HELMHOLTZ
ZENTRUM BERLIN
für Materialien und Energie

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

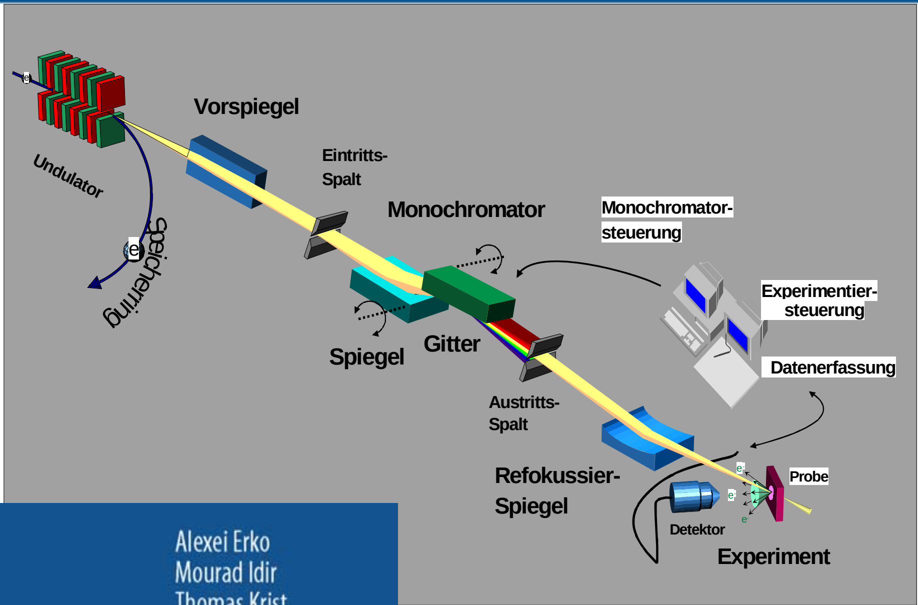
The BESSY RAYTRACE PROGRAM

to calculate (not only)

SYNCHROTRON RADIATION BEAMLINES

Franz Schäfers
(HZB-BESSY)

BESSY

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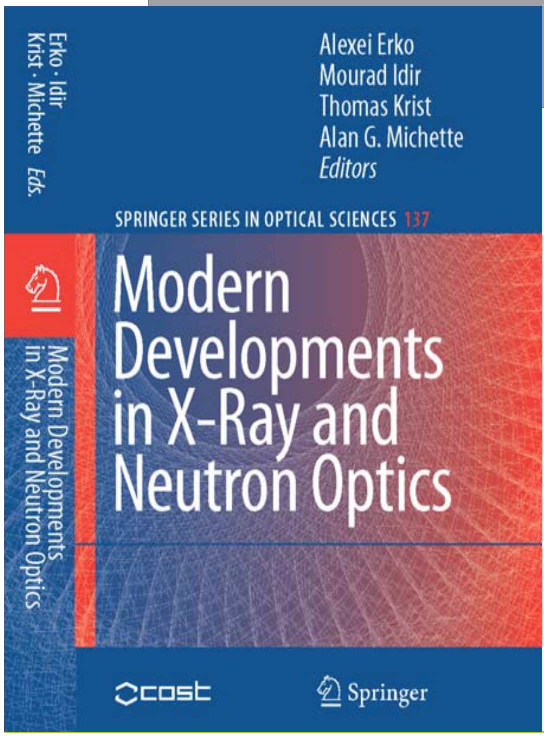
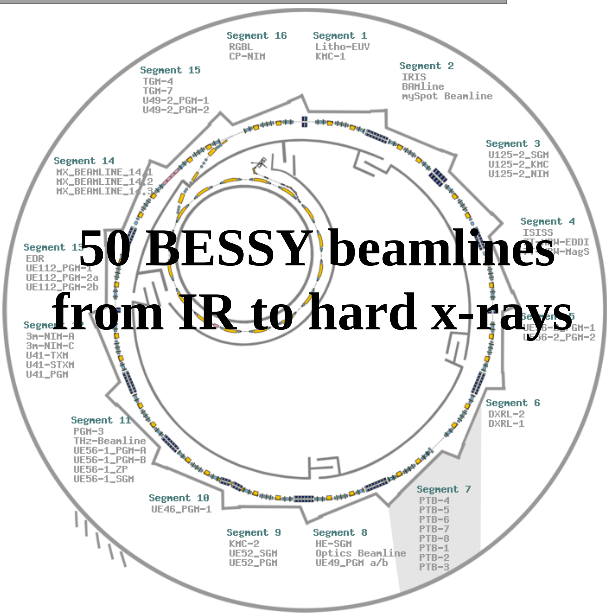

HISTORY

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	Spinger Vol. 137

...

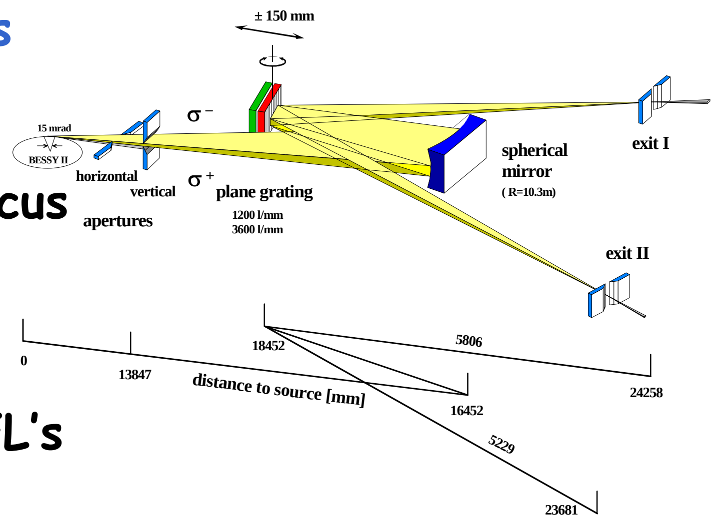




~100 copies worldwide

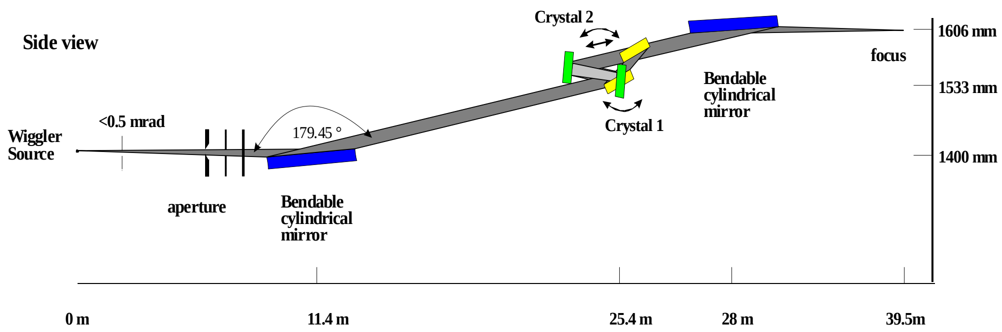
What is raytracing?

- **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**
  - dipole radiation (bending magnets)
  - 3G Wiggler/Undulator beamlines, 4G FEL's
  - 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

photon source
WAVE / URGENT / SMUT

talk M. Scheer

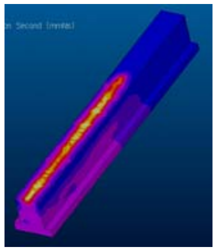
FEM
ANSYS / ProE

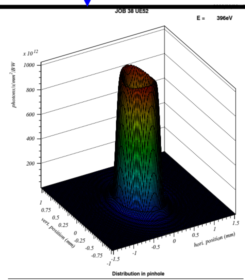
optical elements
REFLEC

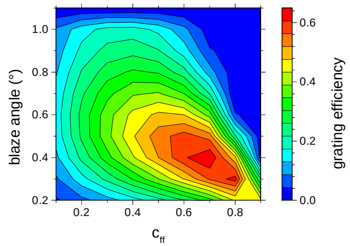
gratings
EFFI

raytracing
RAY / PHASE

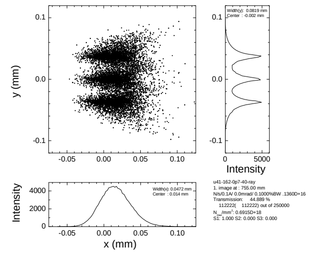
talk J. Bahrdt


temperature distribution


spatial distribution



grating efficiency


spot pattern

What is a ray?

