

SYNCHROTRON RADIATION BEAMLINES

Franz Schäfers
(HZB-BESSY)

HELMHOLTZ
ZENTRUM BERLIN
für Materialien und Energie

```
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##    ##  #######  ##        #######  #######    #####
```

a program

to calculate

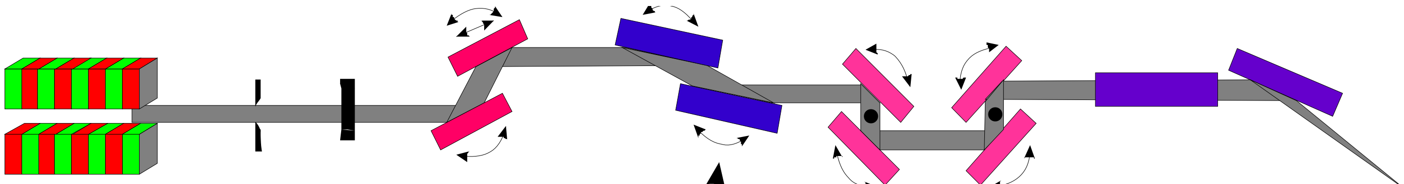
VUV/X-RAY OPTICAL ELEMENTS

and

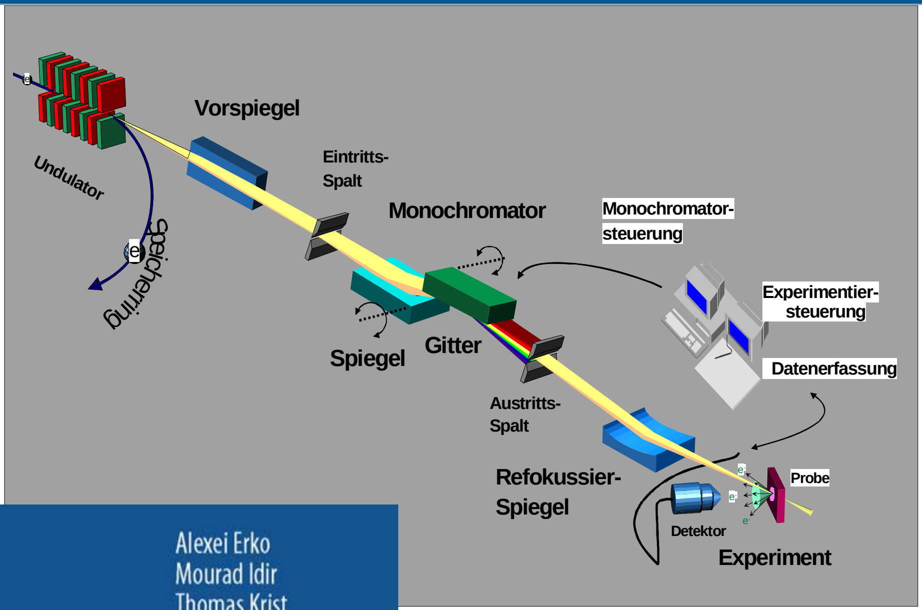
SYNCHROTRON RADIATION

BEAMLINES

Outline



History




```
#######         ###        ##     ##
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##    ##      ##   ##        ## ##
#######      ##     ##        ####
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##     ##    ##     ##         ##
```
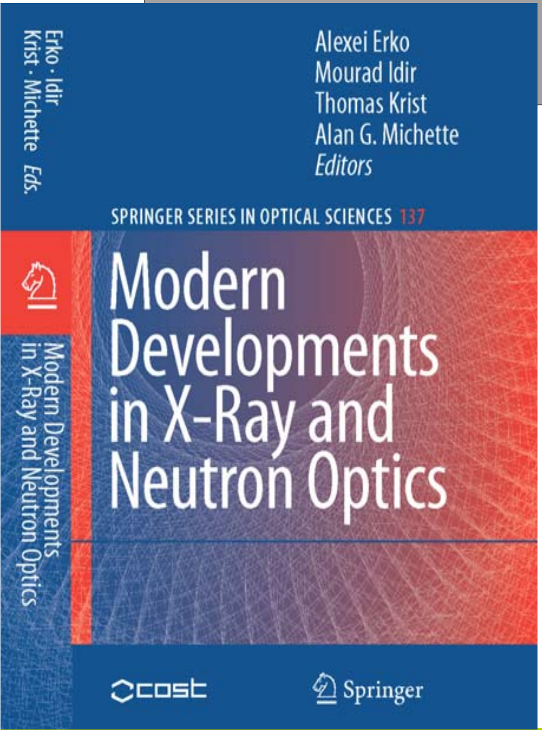
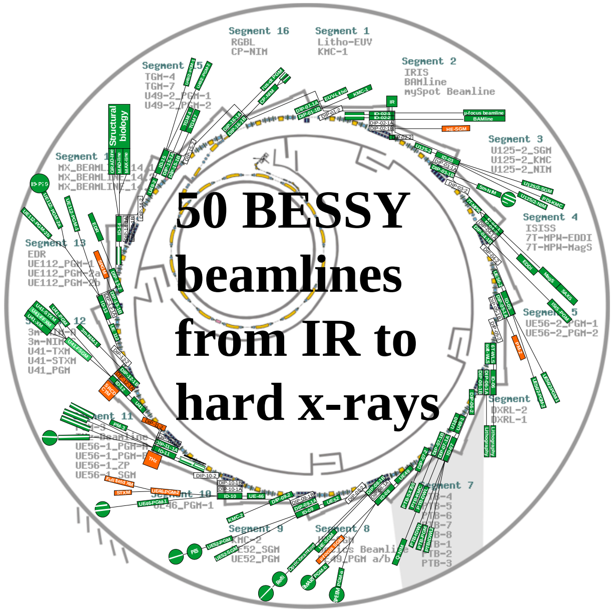

1984	FORTRAN-VMS/PDP-11
1989	VMS / VAX
1990	Surface profiles
1993	Stokes formalism
1994	Crystal optics
1995	Helical Undulators
1996	VMS / Alpha
2000	Multilayers
2002	PC-Windows / LINUX
2003	Pathlength
2005	Wavefront
2006	Expert's Optics
2008	Zoneplates
2008	Springer Vol. 137
2010	ML-Gratings
...	





~100 copies worldwide

Other raytrace tools

Geometric Optics (Intensity raytrace)

XOP Shadow (ESRF)

Xtrace (KIT)

...

Wavefront propagation codes (Fourier Optics)

PHASE (HZB-BESSY)

SRW (ESRF)

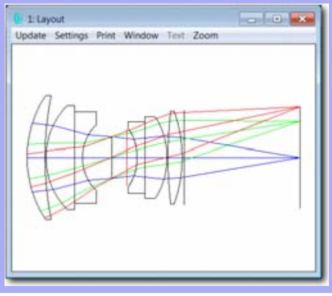
...

Commercial programmes (lenses et al.)

OSLO

(Lambda Research)

ZEMAX



...

Software structure

FORTRAN Source routines on TANGO:
(20.000 lines – 350 pages)

RAY.FOR REFLEC.FOR
Crysub.for
Oeinput.for
Optcon.for
Raylib.for
Source.for

VAX_routines.for

PC_routines.for

LINUX_routines.for

Executable program:

RAY.EXE

RAY.EXE

RAY.EXE

Export:

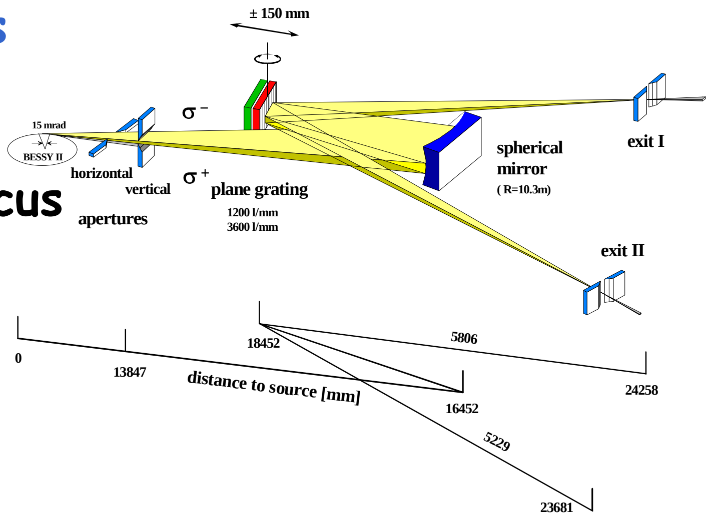
RAY_VAX.ZIP

RAY_PC.ZIP
(12.5 MB)

RAY_LINUX.ZIP

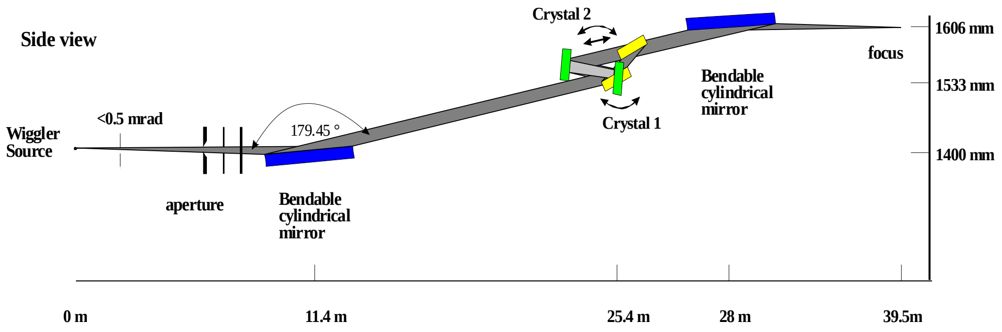
What is raytracing?

- Imaging / focusing properties of optical systems
  - create rays within a source volume
  - trace them through optical elements
  - display geometric distribution at the focus

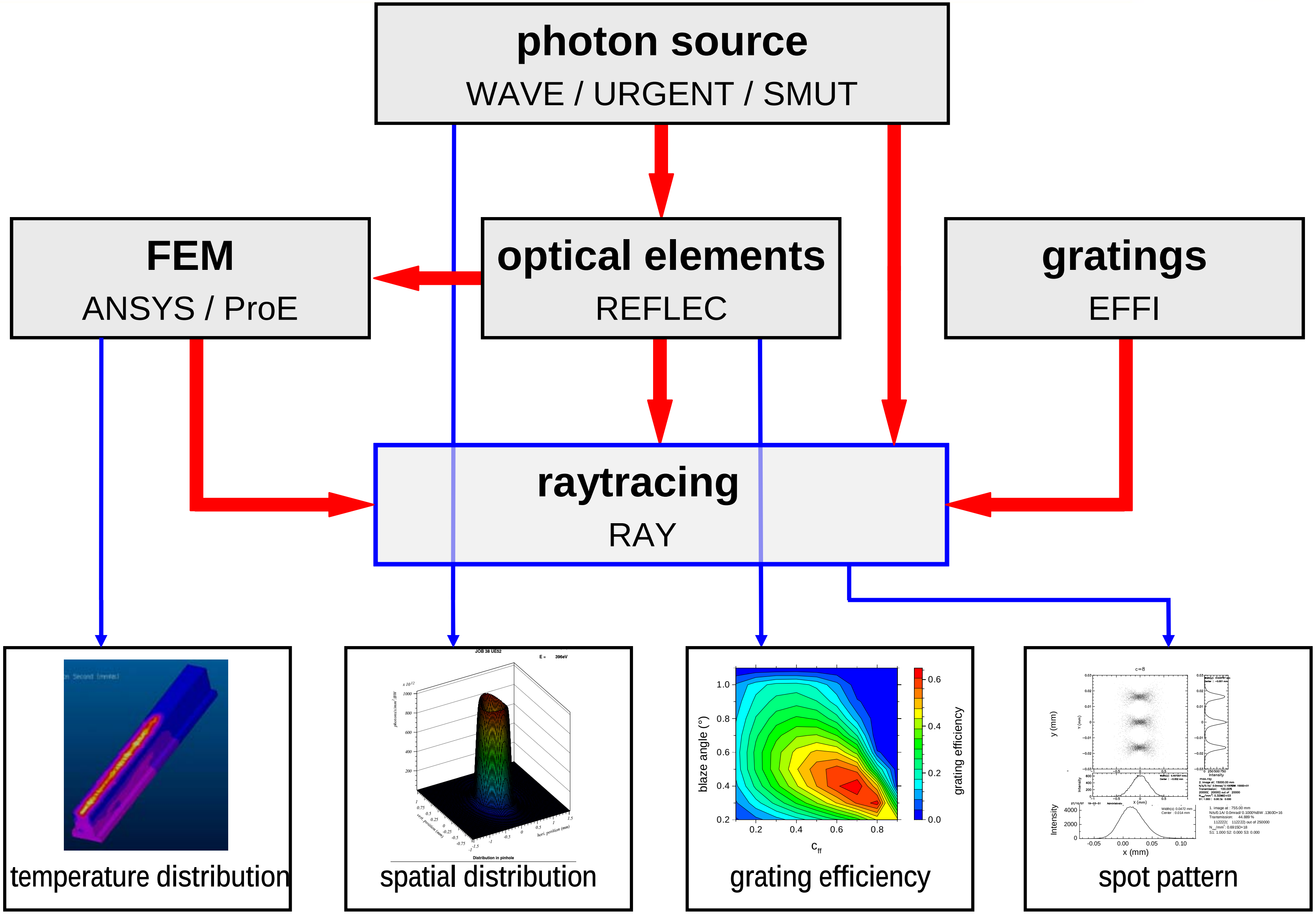


- Design tool for (SR-) beamlines
  - point (extended) sources
  - SR sources (dipole, Wiggler, Undulator)
  - general optical applications
  - predict performance under realistic conditions
  - specify requirements of optical elements before order

- RAY, REFLEC
  - user-friendly
  - easy to learn
  - easy accessible
  - every day use
  - minimum file handling
  - online graphic
  - quick response to new demands



BESSY optics software tools



Flow Chart of RAY

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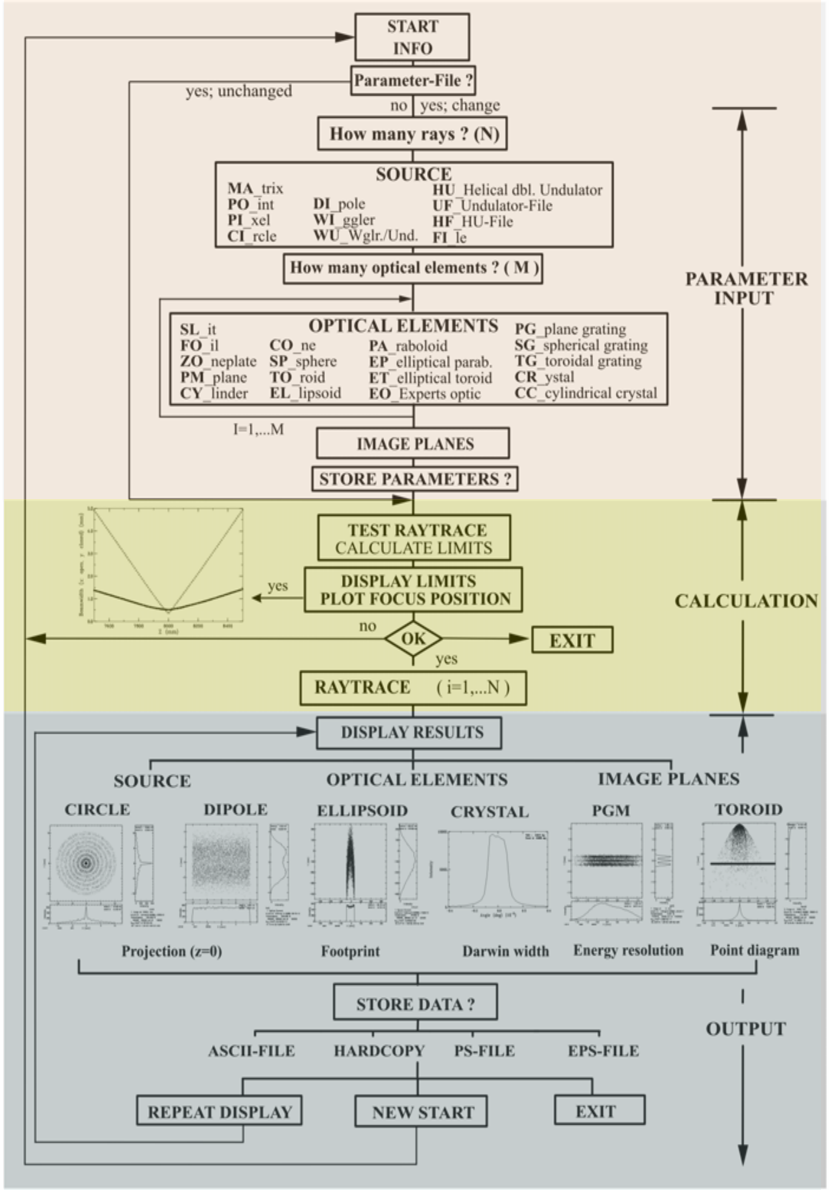
Parameter input

Raytrace

Graphics output



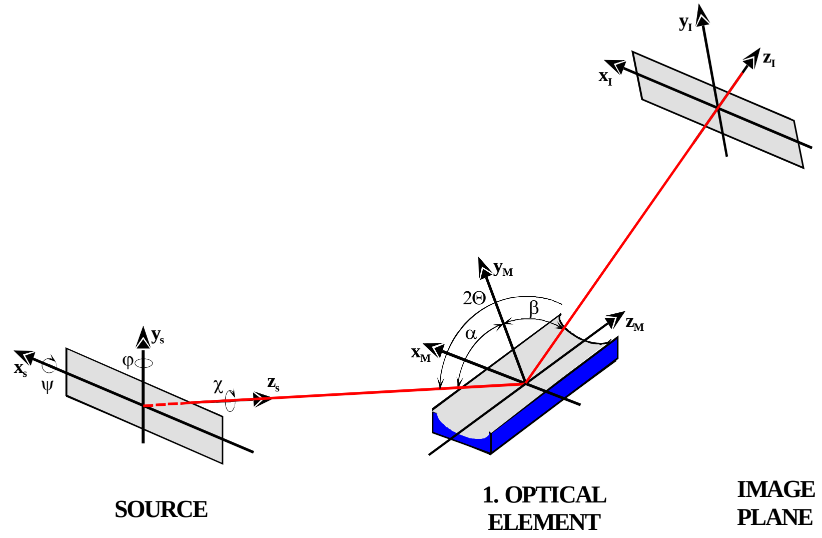
no Graphical User Interface,

but „remotely" attachable to IDL, LABVIEW, PC-Batchfile

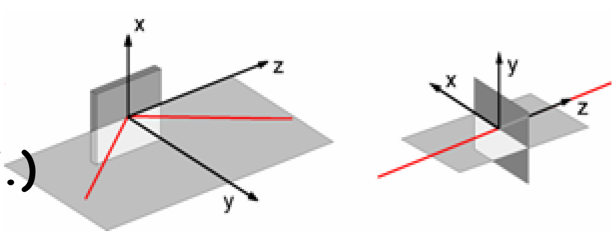
...