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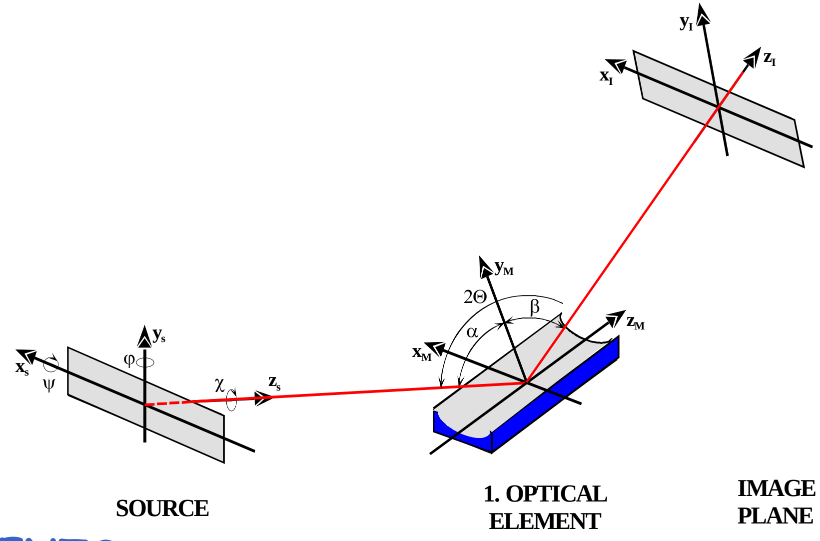
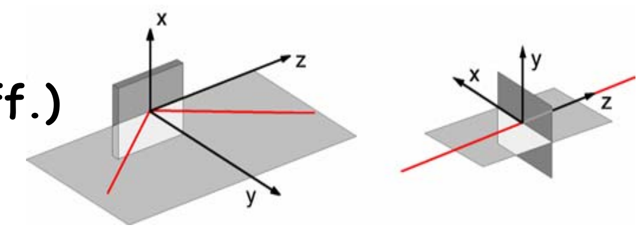
- A RAY is described by 12 parameters
  - geometric coordinates (x,y,z)
  - emission angle (l, m, n)
  - energy (hv)
  - polarisation (S_0, S_1, S_2, S_3)
  - time (pathlength) (t)

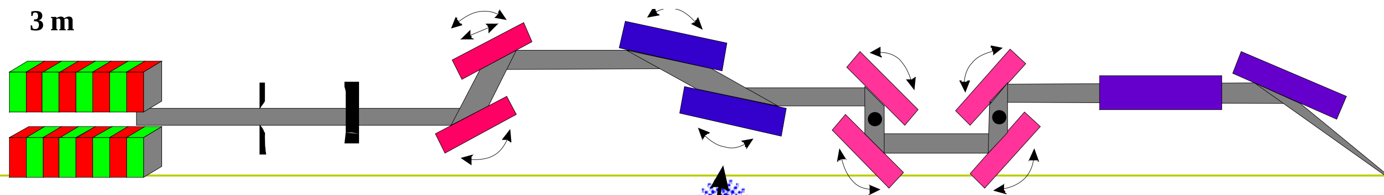


- The RAY starts in a SOURCE-volume
  with defined emission characteristics

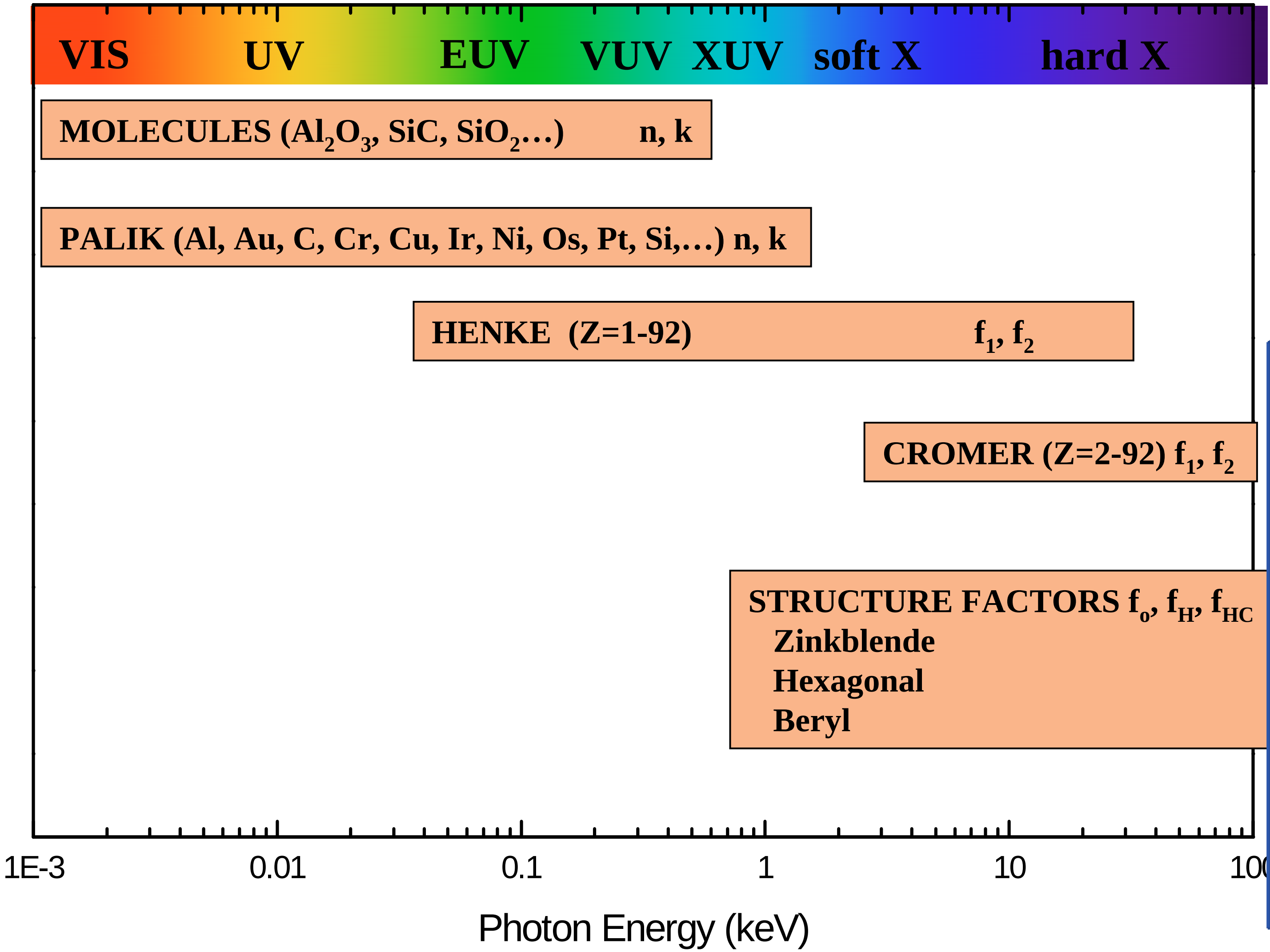
- The RAY is modified by OPTICAL ELEMENTS
  acc. to laws of geometry and optics
  - transmitting - slits, foils (abs.)
  - reflecting - mirrors (refl.)
  - dispersing - gratings, zoneplates (eff.)
  - diffracting - crystals (refl.)



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



OPTICAL DATA TABLES

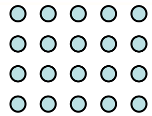


Calculation of

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

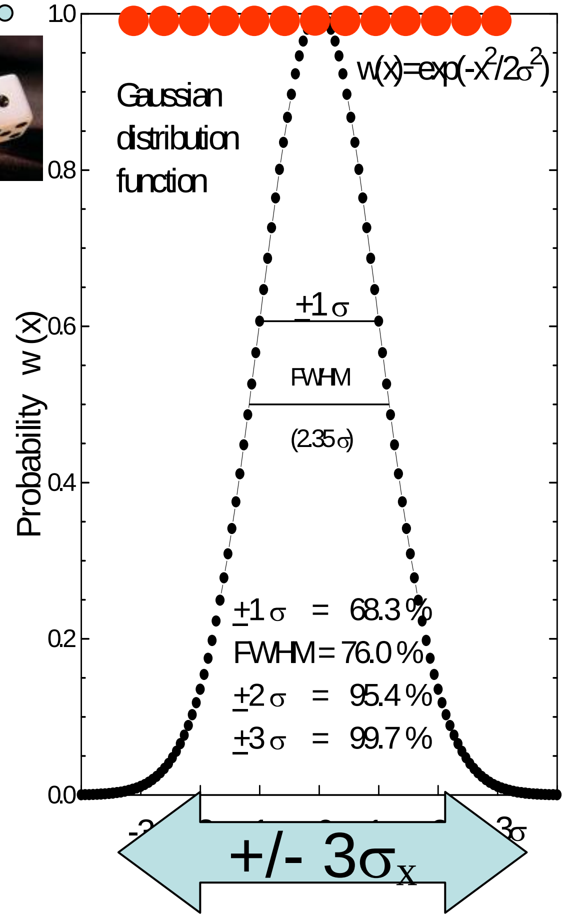
Basic law of RAY:
§1: ALL RAYS HAVE EQUAL PROBABILITY = INTENSITY

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

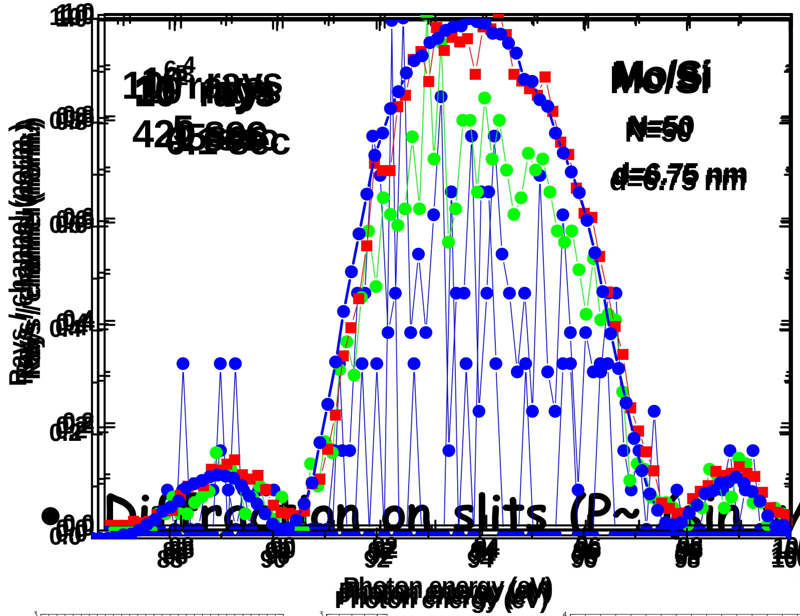


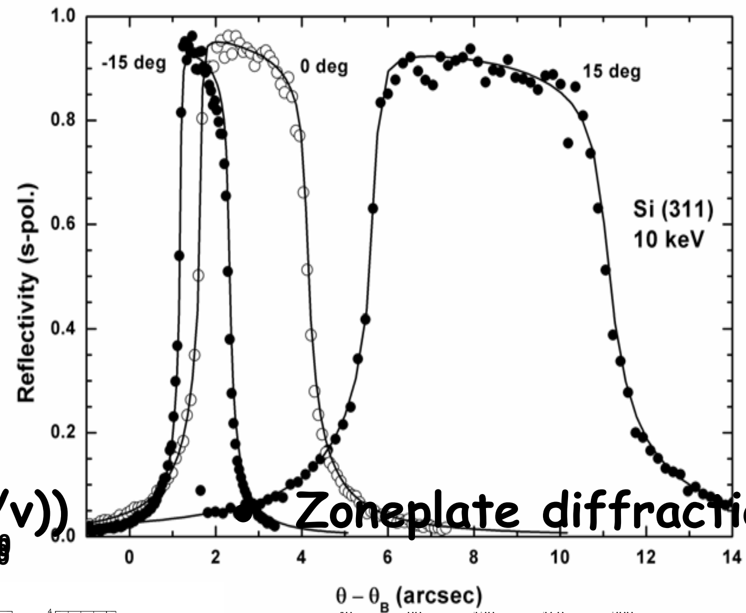
Applicable to ANY probability function

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

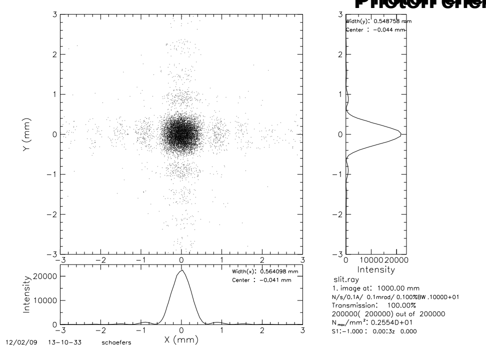
- **Statistical treatment of an ensemble of rays**
  Collective effects (Interference, diffraction…)

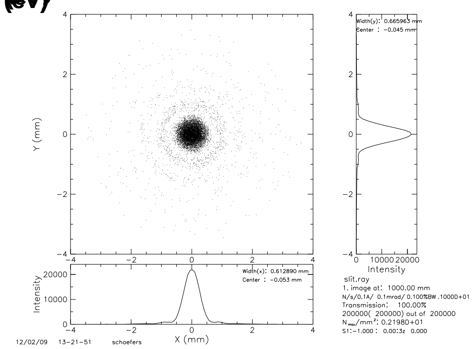
- **Reflectity losses / angle / energy (Rocking curves)**