What is a ray?

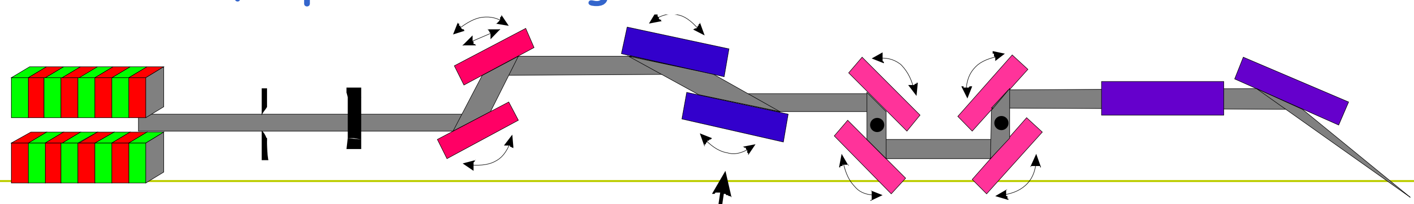
- A RAY is described by 12 parameters
  - geometric coordinates (x,y,z)
  - emission angle (l, m, n)
  - energy (hv)
  - polarisation (S_0, S_1, S_2, S_3)
  - time (pathlength) (t)



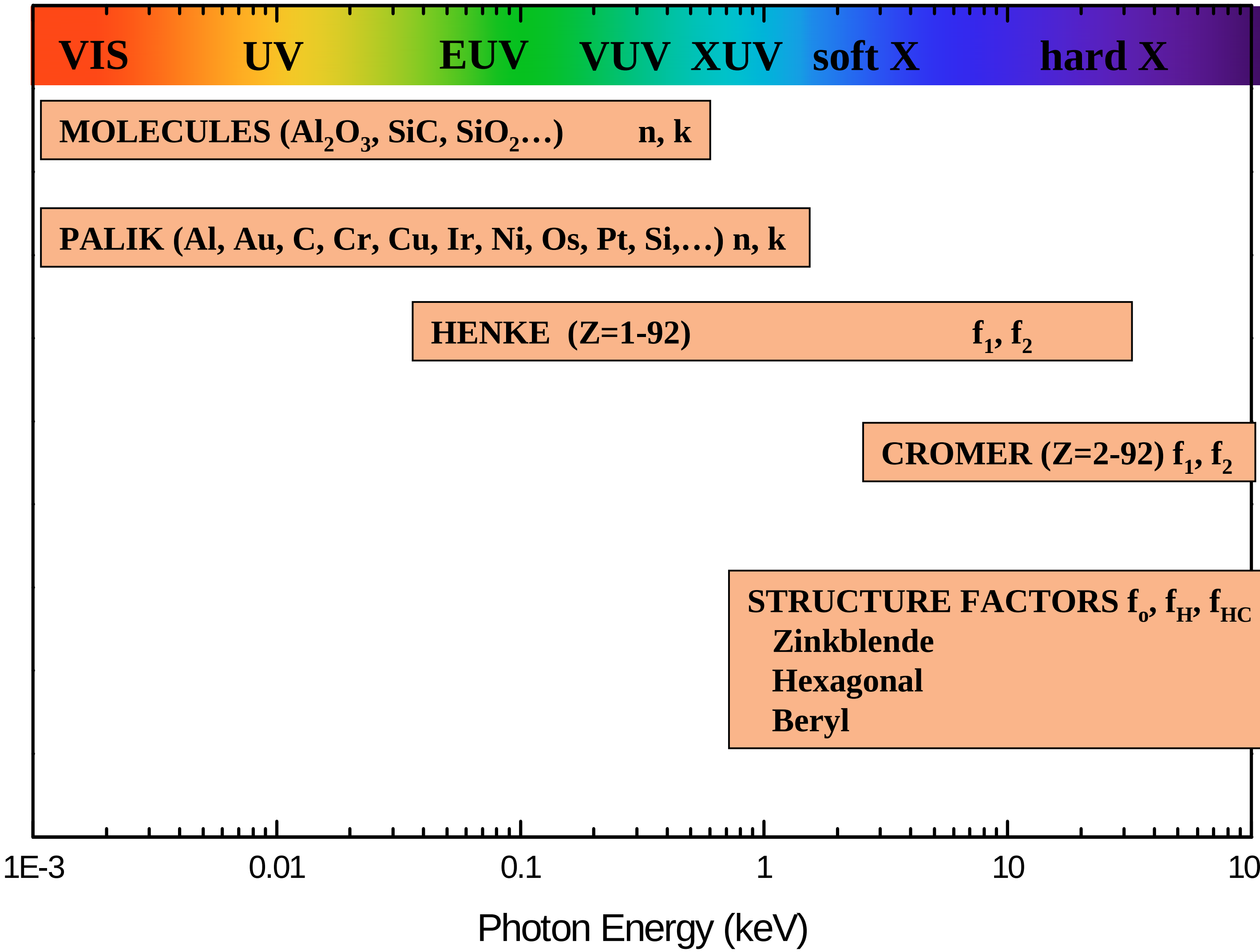
- The RAY starts in a SOURCE-volume with defined emission characteristics
  - point
  - dipole
  - undulator
- The RAY is modified by OPTICAL ELEMENTS acc. to laws of geometry and optics
  - transmitting - slits, foils (abs.)
  - reflecting - mirrors (refl.)
  - dispersing - gratings, zoneplates (eff.)
  - diffracting - crystals (refl.)



- All parameters of the RAY can be visualised at the Source, Optics and Image Planes



OPTICAL DATA TABLES



more than geometry…

Calculation of

- Reflectivity
- Efficiency
- Transmission
- Rocking curves
- Photon Flux
- Resolving power
- Polarisation

LIGHT SOURCE

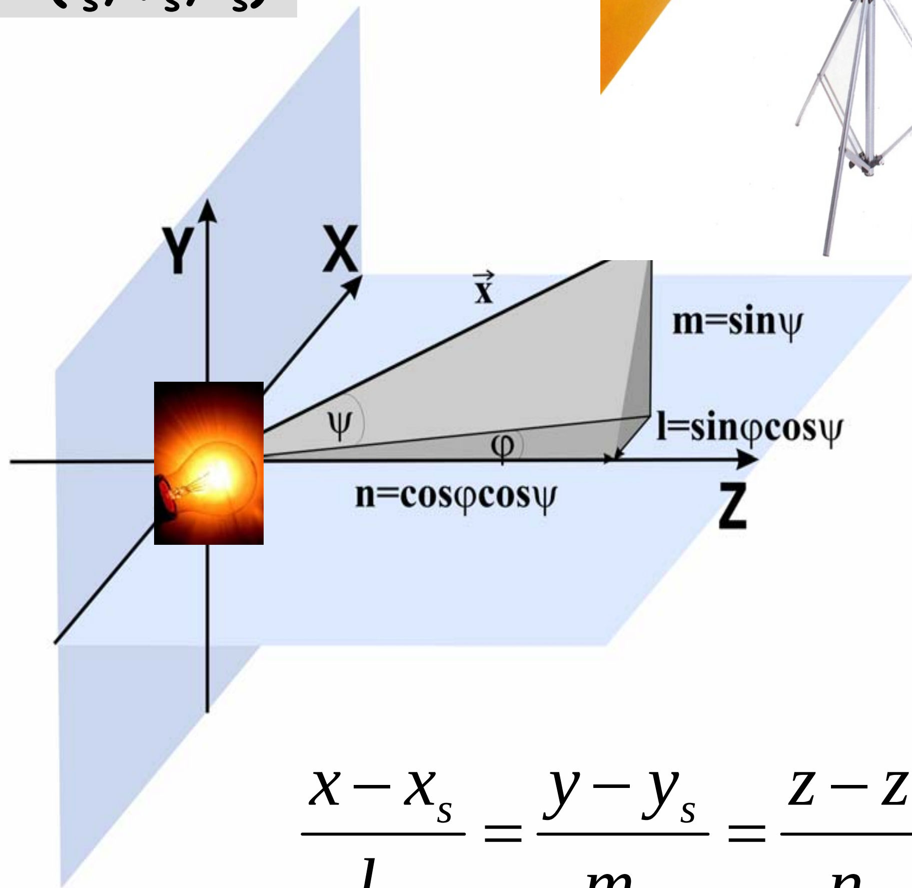
Create a ray

Point (x_s, y_s, z_s) and direction cosini (l_s, m_s, n_s)

$$\vec{x} = \vec{x}_S + t\vec{\alpha}_S$$

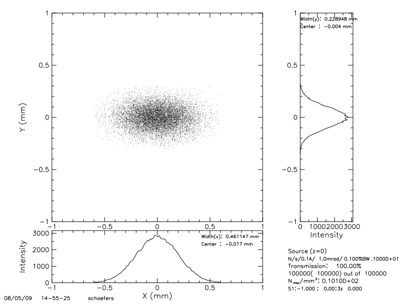
$$\vec{\alpha}_S = \begin{pmatrix} l_S \\ m_S \\ n_S \end{pmatrix} = \begin{pmatrix} \sin\varphi\cos\psi \\ \sin\psi \\ \cos\varphi\cos\psi \end{pmatrix}$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x_s \\ y_s \\ z_s \end{pmatrix} + t \begin{pmatrix} l_S \\ m_S \\ n_S \end{pmatrix}$$

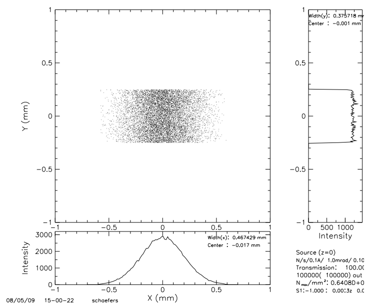


$$\frac{x - x_s}{l_S} = \frac{y - y_s}{m_S} = \frac{z - z_s}{n_S}$$

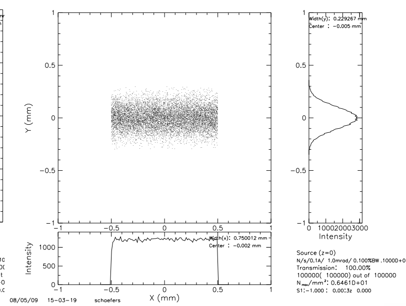
SOURCE TYPES



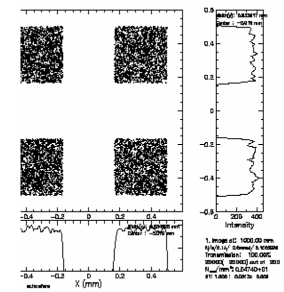
PO_int



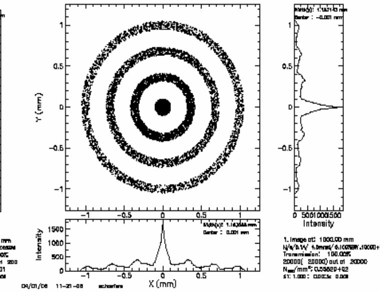
PO_int



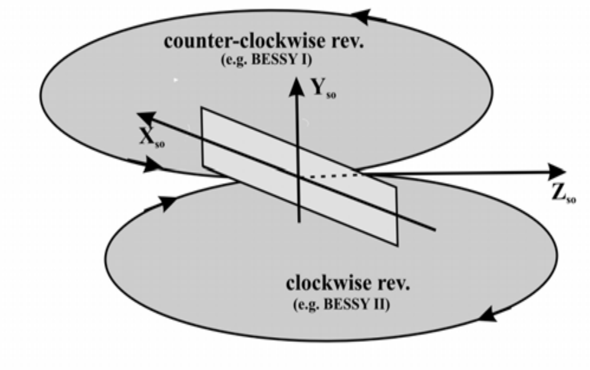
PO_int

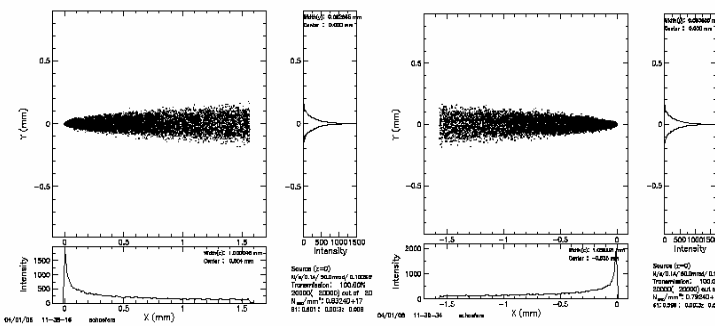


PI_xel

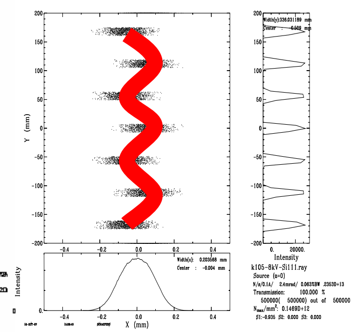


CI_rcle





DI_pole



WI_ggler

- Input by ASCII-data file:

UF_Undulator | HF_Helical Undulator | HU_Helical double Undulator | FI_le

- Realistic simulation of source intensity, volume and emission
- SR sources: polarisation included
  electron beam emittance effects
  detuning effects (orbit change, misalignment)

Basic law of RAY:
§1: ALL RAYS HAVE EQUAL PROBABILITY = INTENSITY

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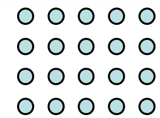
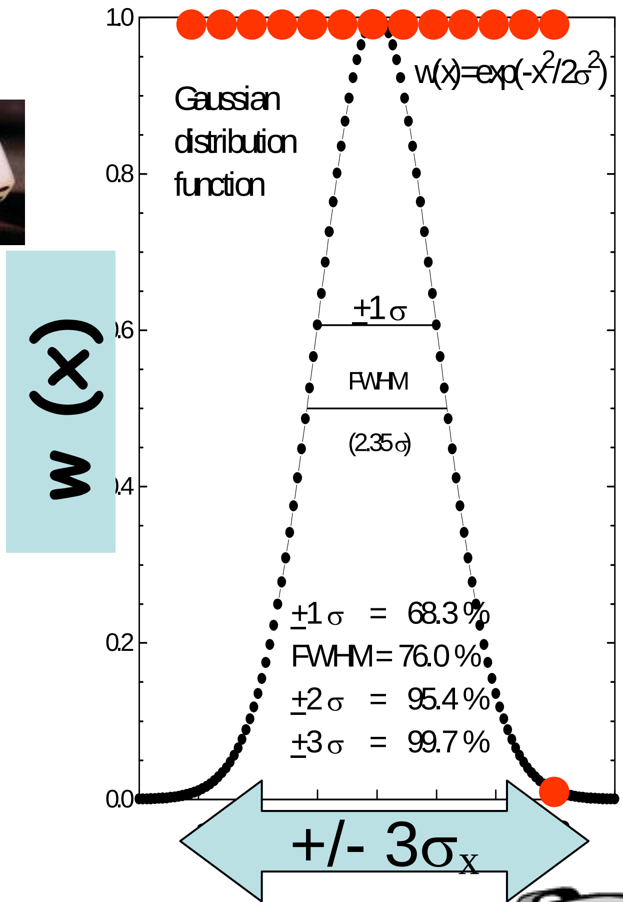


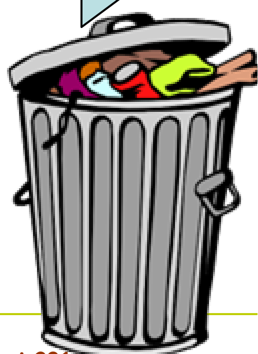
- **Systematic generation or…**
- **Statistical generation of rays within the source**
- **Probability distribution**
  - start coordinates x, y, z
  - emission angles φ, ψ
  - energy, time…
- **Advantages**
  - easy
  - few rays enough for realistic simulation (within given statistics)
  - no systematic errors (only statistical)



- **Example: Gaussian intensity profile**

1. get random number ran1
   $0 \le ran1 \le 1$
2. scale variable, e.g. x
   $x = (ran1 - 0.5)\,\delta x$
   $-\delta x/2 \le x \le \delta x/2$
3. probability for this x value
   $w(x) = \exp(-x^2/2\sigma^2)$
4. get random number ran2
   $0 \le ran2 \ge 1$
5. ACCEPT x ONLY IF
   $w(x) - ran2 \ge 0$
6. if not, goto 1