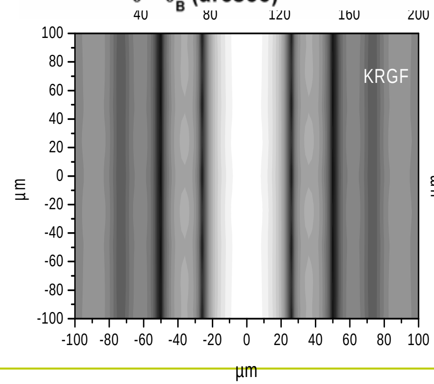


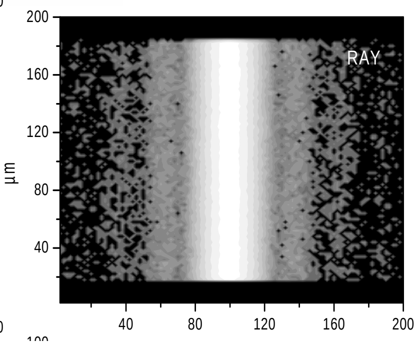


- **Diffraction on slits (P~…/v))**
- **Zoneplate diffraction (A. Erko)**





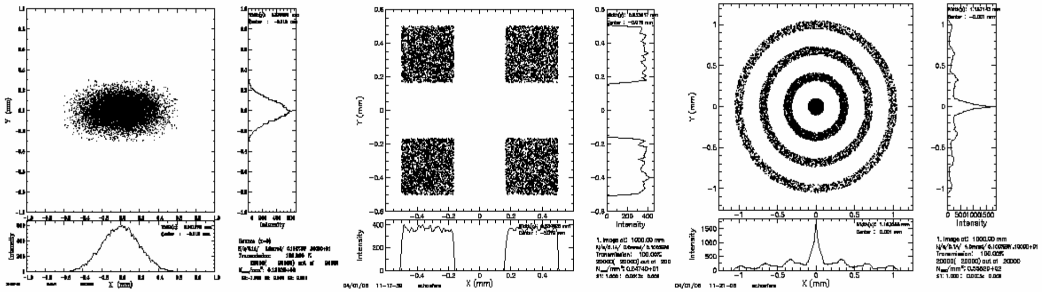




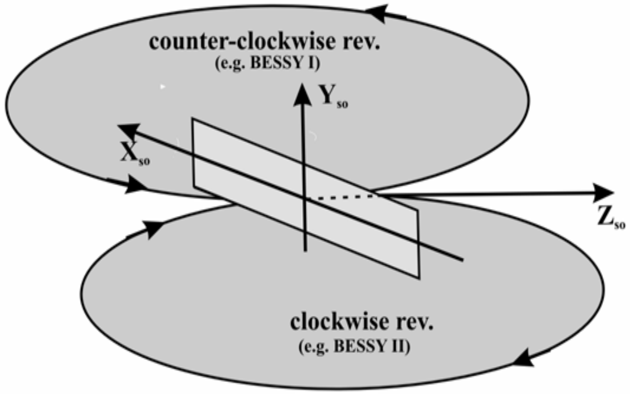
SOURCES

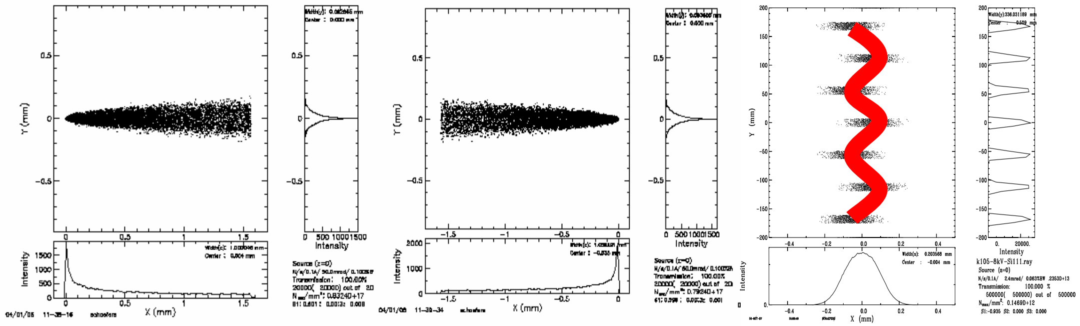
$$\vec{x} = \vec{x}_S + t\vec{\alpha}_S$$

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



PO_int **PI_xel** **CI_rcle**

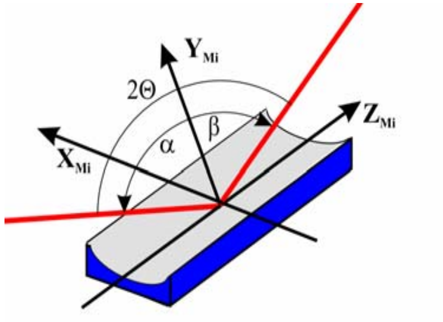




DI_pole **WI_ggler**

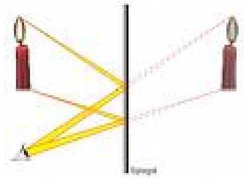
- Realistic simulation of source intensity, volume and emission
- Input by file: create your own source ((helical) undulator…)
- SR sources: polarisation included
  electron beam emittance effects
  detuning effects (orbit change, misalignment)

2nd, 3rd order surfaces

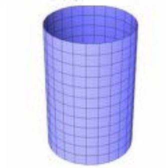


$$F(x,y,z) =$$
$$= a_{11}x^2 + a_{22}y^2 + a_{33}z^2 +$$
$$+ 2a_{12}xy + 2a_{13}xz + 2a_{23}yz +$$
$$+ 2a_{14}x + 2a_{24}y + 2a_{34}z + a_{44}$$
$$+ b_{12}x^2y + b_{21}xy^2 +$$
$$+ b_{13}x^2z + b_{31}xz^2 +$$
$$+ b_{23}y^2z + b_{32}yz^2 = 0$$

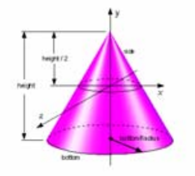
PM_plane m.



CY_linder (x,z)

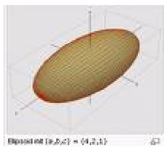


CO_ne

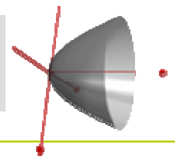


SP_here

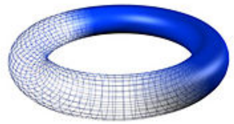
EL_lipsoid



PA_raboloid (circ., ell.)

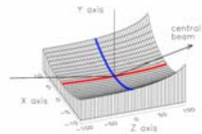


TO_roid



ET_elliptical toroid

DI_aboloid



EO_expert‘s optic

Textbook raytracing

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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

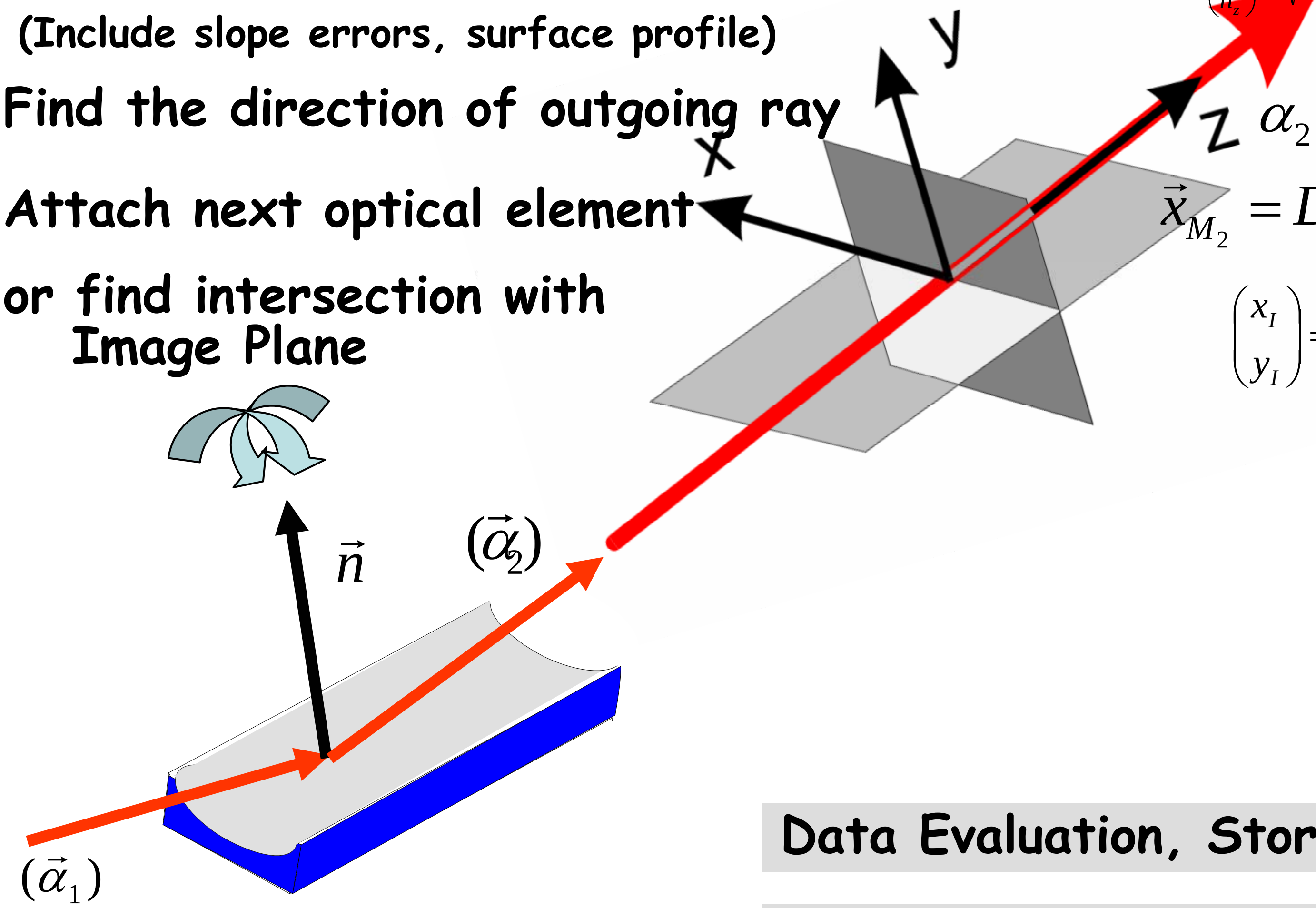
$$\alpha_2 = \vec{\alpha}_1 - 2 \cdot (\vec{n} \circ \vec{\alpha}_1)\vec{n}$$

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

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

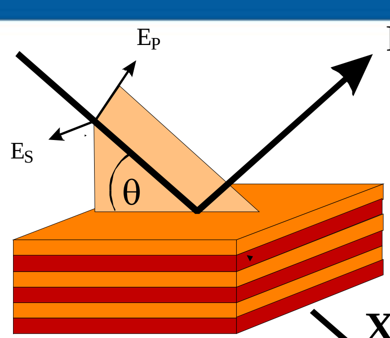


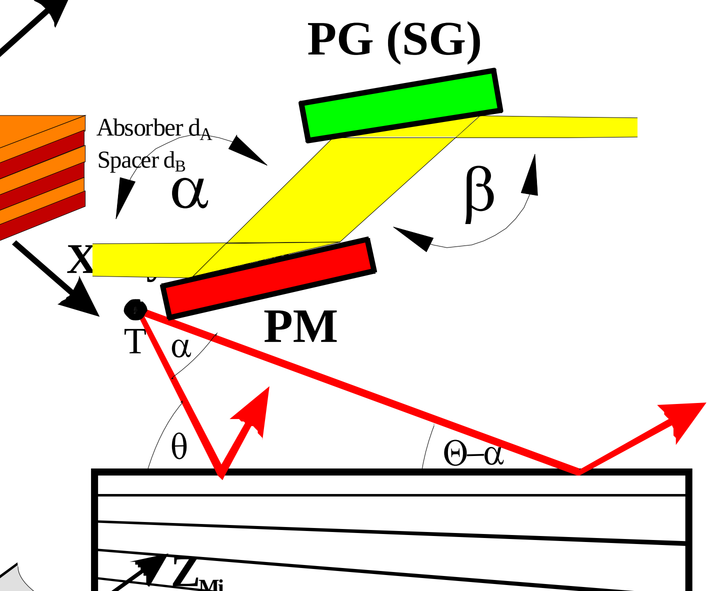
Data Evaluation, Storage, Display

Start with a new ray in the source…

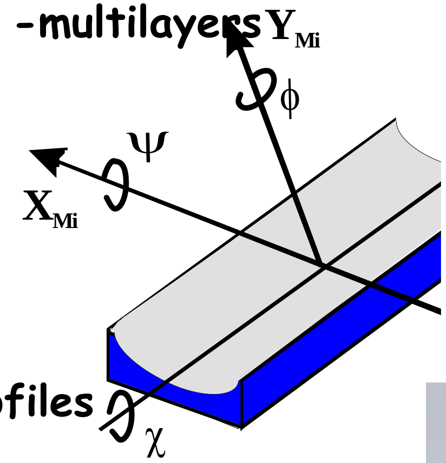
Features of optical elements

- (Multilayer-) Coatings on Optics
- Special monochromator mounts:
  SX700 plane grating PGM
  Spherical grating SGM

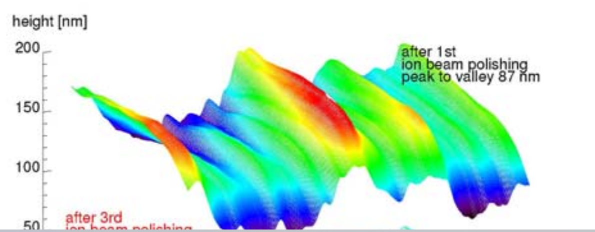




Varied Line Spacing-(VLS-) gratings
Laterally graded crystals, -multilayers



- Miscellaneous: Misalignment



Measured, calc. surface profiles

- Rectangular, circular shape or rings (capillaries)

Reflection Gratings (plane, spherical, toroidal)

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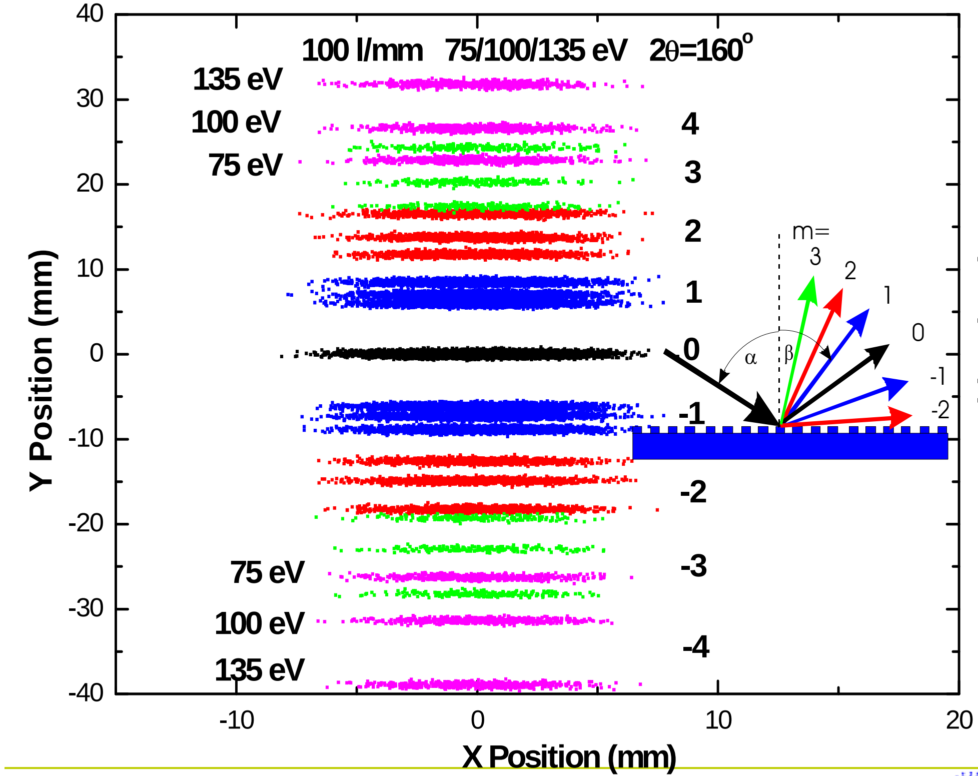
$$k\lambda = d(\sin\alpha + \sin\beta)$$