Applicable to ANY probability function

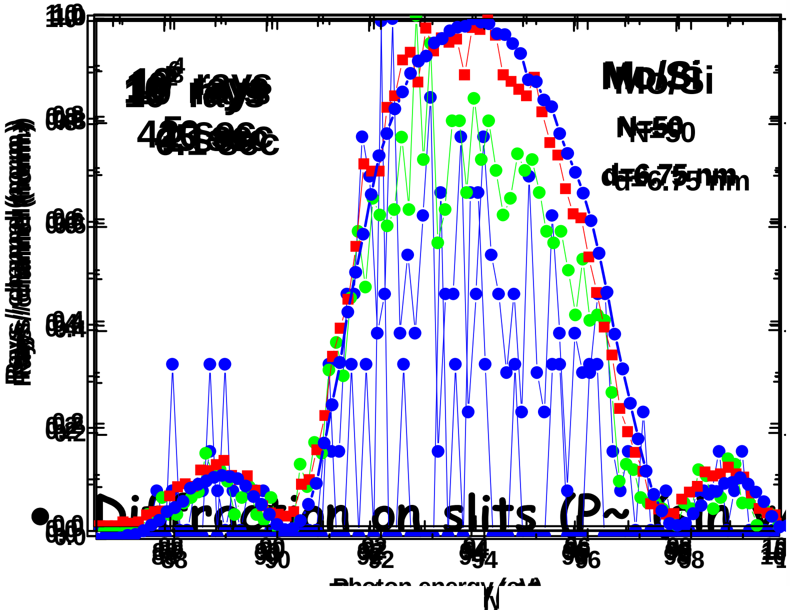


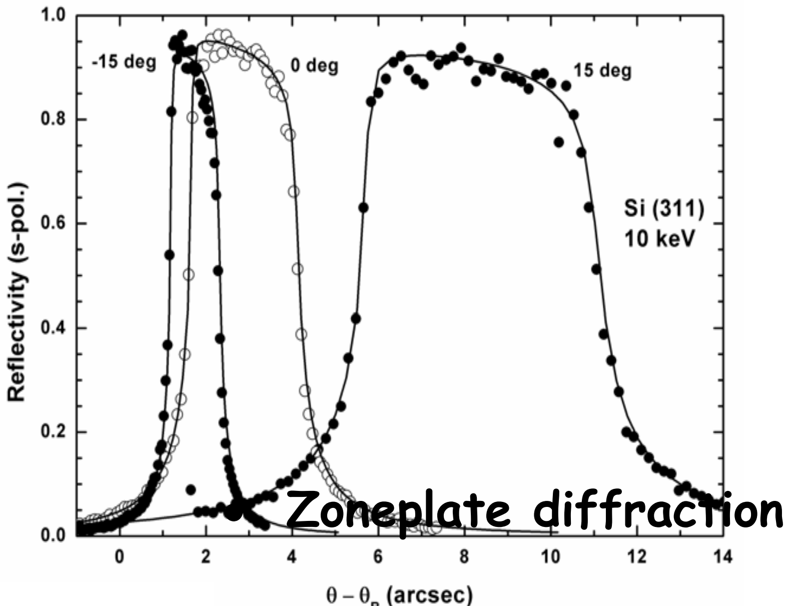
§2: ALL RAYS ARE INDEPENDENT, but… (Particles and Waves)

- Statistical treatment of an ensemble of rays

  Collective effects (Interference, diffraction…)

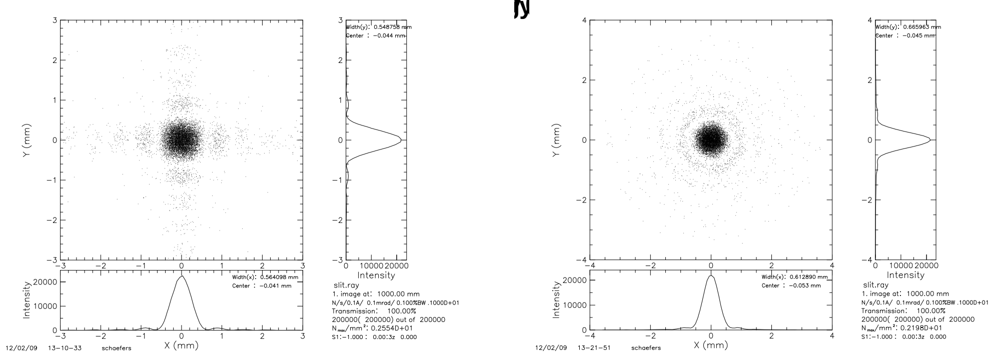
- Reflectivity loss / angle / energy (Rocking curves)

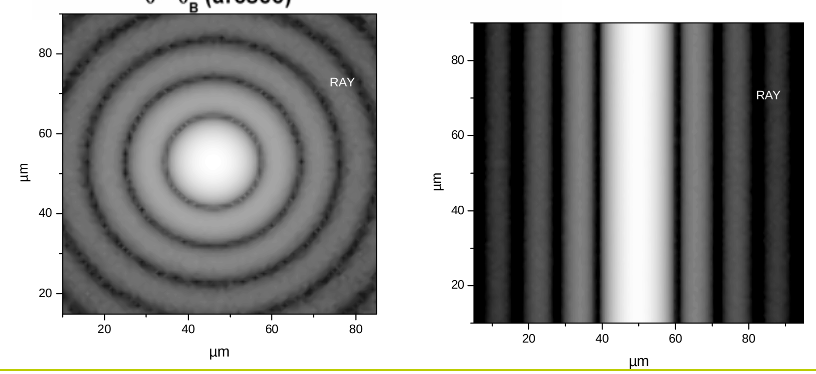




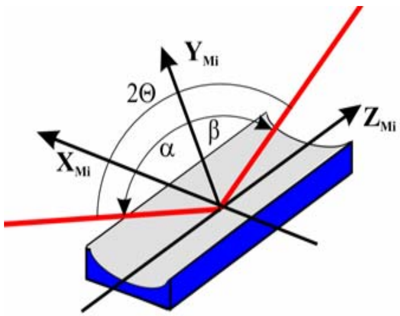
- Diffraction on slits

Zoneplate diffraction





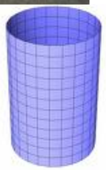
2nd, 3rd order surfaces (MI, GR, CR)



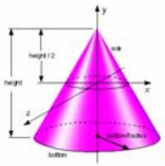
$$F(x,y,z) =$$
$$= a_{11}x^2 + a_{22}y^2 + a_{33}z^2 +$$
$$+ 2a_{12}xy + 2a_{13}xz + 2a_{23}yz +$$
$$+ 2a_{14}x + 2a_{24}y + 2a_{34}z + a_{44}$$
$$+ b_{12}x^2y + b_{21}xy^2 +$$
$$+ b_{13}x^2z + b_{31}xz^2 +$$
$$+ b_{23}y^2z + b_{32}yz^2 = 0$$

PM_plane m.

CY_linder (x,z)



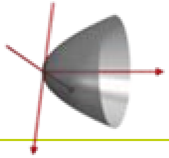
CO_ne



SP_here

EL_lipsoid

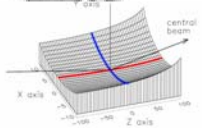
PA_raboloid (circ., ell.)



TO_roid

ET_elliptical toroid

DI_aboloid



EO_expert's optic

Textbook raytracing

Find the intersection point x_M, y_M, z_M

Find the local normal vector

(Include slope errors, surface profile)

$$\vec{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} = \frac{1}{\sqrt{f_x^2 + f_y^2 + f_z^2}} \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} \qquad \vec{f} = \nabla F$$

Find the direction of outgoing ray

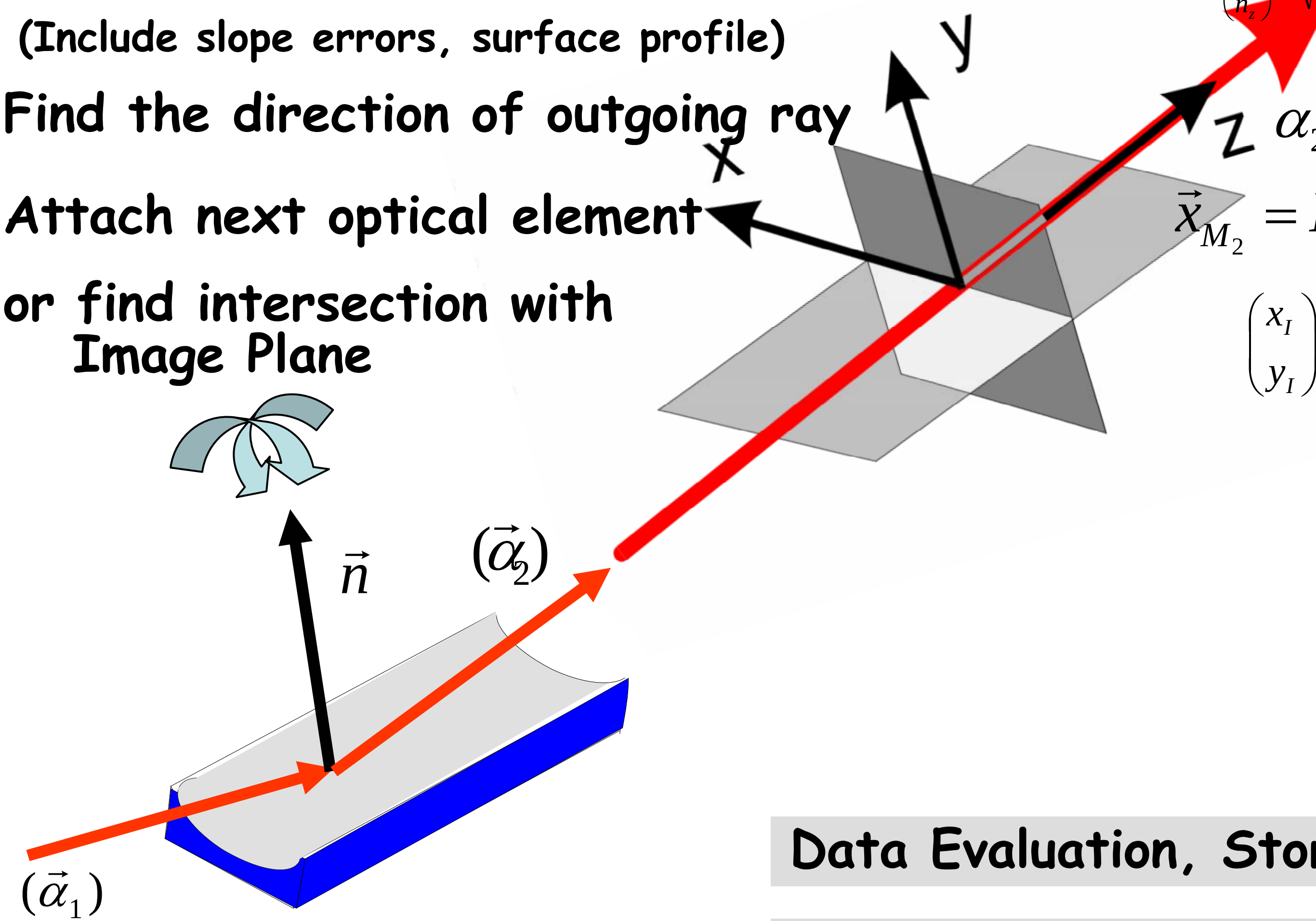
$$\vec{\alpha}_2 = \vec{\alpha}_1 - 2 \cdot (\vec{n} \circ \vec{\alpha}_1)\vec{n}$$

Attach next optical element

$$\vec{x}_{M_2} = D_{\tilde{x}}(\theta) D_z(\chi) T_z(z_q) \cdot \vec{x}_{M_1}$$

or find intersection with Image Plane

$$\begin{pmatrix} x_I \\ y_I \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} + \frac{1}{n} \begin{pmatrix} l \\ m \end{pmatrix} (z_{I_{1,2,3}} - z)$$

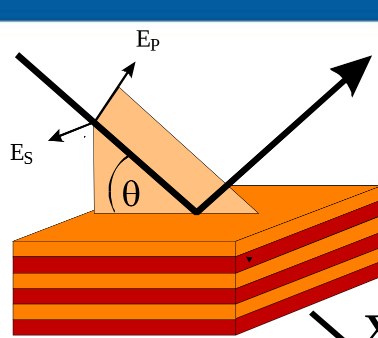


Data Evaluation, Storage, Display

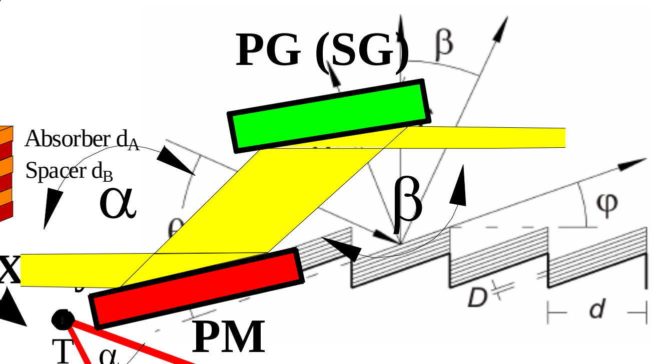
Start with a new ray in the source…

Features of optical elements

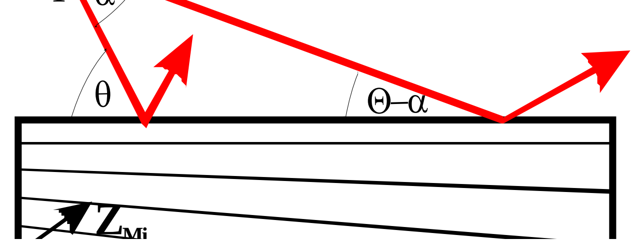
- (Multilayer-) Coatings on Optics



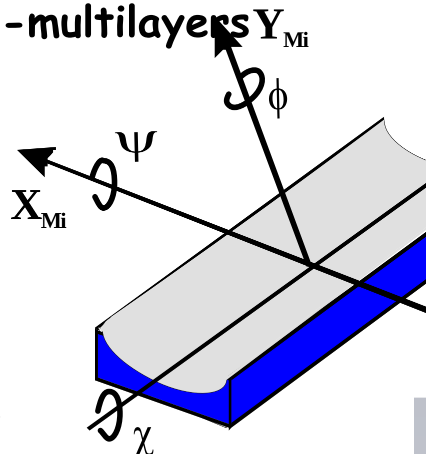
- Special monochromator mounts:
  SX700 plane grating PGM
  Spherical grating SGM



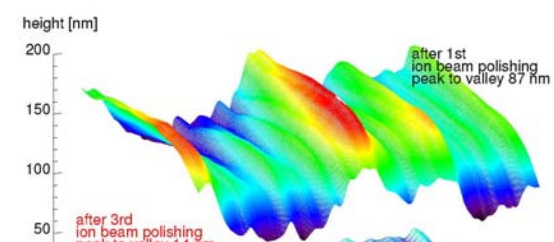
Varied Line Spacing-(VLS-) gratings
Laterally graded crystals, -multilayers



- Miscellaneous: Misalignment



- Measured, calc. surface profiles



- Rectangular, circular shape or rings (capillaries)

AXO

APPLIED X-RAY OPTICS

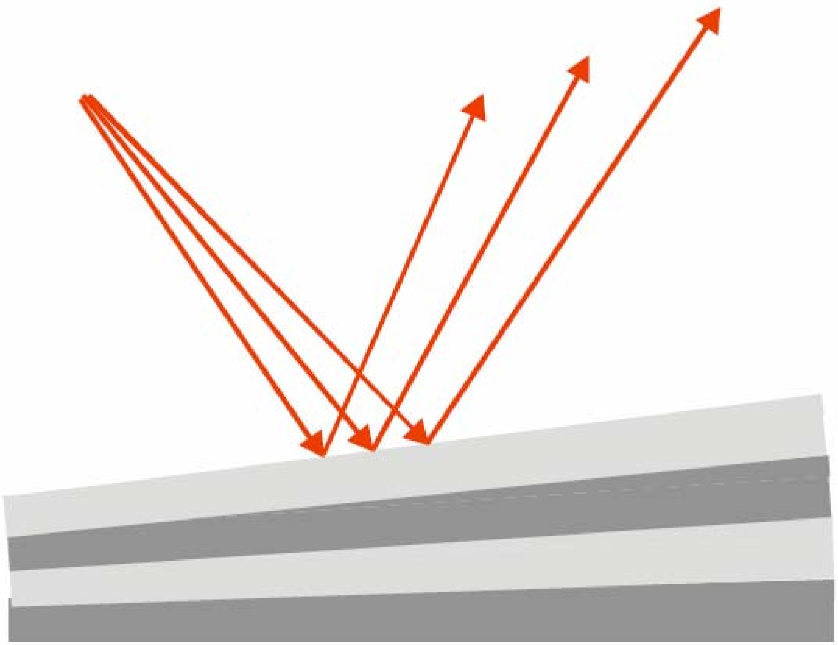
AXO DRESDEN GmbH Applied X-ray Optics Röntgenoptik und Präzisionsbeschichtung

Laterally graded multilayers

BRAGG's law: $\lambda = 2d \sin\theta$

$\Rightarrow$ smaller incidence angle requires larger layer thickness

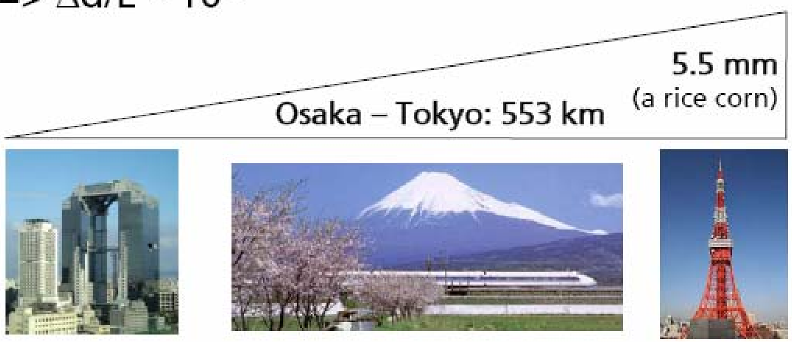
$\Rightarrow$ laterally graded multilayer (for point sources or bended optics)