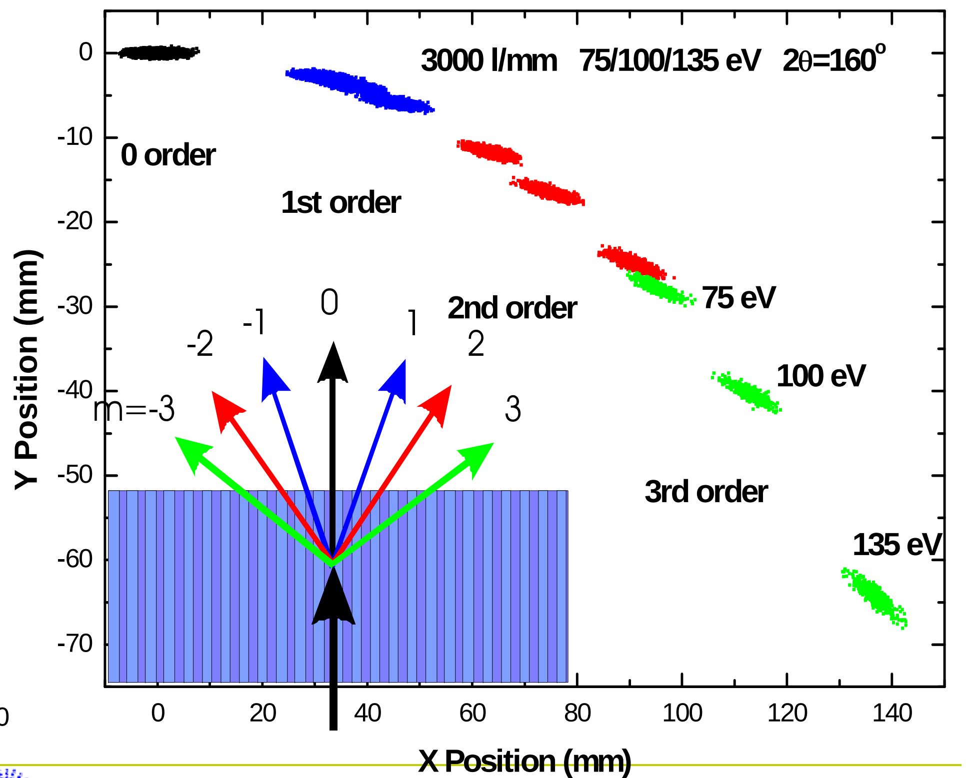
$$(\vec{\alpha}_2) = \begin{pmatrix} l_2 \\ m_2 \\ n_2 \end{pmatrix} = \begin{pmatrix} l_1 \\ \sqrt{m_1^{\,2} + n_1^{\,2} - (n_1 - a_1)^2} \\ n_1 - a_1 \end{pmatrix} \qquad a_1 = kl/d$$

VLS-Grating:

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



conical diffraction



KMC-1 beamline performance

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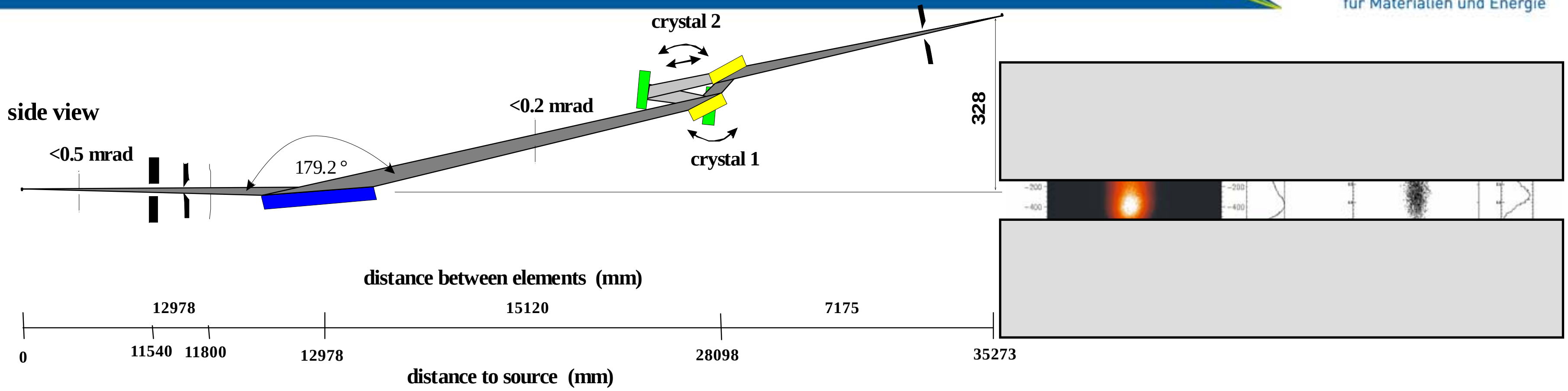
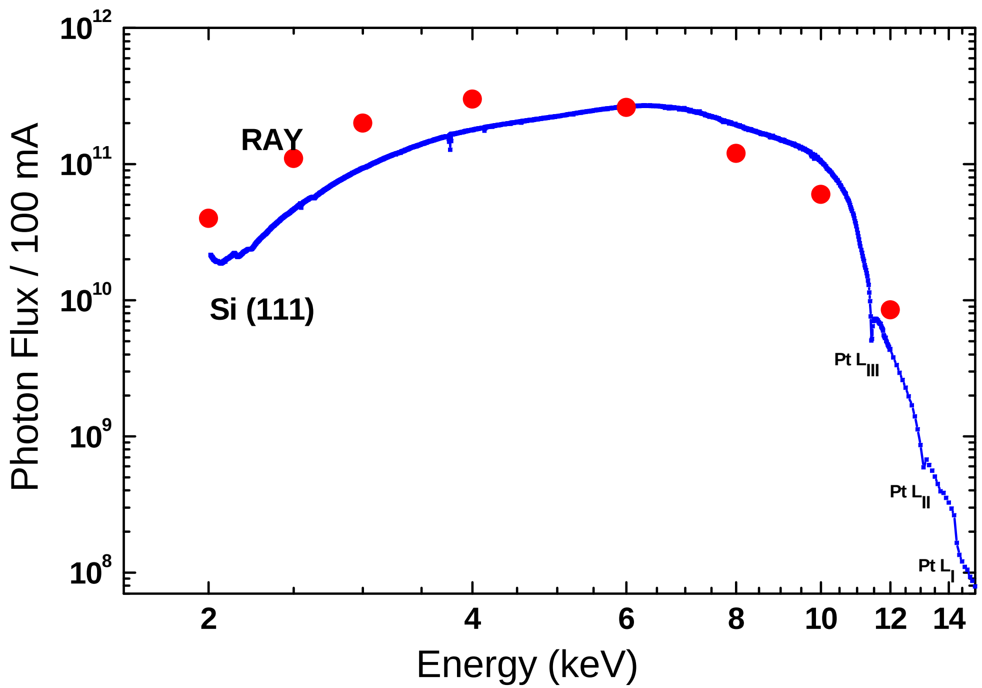
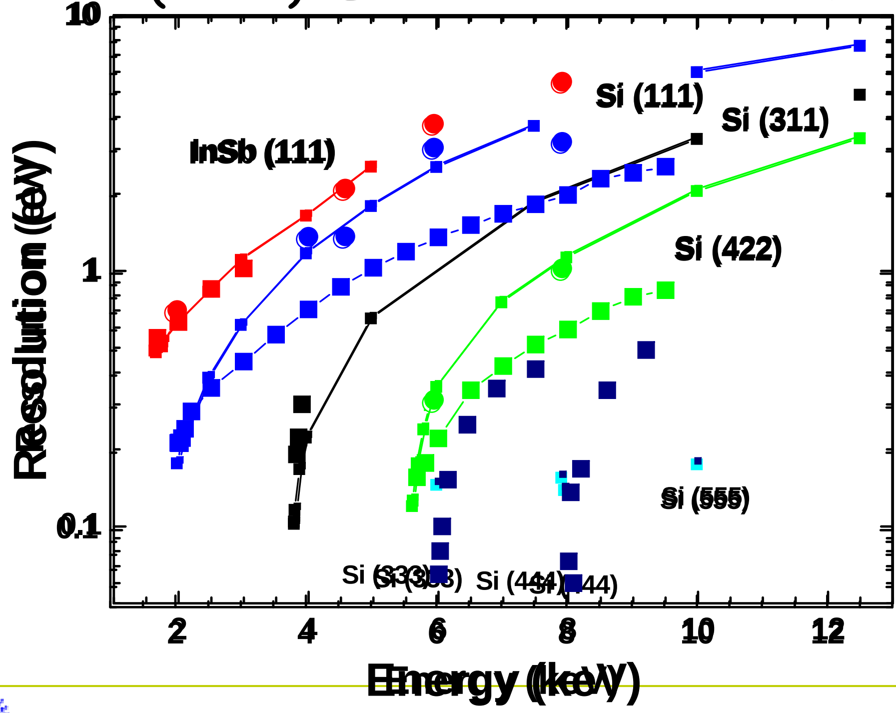




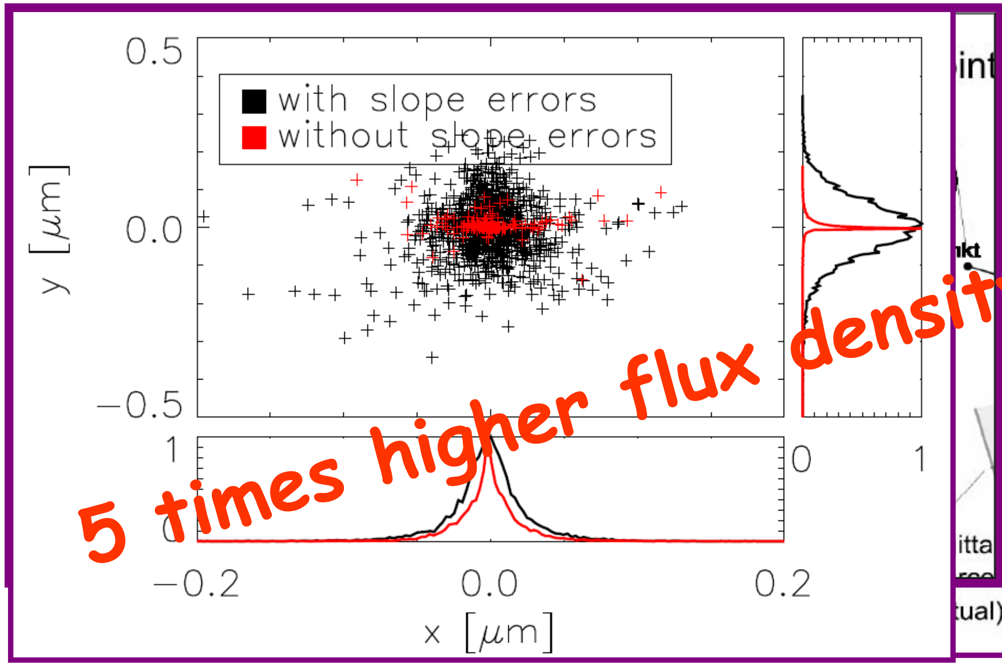
(HAX)PES better than calc.

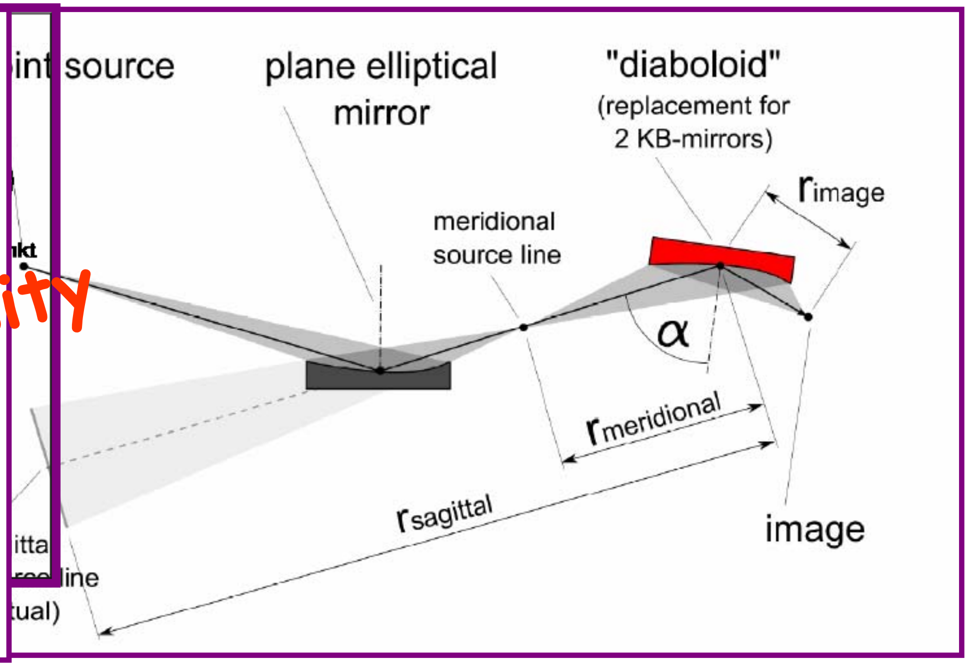


Diaboloid - optics

Stigmatic Imaging of an astigmatic source

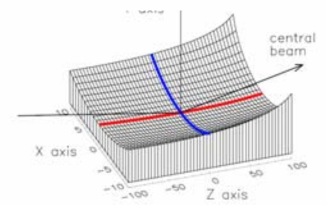
(Convert toroid to spherical wavefront)





slope error (σ)		0.5 μm x 0.2 μrad
spot size (fwhm)	red	0.028 μm x 0.005 μm
spot size with slope errors (fwhm)	black	0.037 μm x 0.162 μm

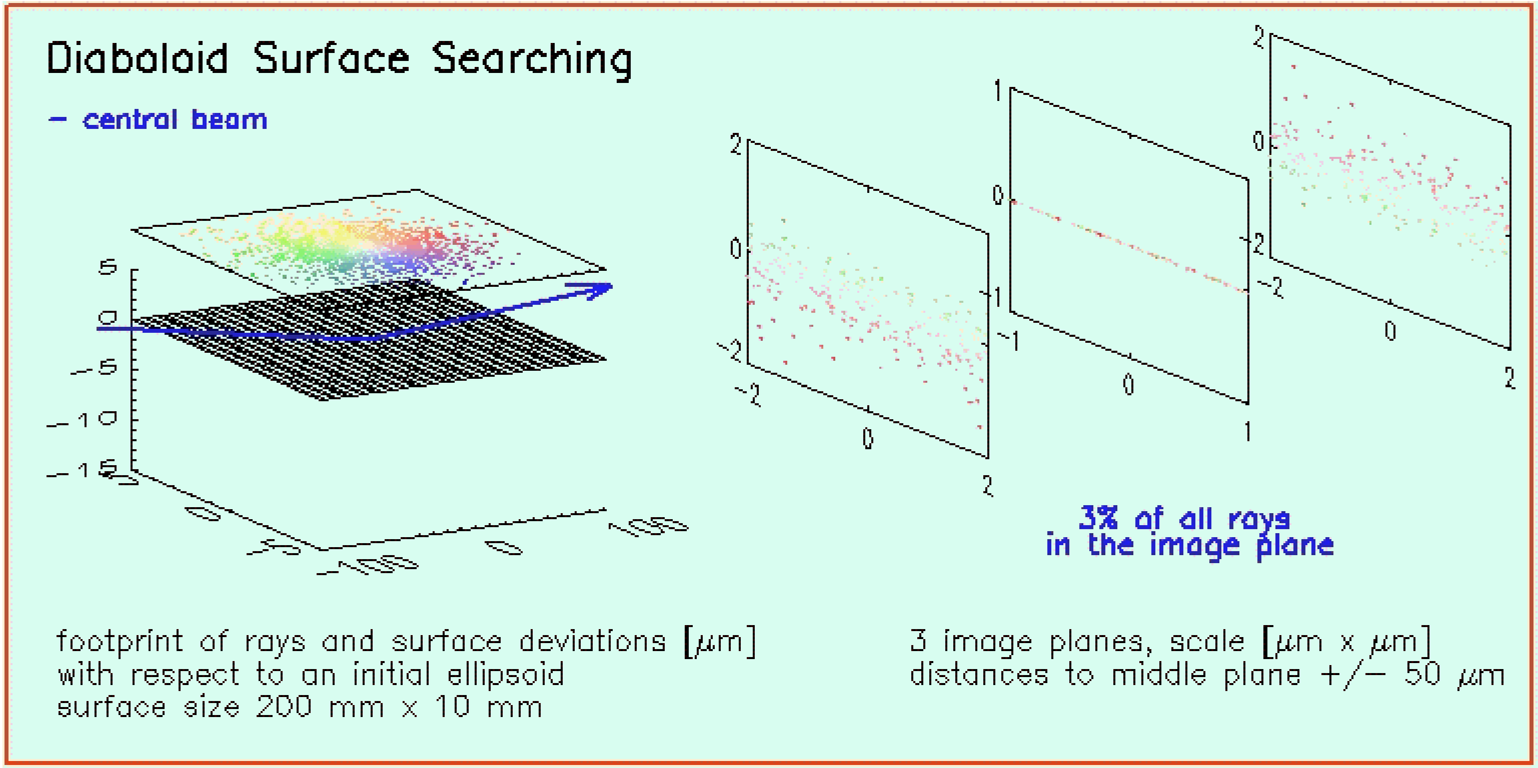
$r_{meridional}$	10 m
$r_{sagittal}$	33 m
α	87.5 °
r_{image}	180 mm
mirror size	200 mm x 10 mm