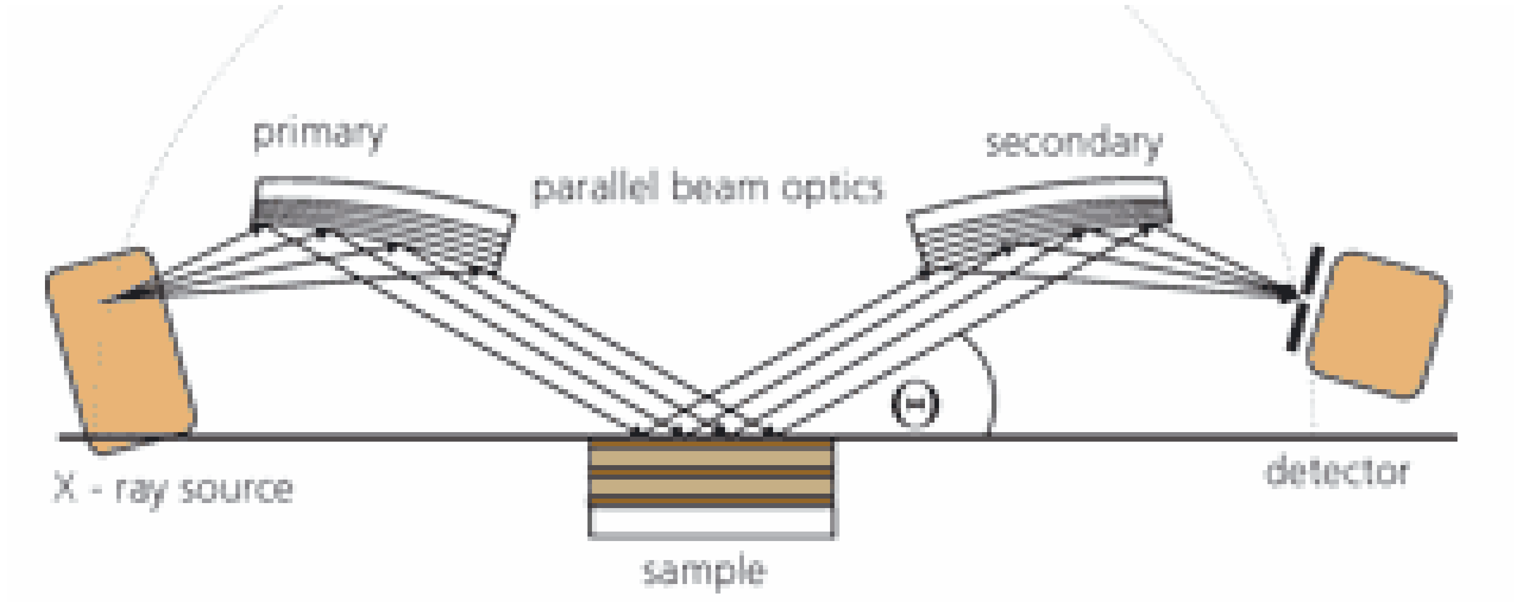


Typical application:

d = 2.88-3.52 nm for a distance of 60 mm

=> $\Delta d/L \approx 10^{-8}$

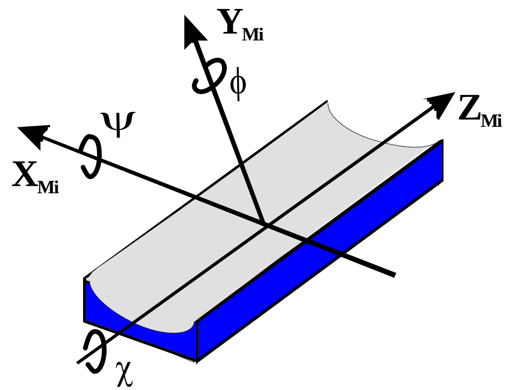




2-dim. thickness variation in material A and/or B

$$d_{(A,B)(x,z)} = d_{(A,B)(0,0)} * (1 + b1z + b2z^2 + b3z^3 + b4z^4 + $$

$$+ b5x + b6x^2 + b7x^3 + b8x^4)$$



Reflectivity and Polarisation

- Each ray has an energy (E) and a polarisation $\vec{S}_{ini} = (S_0, S_1, S_2, S_3)$

  (Given by input or calculated (DI_pole, WI_ggler, Undulator))

- E and S can be different for different rays

- Polarisation is traced through the entire optical system

➡ Determination of energy resolution

Determination of (de)polarisation effects

$$\vec{S}_{final} = R(-\chi)MR(\chi)\vec{S}_{ini}$$

$$\vec{S}_M = \begin{pmatrix} S_{0M} \\ S_{1M} \\ S_{2M} \\ S_{3M} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\chi & \sin 2\chi & 0 \\ 0 & -\sin 2\chi & \cos 2\chi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \bullet \begin{pmatrix} S_{0ini} \\ S_{1ini} \\ S_{2ini} \\ S_{3ini} \end{pmatrix}$$

$$\begin{pmatrix} S_{0\,final} \\ S_{1\,final} \\ S_{2\,final} \\ S_{3\,final} \end{pmatrix} = \begin{pmatrix} \frac{R_s + R_p}{2} & \frac{R_p - R_s}{2} & 0 & 0 \\ \frac{R_p - R_s}{2} & \frac{R_s + R_p}{2} & 0 & 0 \\ 0 & 0 & R_s R_p \cos\Delta & R_s R_p \sin\Delta \\ 0 & 0 & -R_s R_p \sin\Delta & R_s R_p \cos\Delta \end{pmatrix} \circ \begin{pmatrix} S_{0M} \\ S_{1M} \\ S_{2M} \\ S_{3M} \end{pmatrix}$$

Rotation matrix

Müller matrix

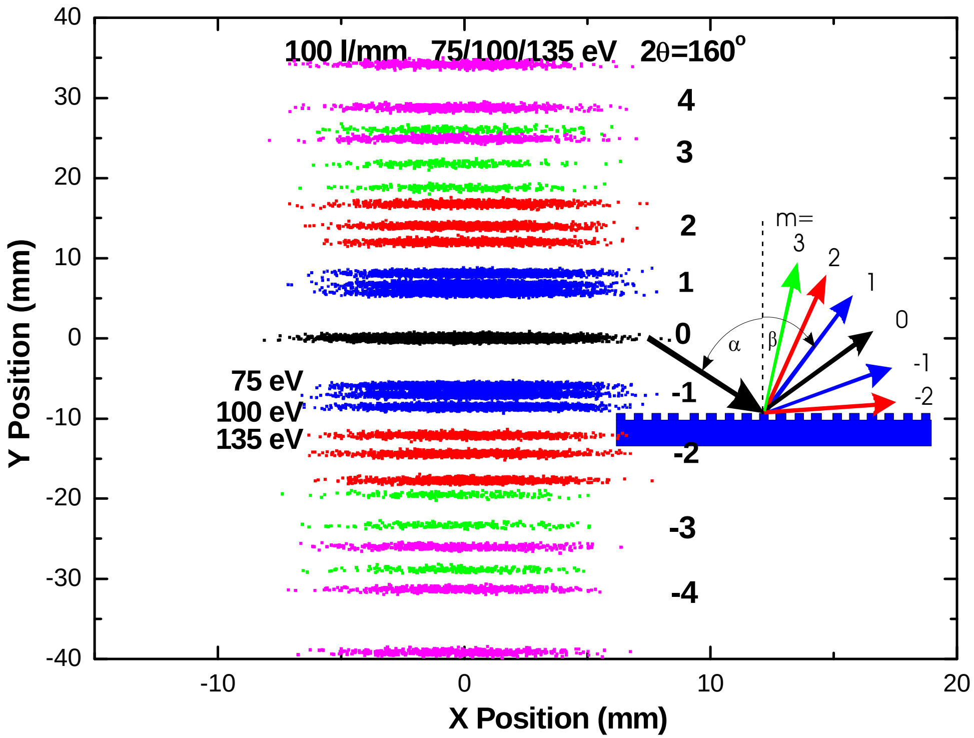
Reflection Gratings (plane, spherical, toroidal)

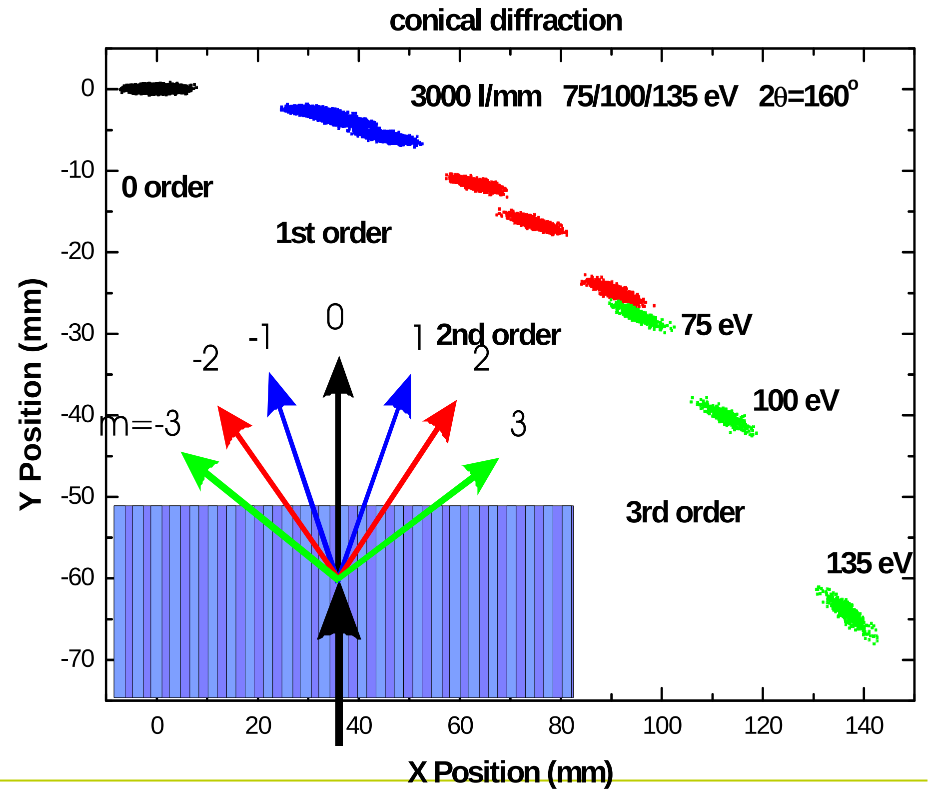
$$k\lambda = d(\sin\alpha + \sin\beta)$$

$$(\vec{\alpha}_2) = \begin{pmatrix} l_2 \\ m_2 \\ n_2 \end{pmatrix} = \begin{pmatrix} l_1 \\ \sqrt{m_1^{\ 2} + n_1^{\ 2} - (n_1 - a_1)^2} \\ n_1 - a_1 \end{pmatrix} \qquad a_1 = kl/d$$

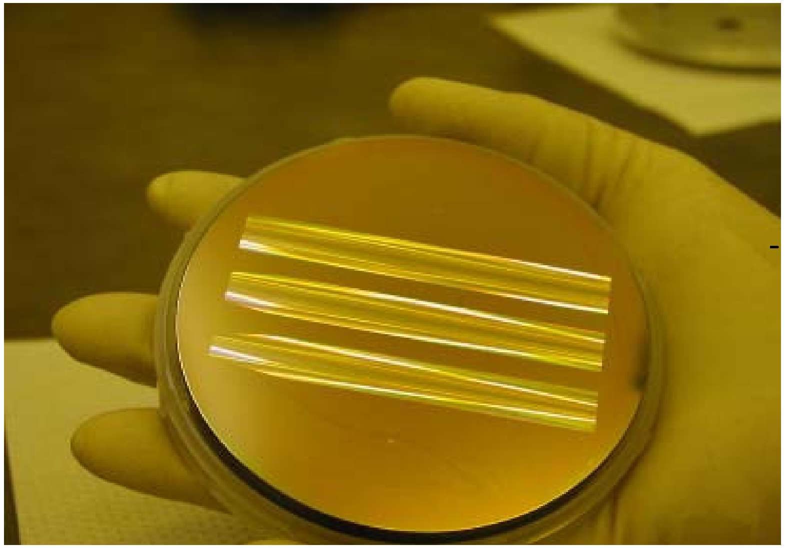
VLS-Grating:

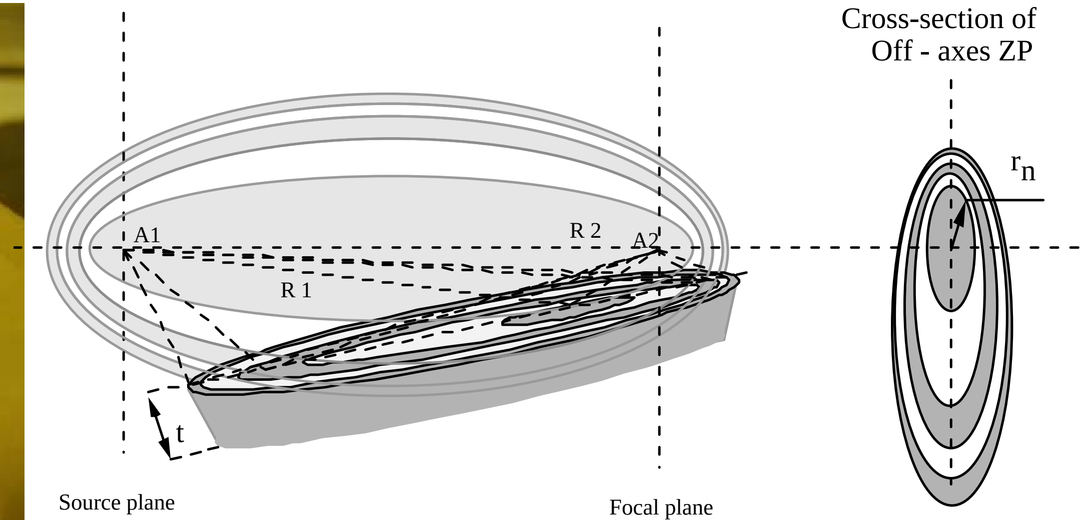
$$1/d = n = n_0 \cdot \left(1 + 2b_2 z + 3b_3 z^2 + 4b_4 z^3 + 2b_5 x + 3b_6 x^2 + 4b_7 x^3\right)$$





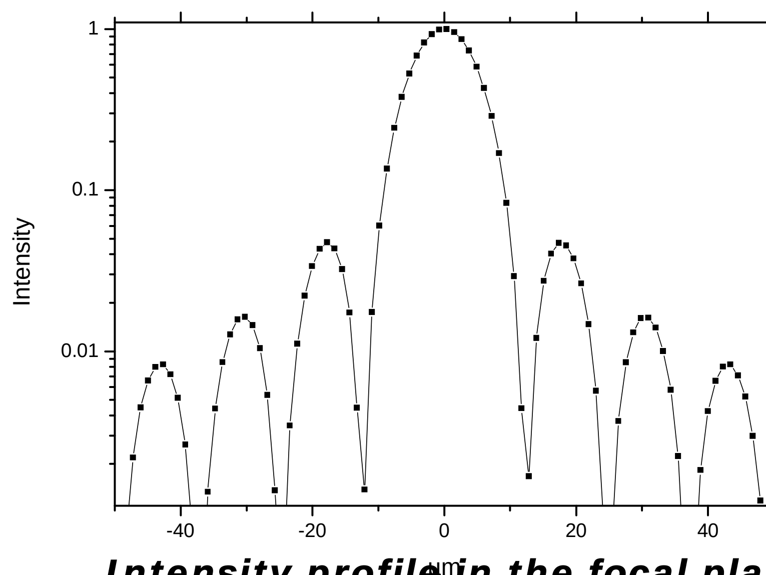
Special optics: Zoneplates (transmission, reflection)





Elliptical Reflection (Bragg-Fresnel) zone plate for reflection, focussing, monochromatisation

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

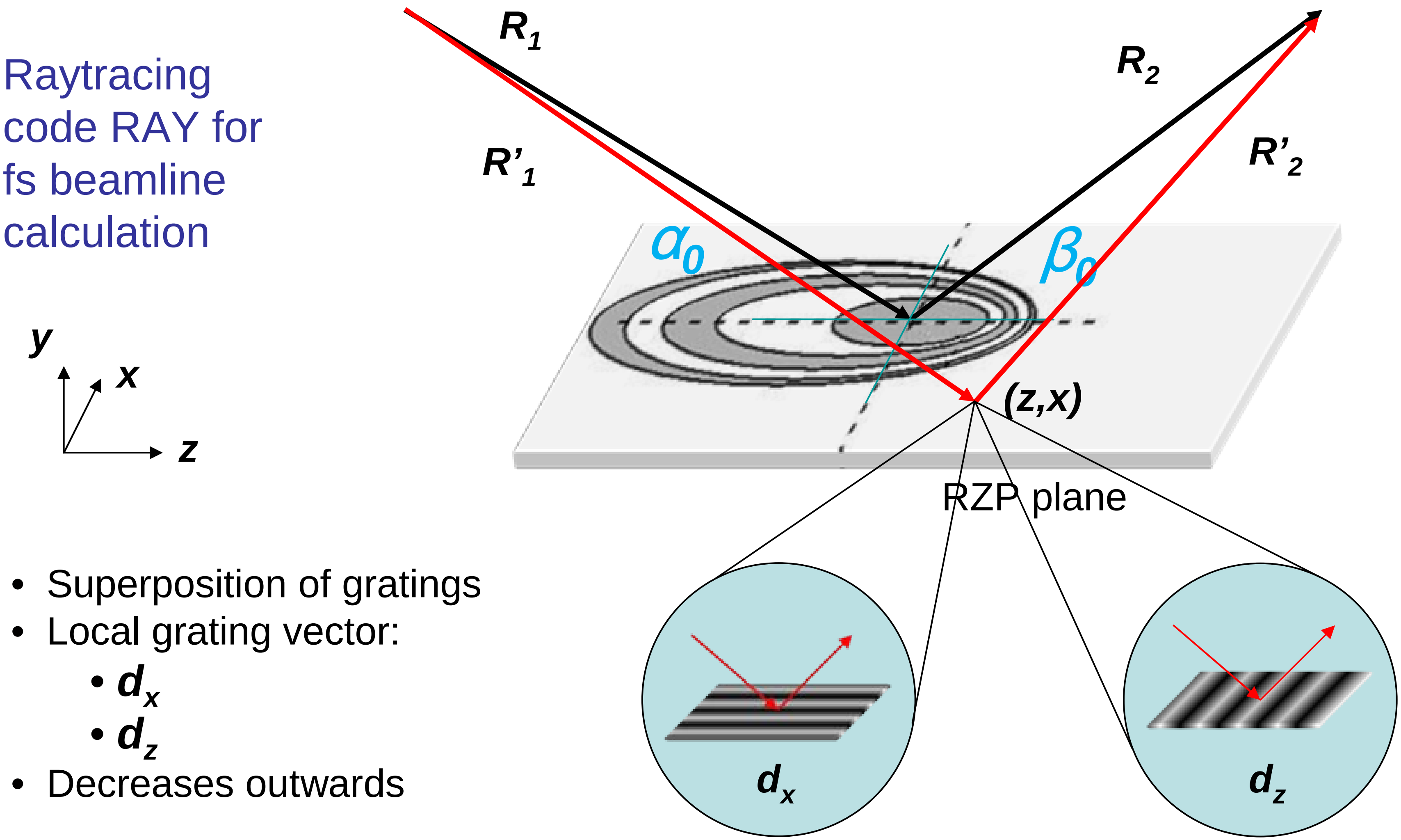


Intensity profile in the focal plane calculated with 100 000 000 rays

Special optics: Zoneplates (transmission, reflection)

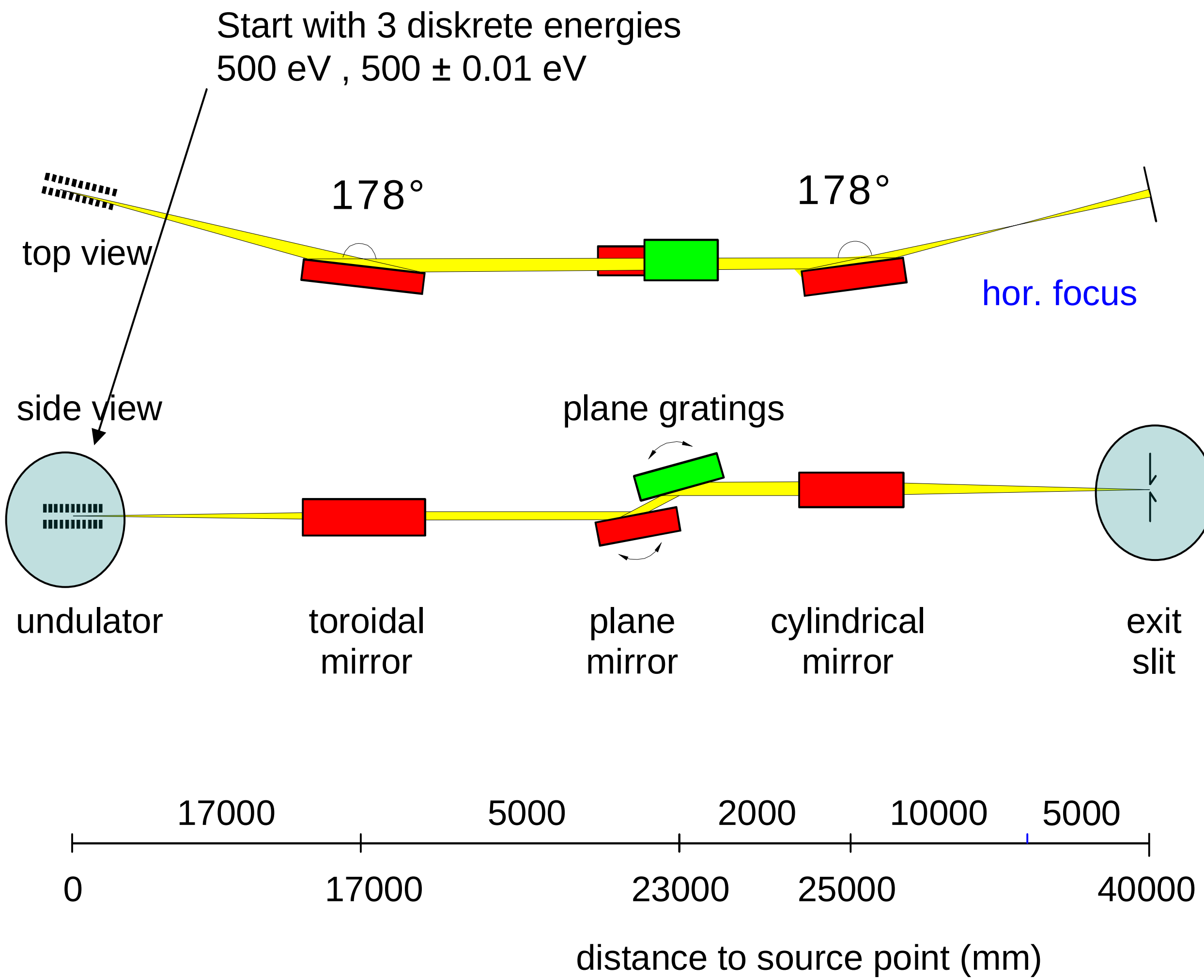
Courtesy Shahin Shahraei
Courtesy Alexei Erko

Raytracing code RAY for fs beamline calculation



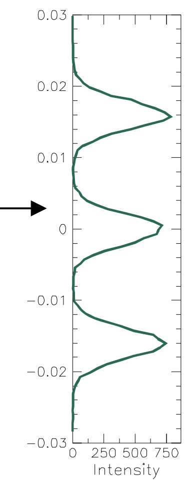
- Superposition of gratings
- Local grating vector:
  - d_x
  - d_z
- Decreases outwards

Impact of c-value: Beamline study MAX IV



RAYtracing

Watch pattern at exit slit



Vary magnification ratio c

$c = \cos\beta / \cos\alpha$

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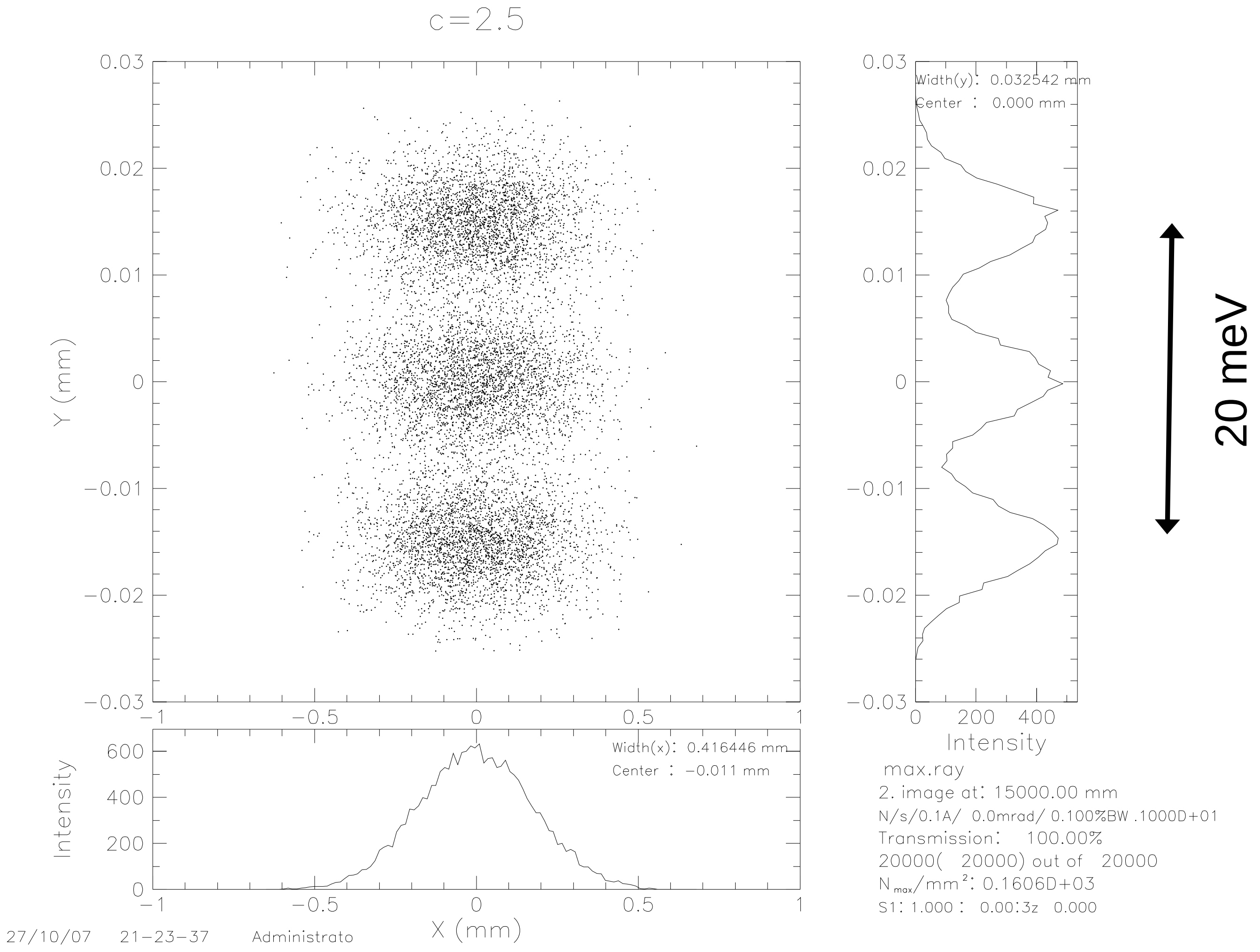
Beamline study MAX IV

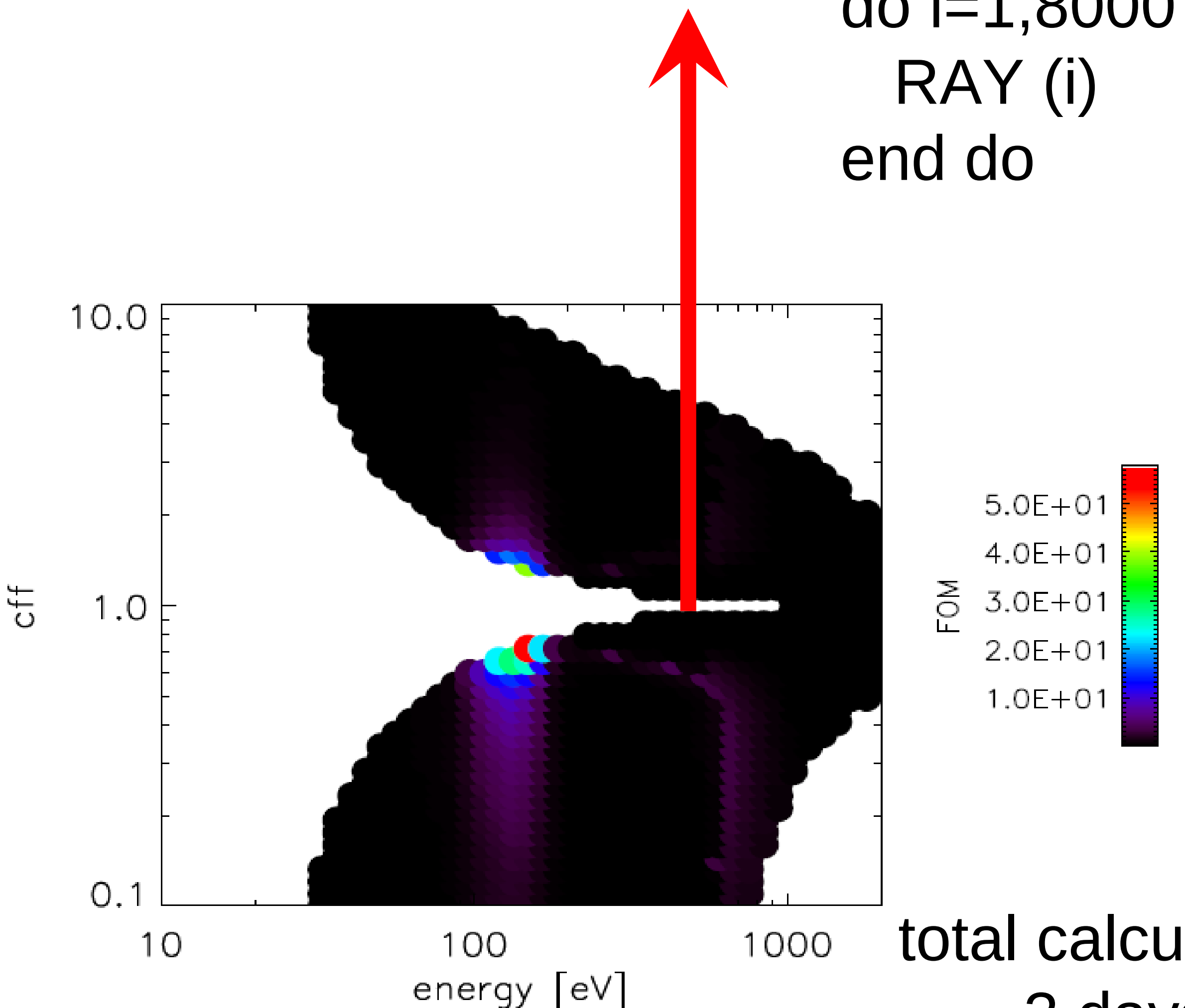
No slope errors



500 eV

Demagnified source improves energy resolution

2.10 „Figure of Merit“ 2

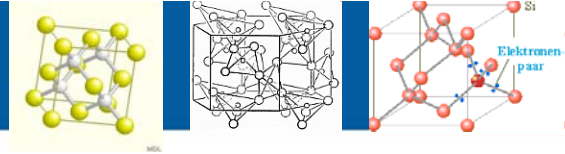


RAY in IDL surrounding

```
do i=1,8000
   RAY (i)
end do
```

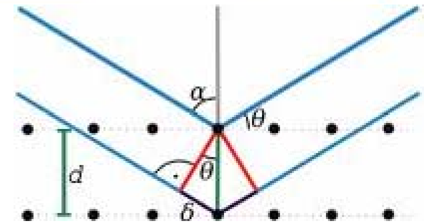
total calculation time ~3 days

Crystals



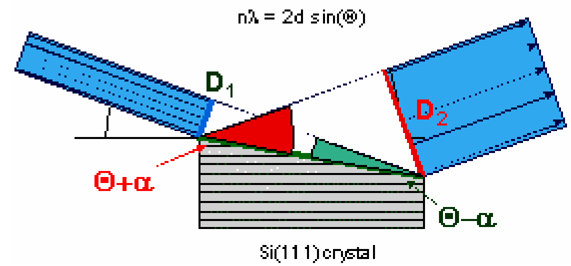
- **Bragg-reflection at crystal lattice planes:**

$$\lambda = 2d\sin\theta$$

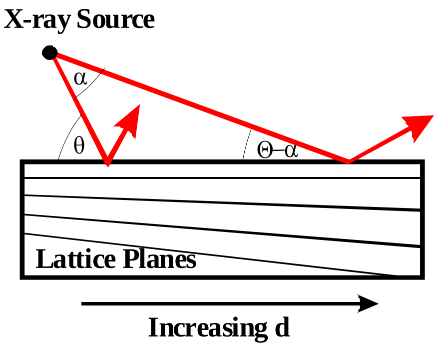


- ***Asymmetric crystals (offset to surface):***

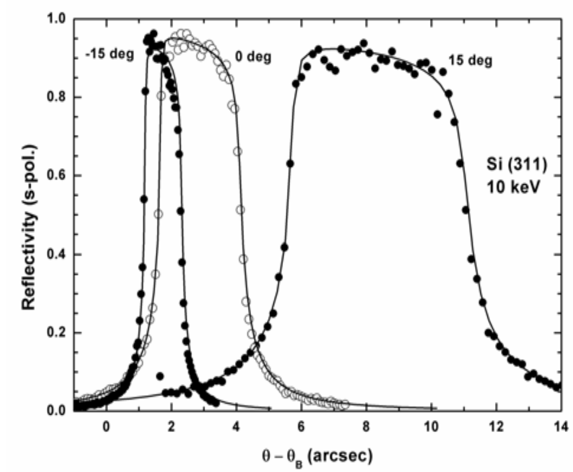
$$b = (\sin(\theta_B - \alpha))/(\sin(\theta_B + \alpha))$$