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

IDL-Animation
(Thomas Zeschke, BESSY)

Diaboloid - optics



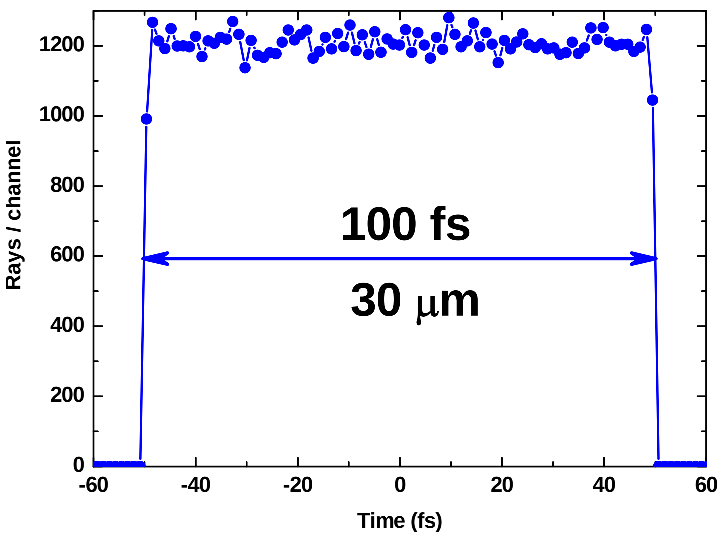
Time Evolution of beams - controlling the pulse shape & broadening

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

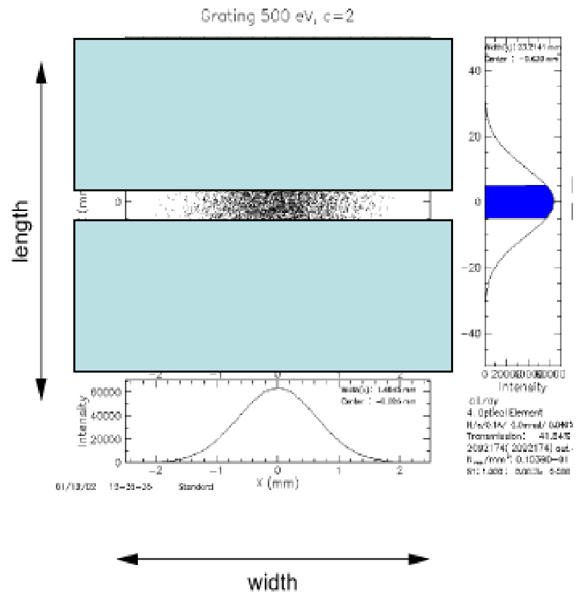
Phase $$\varphi = \frac{2\pi}{\lambda} pl$$

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

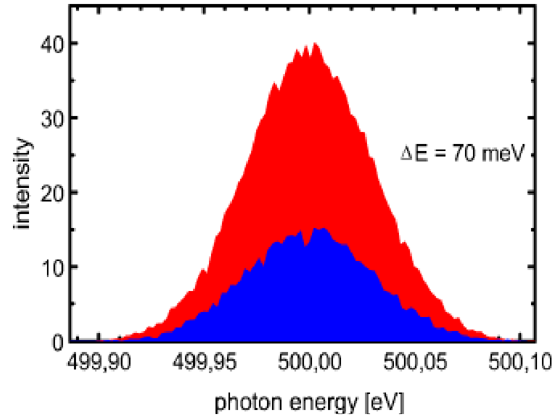
Source

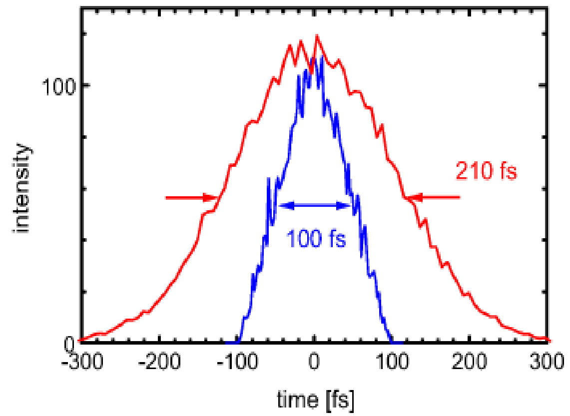


Grating



Focus





(source: 100 fs rectangular)

Confining illuminated grating length: pulse length unchanged

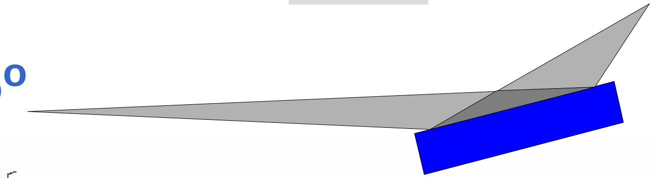
Wavefronts, Coherence

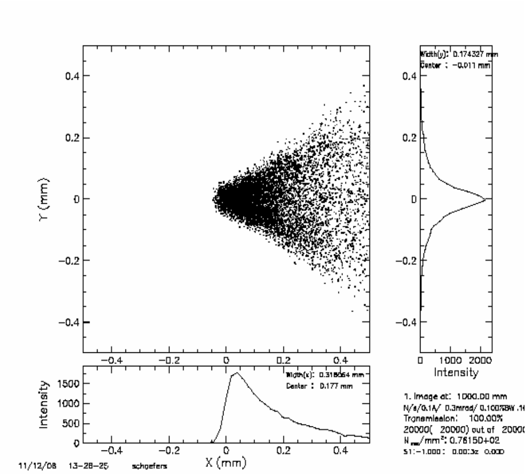
Path length $pl = \sqrt{((x - x_{old})^2 + (y - y_{old})^2 + (z - z_{old})^2)} - zq$

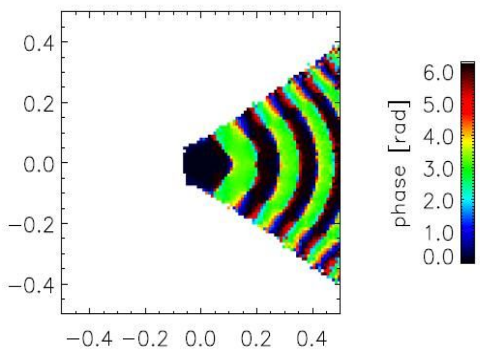
Phase $\varphi = \frac{2\pi}{\lambda} pl$

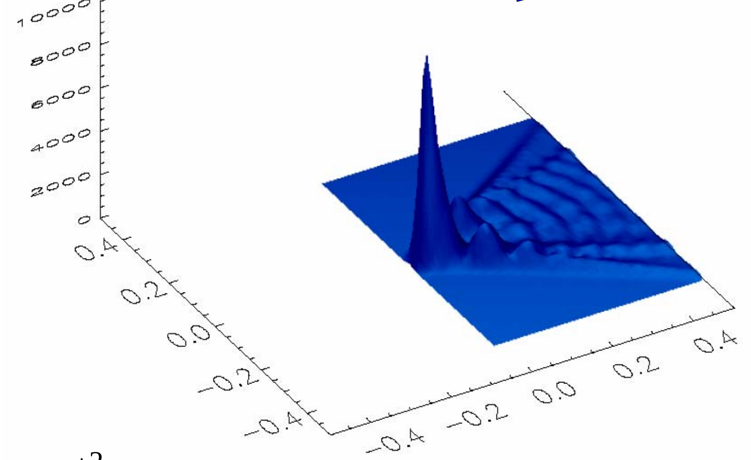
Travel time $t = \frac{pl}{c}$

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

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 !!!

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