- **Graded crystals (d=d(z))**



$$\Delta\Theta_{out} = b\Delta\Theta_{in}$$



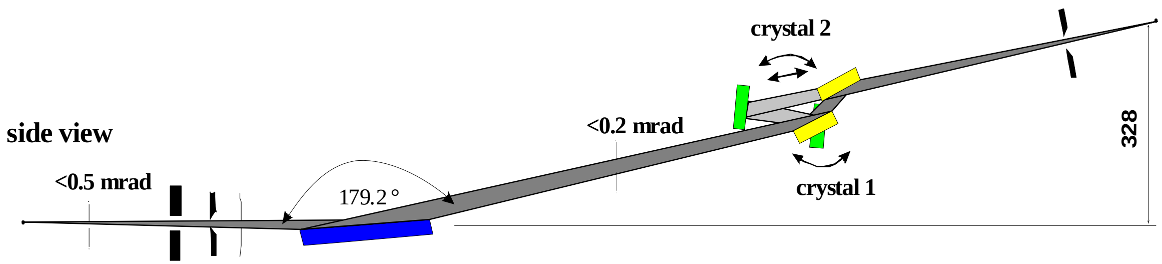
- **Plane and cylindrical crystals**
- **Darwin-Prins formalism**
- **Crystal structure factors *F_0, F_h, F_{hc}***

  (geometric properties – element specific scattering factors

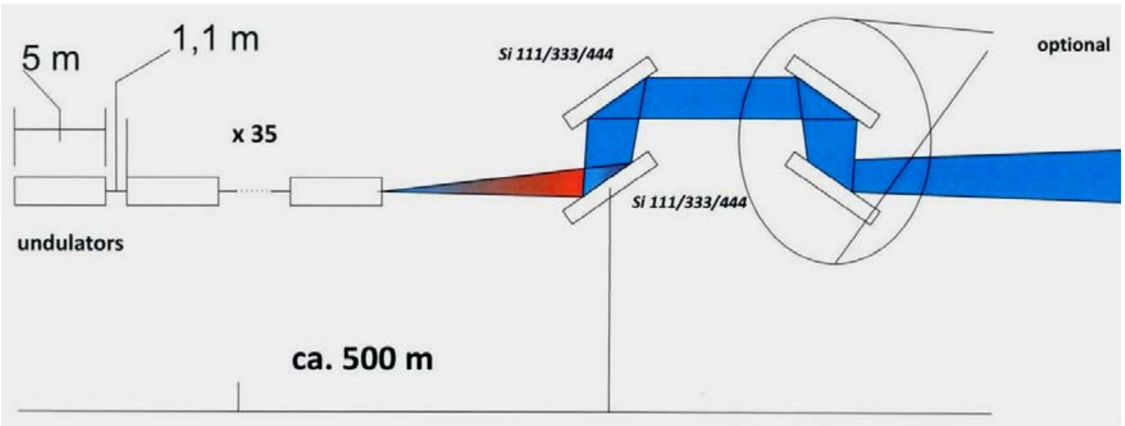
  (Miller indices hkl, elements, lattice constant, $f=f_0+\Delta f_1+\Delta f_2$)

- **Calculated for zink blende, quartz**

Crystals



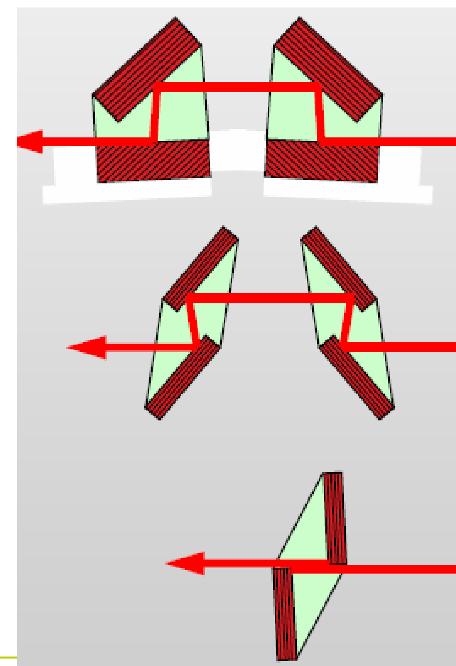
Double Crystal Mono DCM

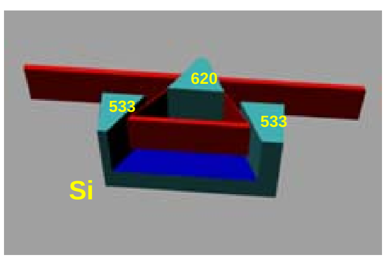


4-bounce Bartels Monochromator

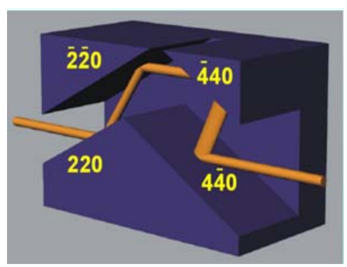
Four Crystal Mono FCM

High Resolution Mono HRM



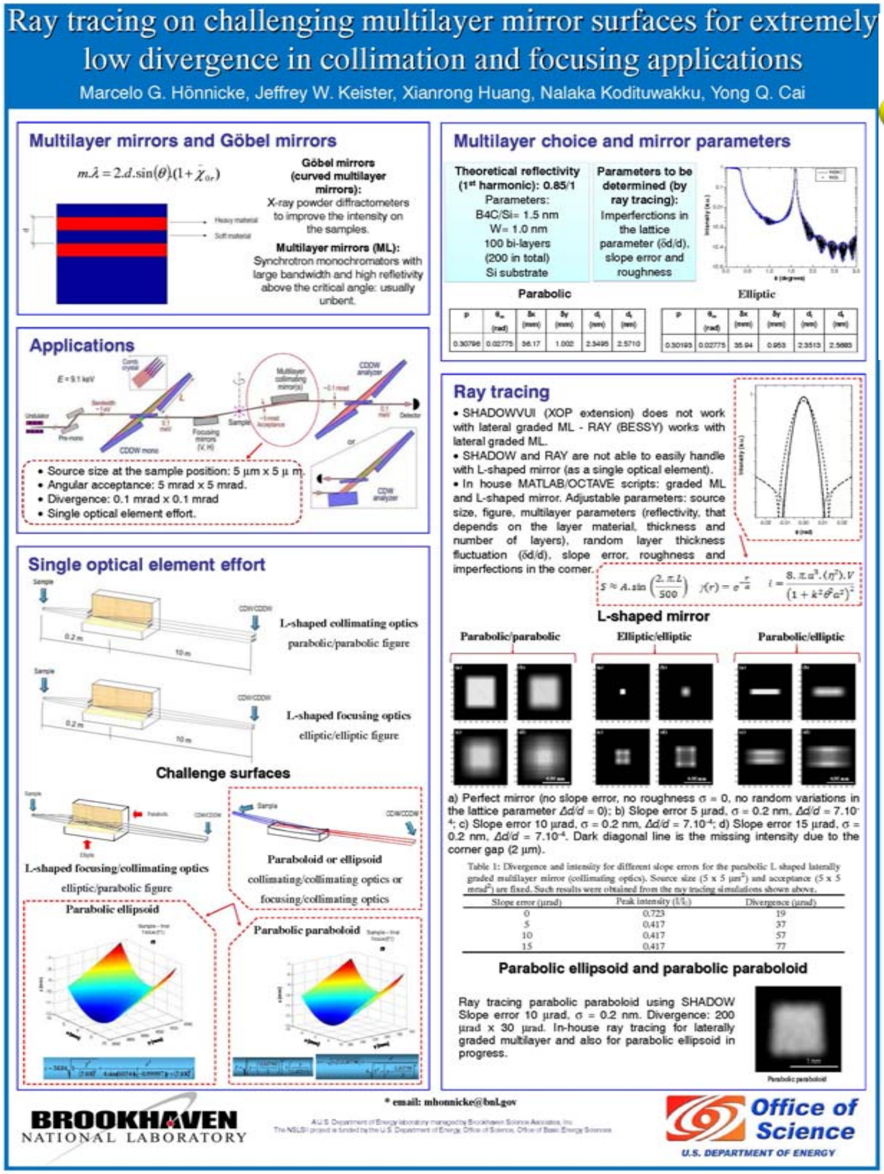


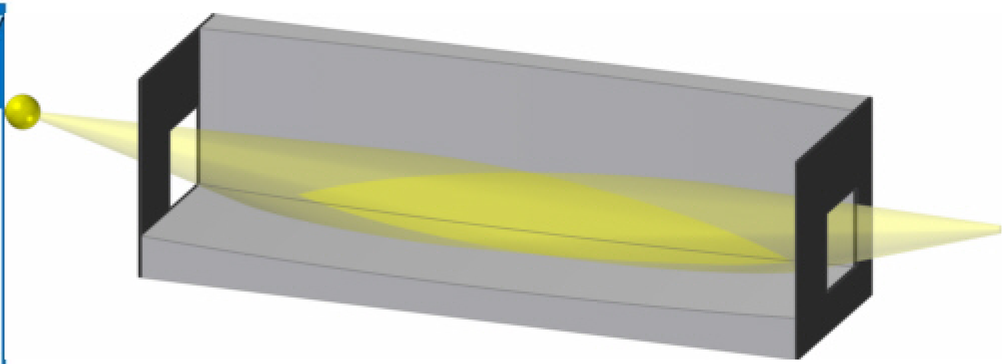
asymmetric (60°) diffractions
E= 8.03996 keV,
ΔE= 14.685 meV

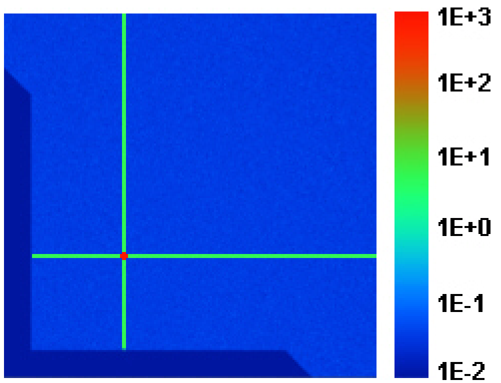


Miniature monolithic Ge
4-bounce monochromator
for Co Kα1 radiation

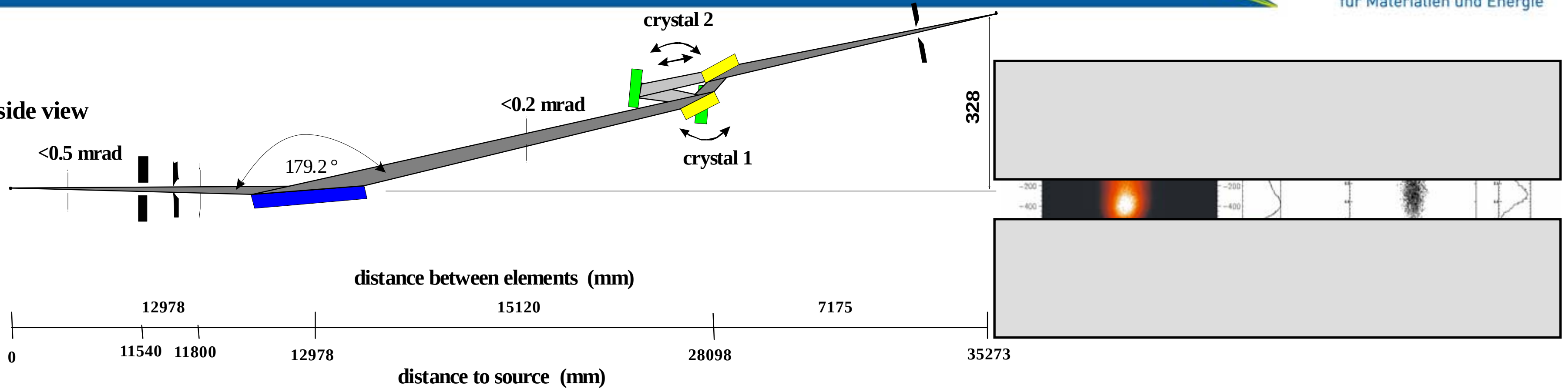
Montel Optics (still to be done…)

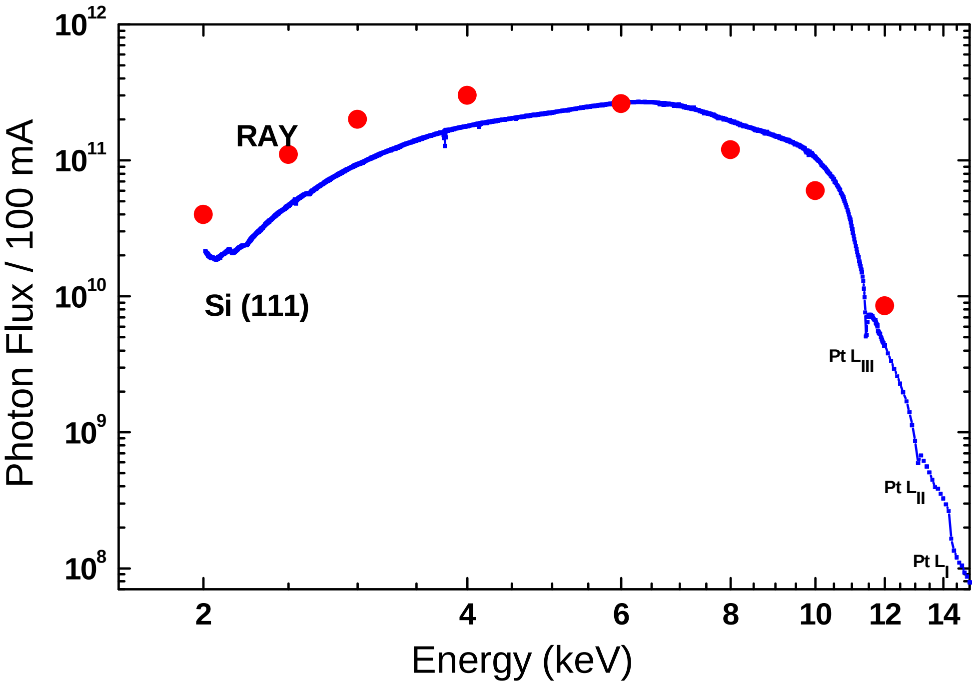




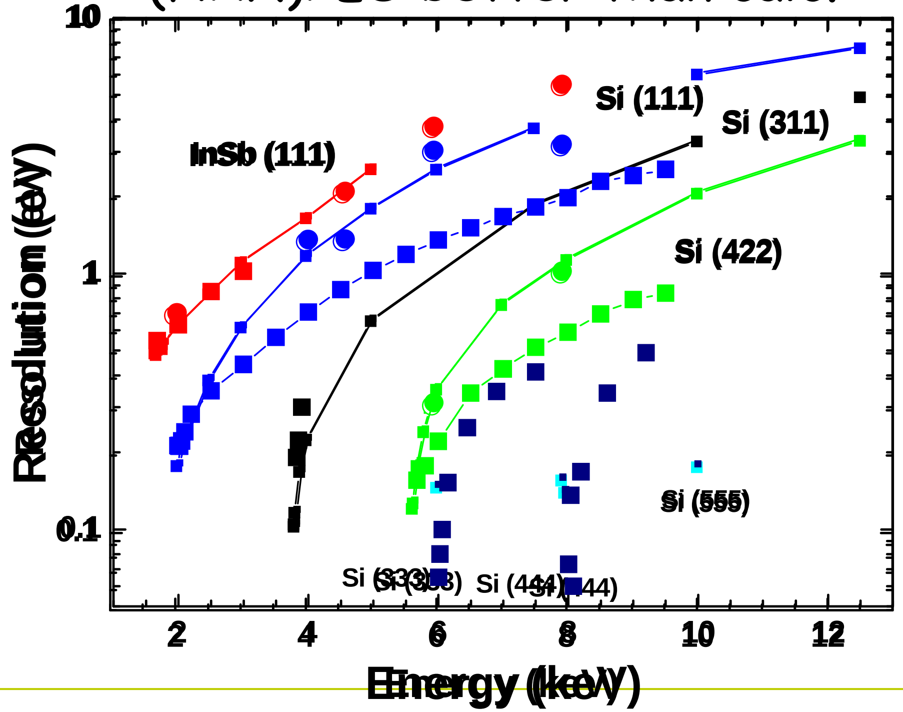


KMC-1 beamline performance



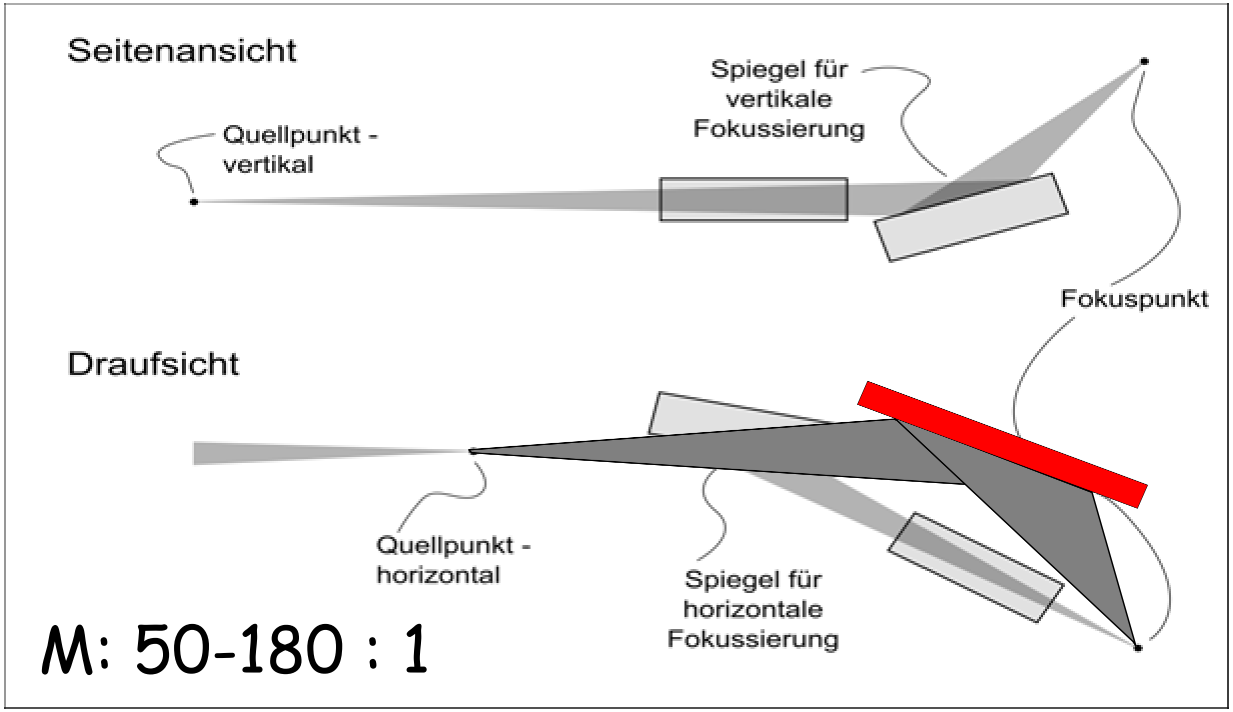


(HAX)PES better than calc.

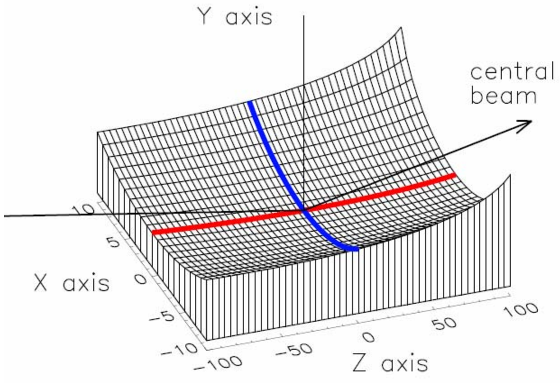


Diaboloid - optics

Stigmatic Imaging of an astigmatic source
(Convert toroidal to spherical wavefront)



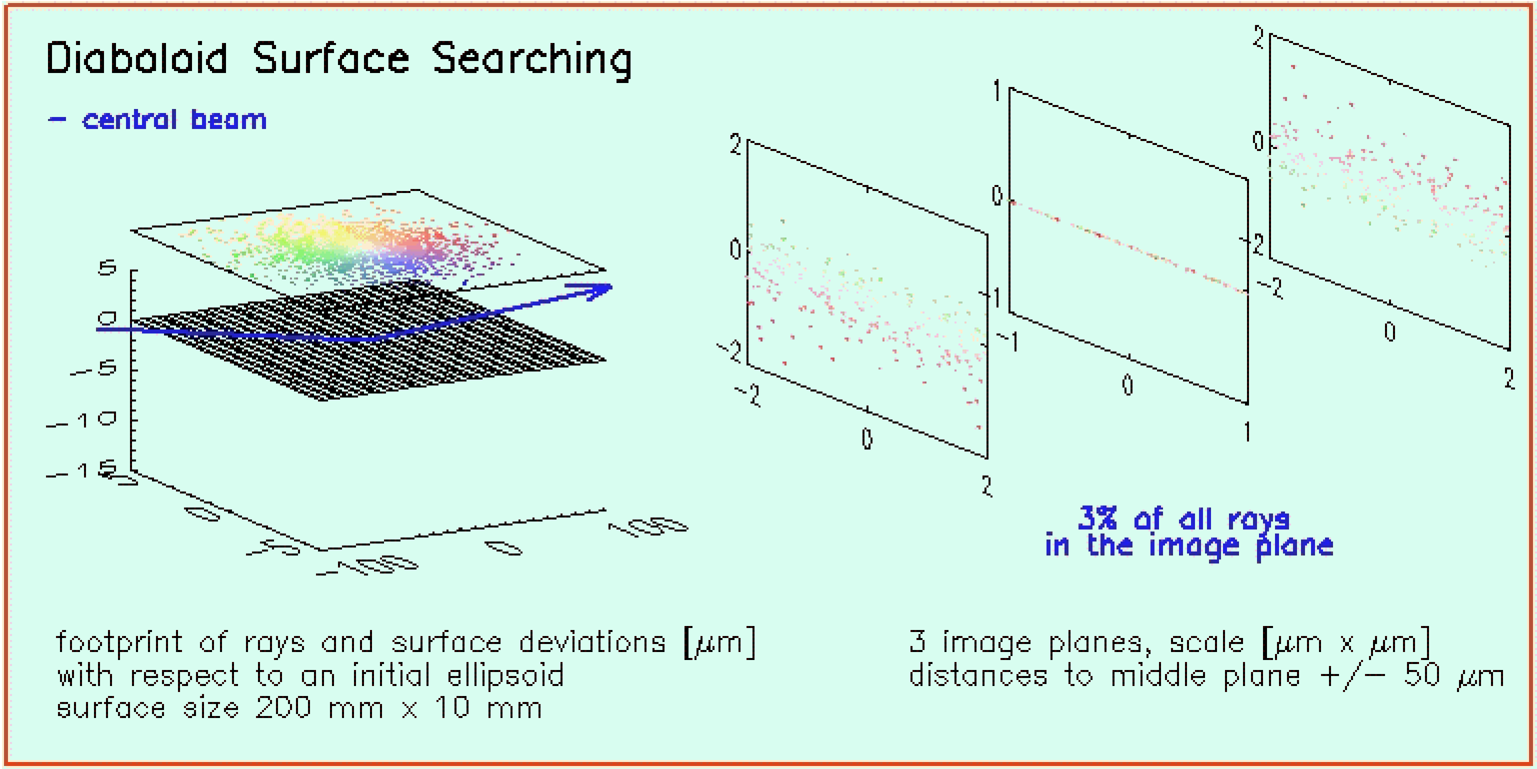
Diaboloid



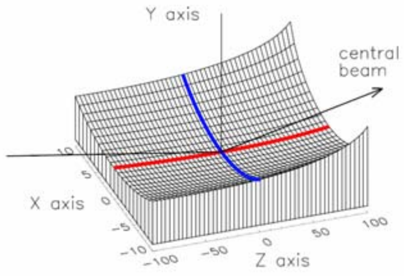
$$F(x,y,z)=0 \;=\; a_{11}x^2+a_{22}y^2+a_{33}z^2+ 2a_{23}yz+2a_{24}y+2a_{34}z+ a_{44} + b_{13}x^2z$$

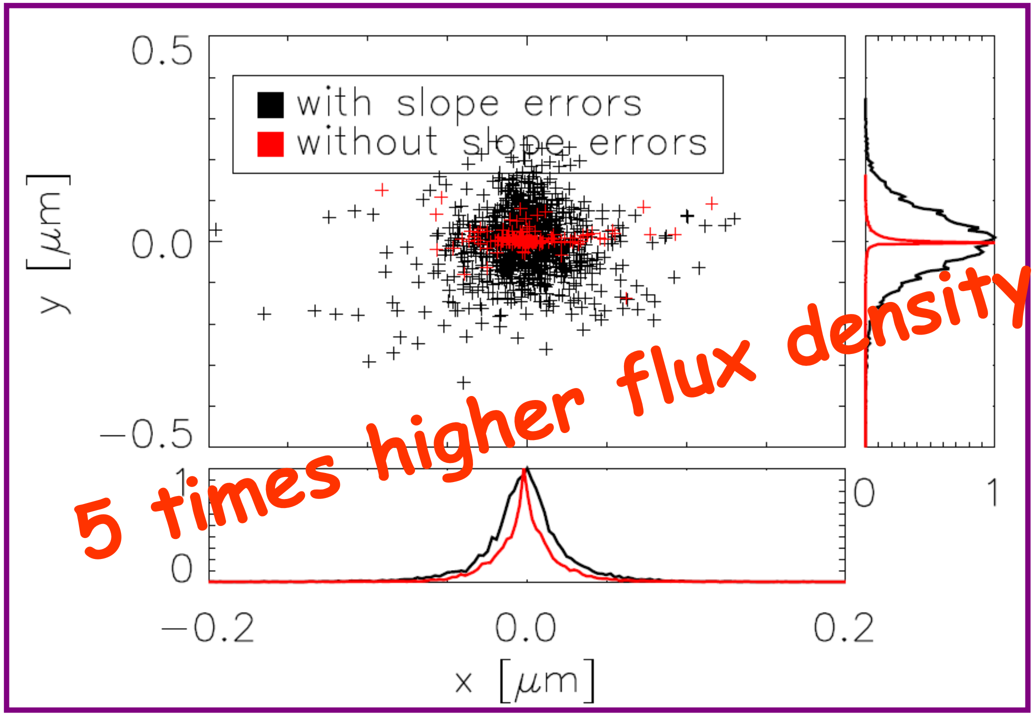
focussing properties: IDL-Animation
(Thomas Zeschke, BESSY)

Diaboloid - optics



Diaboloid - optics





slope error (σ)   0.5 μm x 0.2 μrad
spot size (fwhm) 0.037 μm x 0.162 μm

$$\begin{aligned} F(x,y,z)=0 \quad = \quad & a_{11}x^2 + a_{22}y^2 + a_{33}z^2 + \\ & 2a_{23}yz + 2a_{24}y + 2a_{34}z + \\ & a_{44} \qquad\qquad + b_{13}x^2 z \end{aligned}$$

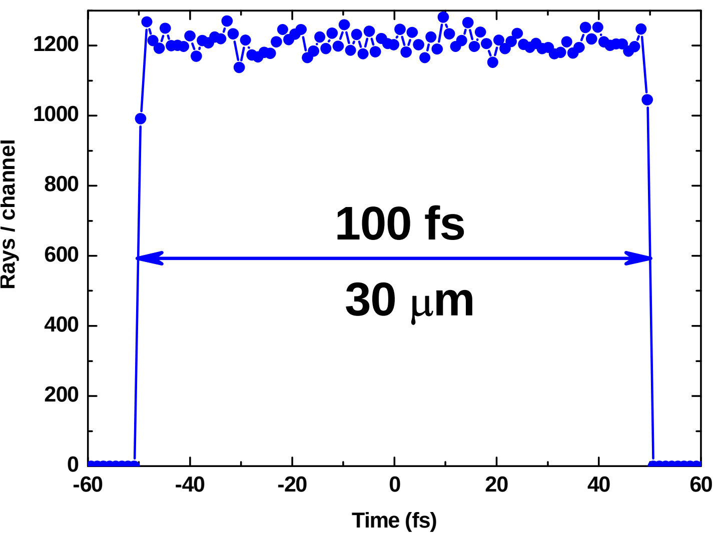
Time Evolution of beams - controlling the pulse shape & broadening

Path length $$pl = \sqrt{((x - x_{old})^2 + (y - y_{old})^2 + (z - z_{old})^2)} - zq$$

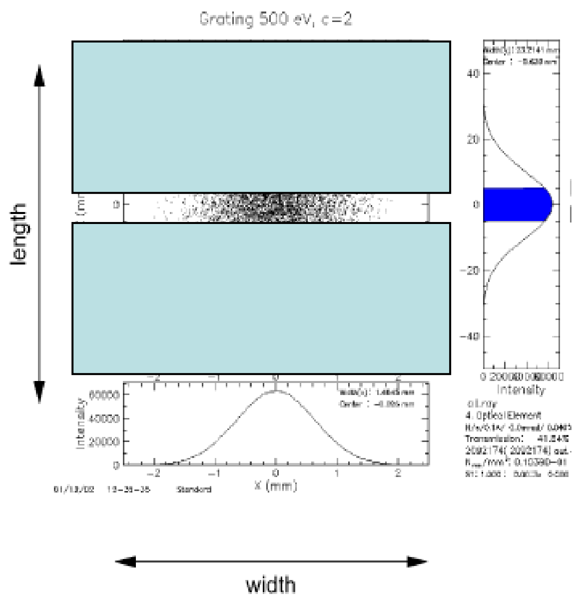
Phase $$\varphi = \frac{2\pi}{\lambda} pl$$

Travel time $$t = \frac{pl}{c}$$

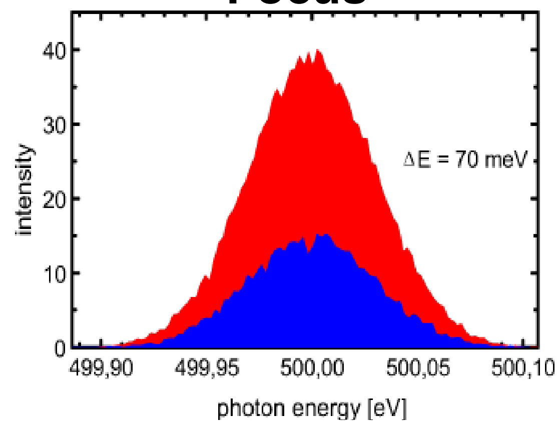
Source

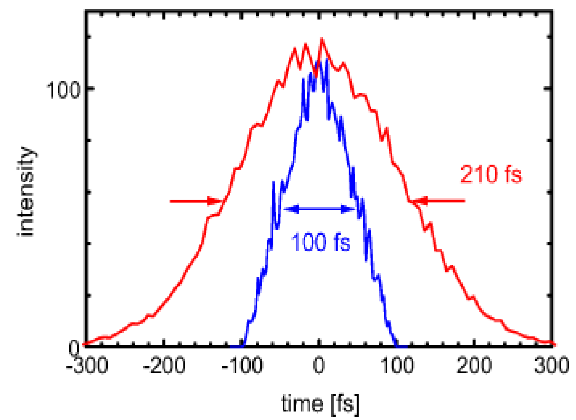


Grating



Focus





(source: 100 fs rectangular)

Confining illuminated grating length: pulse length unchanged

Wavefronts, Coherence

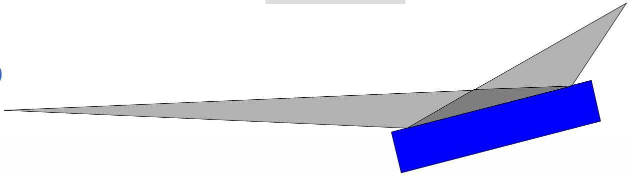
Path length

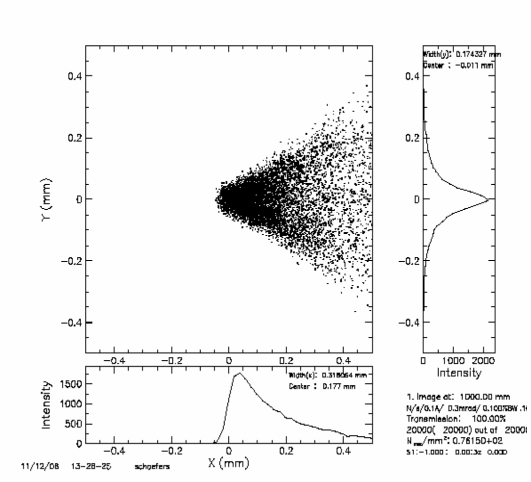
$$pl = \sqrt{((x - x_{old})^2 + (y - y_{old})^2 + (z - z_{old})^2)} - zq$$

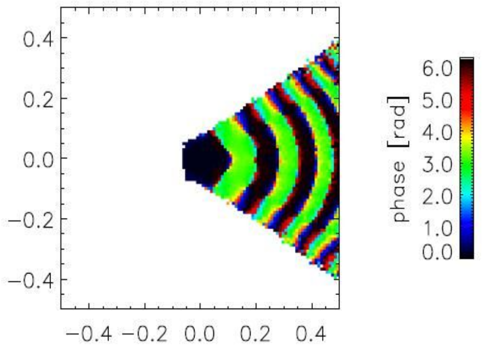
Phase $\varphi = \frac{2\pi}{\lambda} pl$

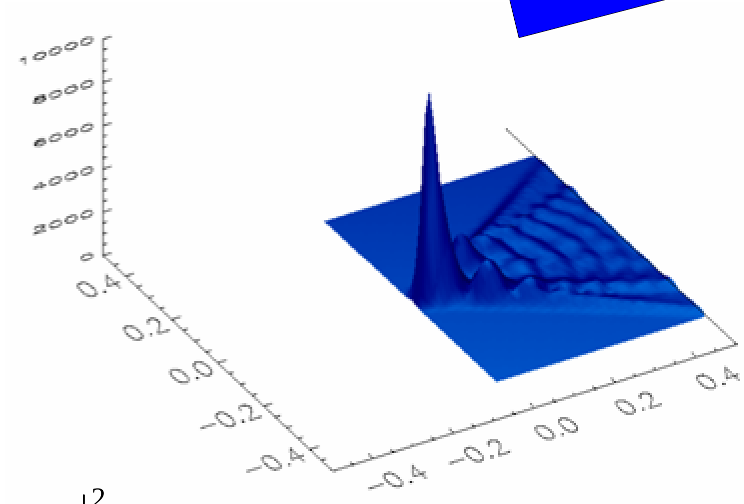
Travel time $t = \frac{pl}{c}$

Coherent illumination of toroid, 10:1, θ=2.5º









Geometric Intensity **Phase** $I = \left|\sum_j e^{i\varphi_j}\right|^2$ **=** **Interference**

- Similar to "real" wavefront codes: PHASE, SRW
- Phasespace, time, energy, polarisation:

  → Identify sections of equal phase: Coherence

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für Materialien und Energie

```
######    #######  #######   ##       #######    #####
##   ##   ##       ##        ##       ##       ##   ##
##   ##   ##       ##        ##       ##       ##
######    #######  #######   ##       #######  ##
##  ##    ##       ##        ##       ##       ##
##   ##   ##       ##        ##       ##       ##   ##
##    ##  #######  ##        #######  #######   #####
```

a program

to calculate

VUV/X-RAY OPTICAL ELEMENTS

and

SYNCHROTRON RADIATION
BEAMLINES

BESSY

Other reflectivity codes

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IMD (D. Windt)

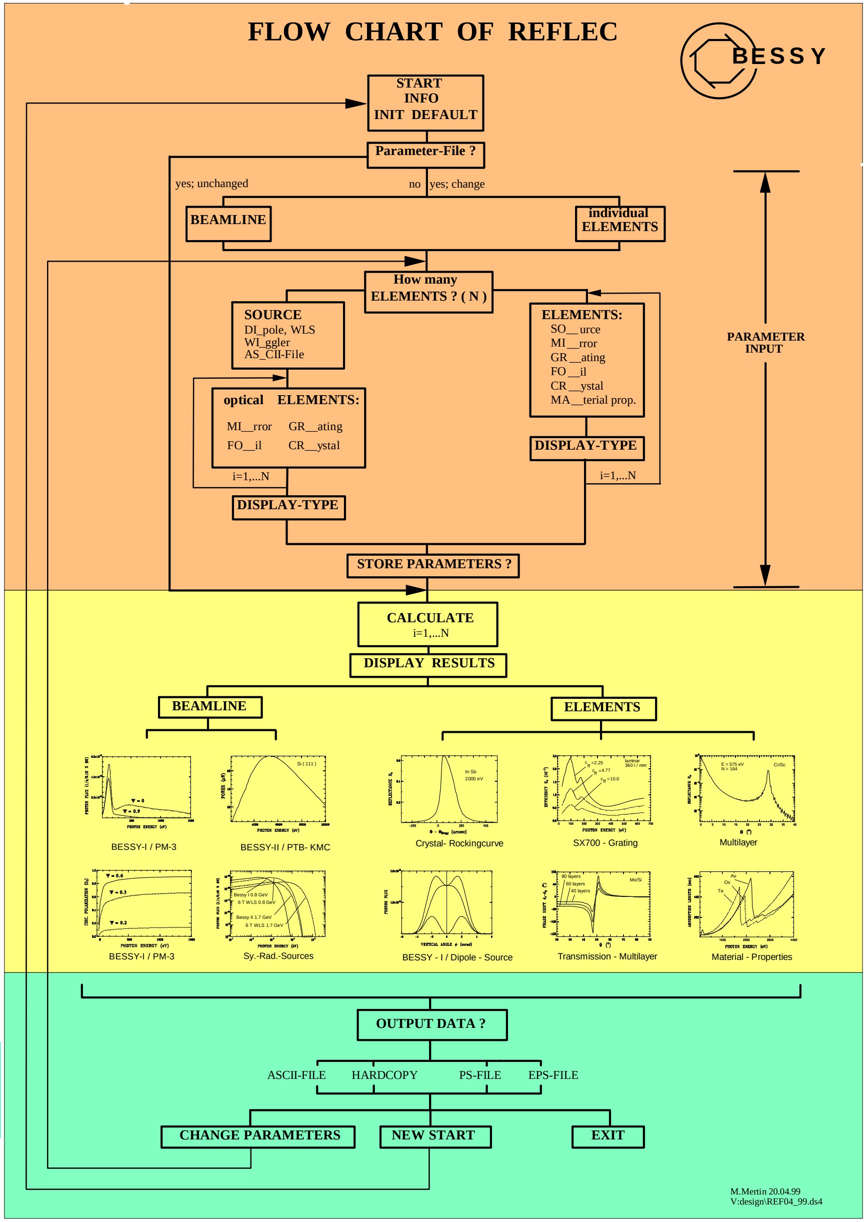
CXRO webpage (E. Gullickson)

…

Parameter input

Calculation

Graphics output



Beamlines or Elements (<10)

- SR-Sources
- Mirrors
- Gratings
- Foils
- Crystals
- Windows
- Multilayers

Beamlines, sources:

- Photon flux
- Resolution
- Angular distribution

Elements:

- Reflectivity $R_{s,p}$
- Efficiency $E_{s,p}$
- Rocking curves
- Polarisation prop.
- Phase retardance
- Optical constants
- Absorption prop.

… as fct. of angle, energy

LIMITATIONS / WARNINGS

- The program has NO intelligence - even after 25 years of programming
- The program will NOT give any ideas for the kind of beamline you want to have
- Nor does it have any idea of good experiments at a beamline
- The program performs only what was programmed -
  The results are valid only within the mathematical or physical model implemented
- The program may still have errors (it has - definitely!!)
- The designer may have made typing errors in the input menue
- The designer may have misunderstand the program's language or a result

YOU ARE THE EXPERT - NOT RAY !!!

Acknowledgements

Programming

Josef Feldhaus (Start)
Michael Krumrey (CR)
K.J.S. Sawhney (EPU)
Dirk Abramsohn (PC)
Shahin Sahraei (RZP)

Special features implementation

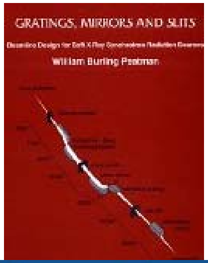
Alexei Erko (micro-, nano stuff)
Rolf Follath (time)
Gerd Reichardt (GR)
Fred Senf (CO)
Thomas Zeschke (IDL, Diab., Phase)

Users

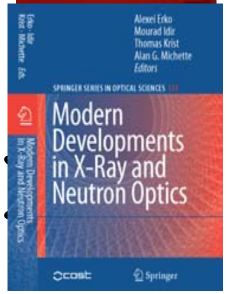
BESSY optics group
Worldwide usage

Advertisement

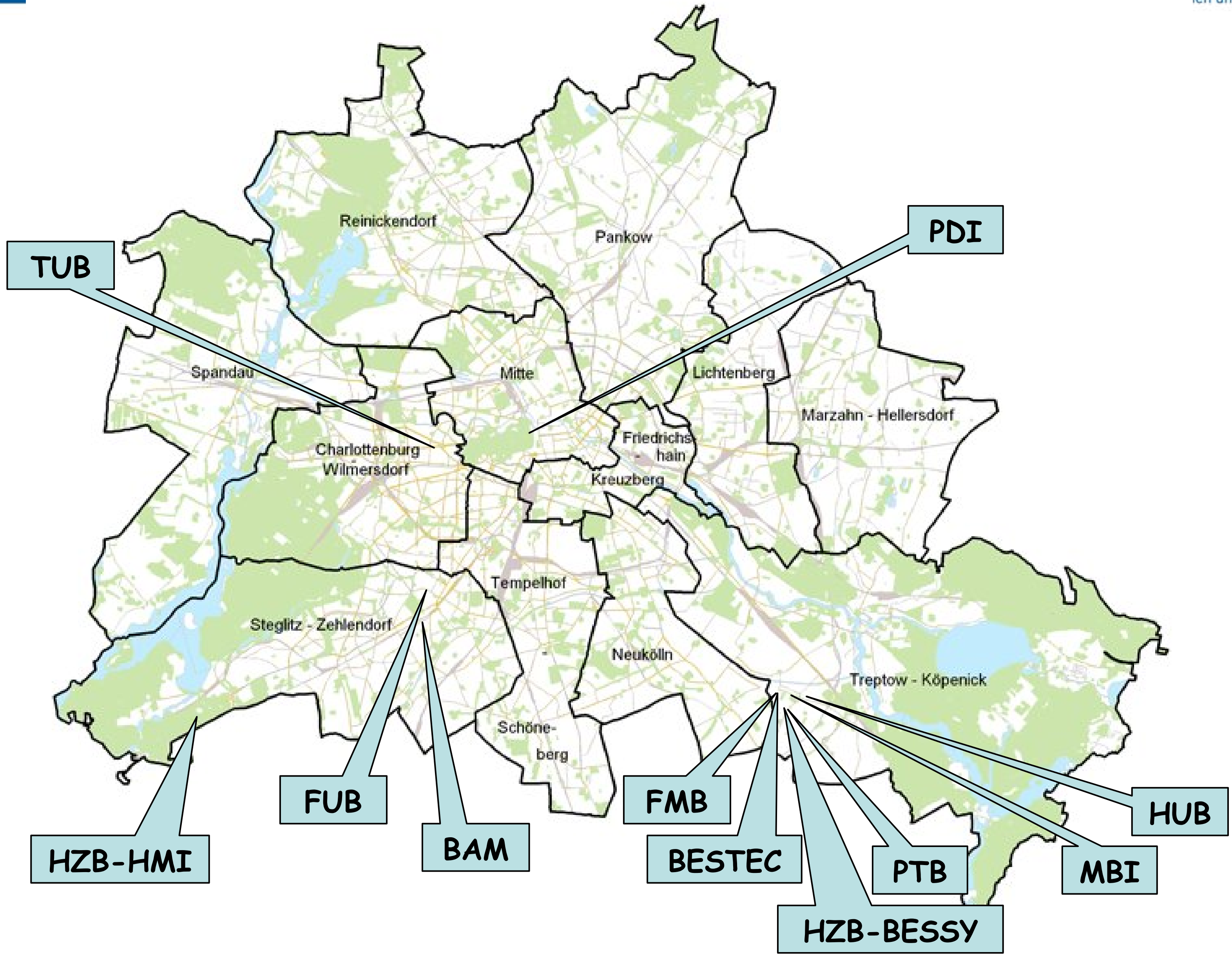
William Peatman
("Gratings, Mirrors and Slits")



Alexei Erko,
Mourad Idir et al.(ed.)
("Modern Developments…")



RAY users in Berlin



RAY users in Germany

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- Uni Bielefeld
- Uni Münster
- DELTA/Uni Dortmund
- Uni Kassel
- FZ Jülich
- Uni Bonn
- Uni Giessen
- Uni Mainz
- FZ Karlsruhe
- Uni Freiburg
- DESY/HASYLAB FLASH/XFEL
- Uni Hamburg
- GKSS Geesthacht INCOATEC
- Uni Potsdam
- MPI Potsdam
- Uni Göttingen
- Uni Cottbus
- Dünne Schichten
- AXO / IWS
- Jenoptik
- Uni Würzburg
- ZEISS Oberkochen
- LM-Uni München

RAY users in Europe

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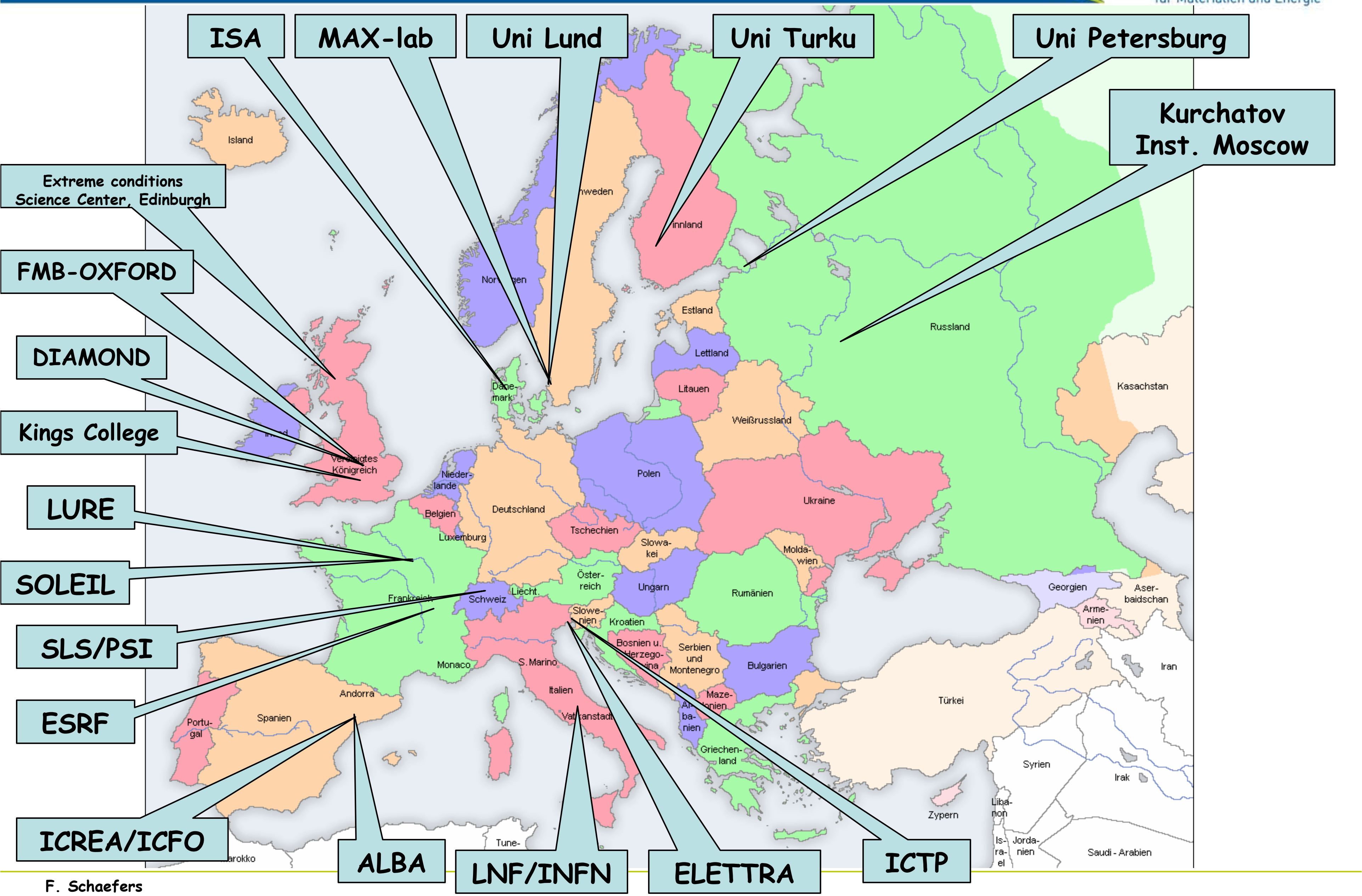

RAY users worldwide

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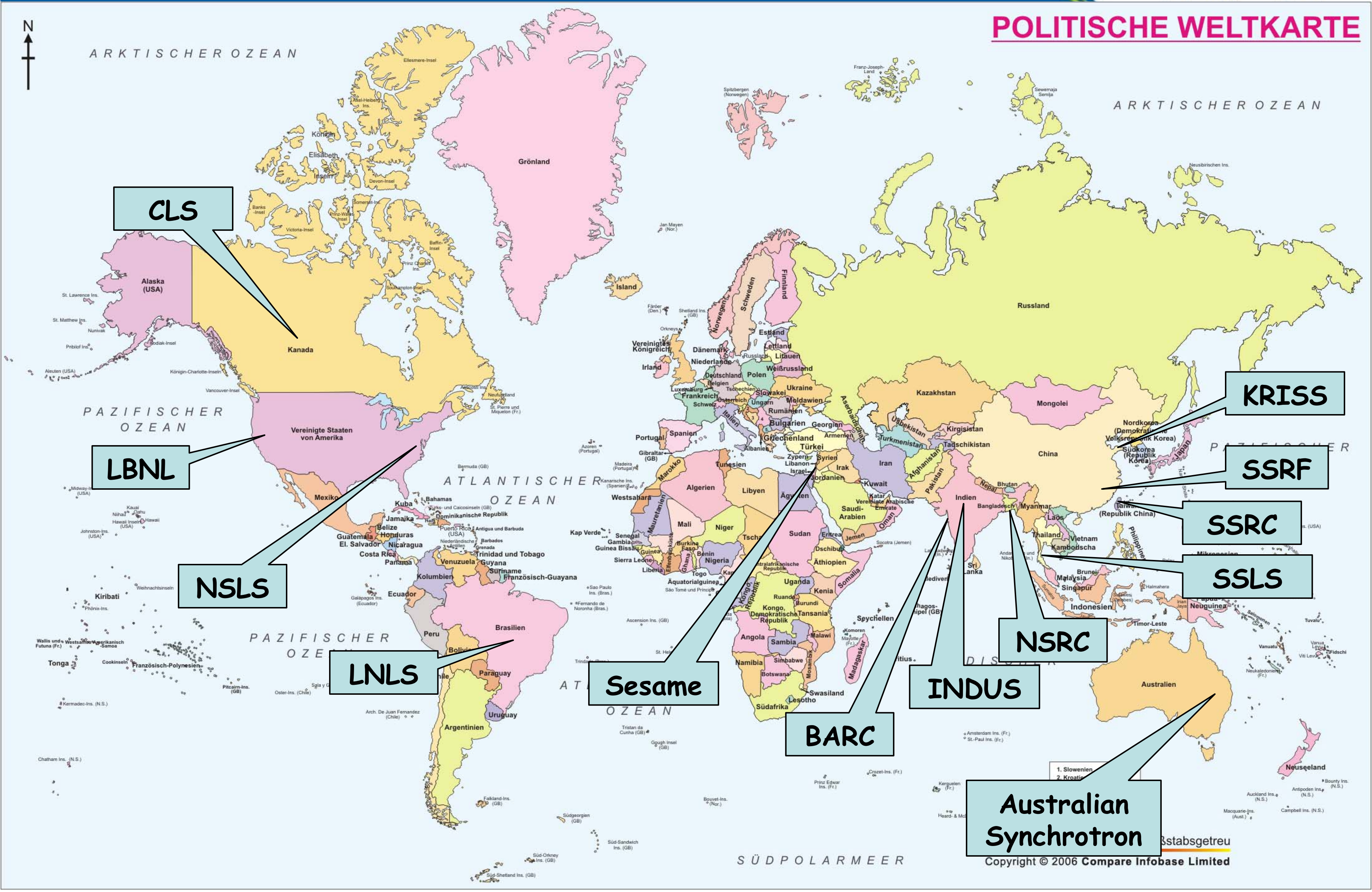

Thanks for listening

Examples

- Illumination of a screen at 10 m behind a divergent source
- Vertical intensity distribution of Synchrotron radiation
- Illumination of a grazing incidence mirror
- Focussing/demagnification of a point source by different mirror types (CY, SP, TO, EL)
- Effect of mirror slope errors on focussing
- Effect of misalignment of optics on focussing
- Wavelength response of a Mo/Si multilayer mirror
- Energy-resolution of a plane grating monochromator
- Crystal DCM throughput
- Heatload on optics

see W.B. Peatman, Gratings, Mirrors and Slits, Gordon & Breach, NY 1997