Simulating Hard-Xray beamlines by ray-tracing using ShadowOui

Manuel Sanchez del Rio

OUTLOOK

- Introduction to ray tracing
- Sources
- Optics for Hard X-rays
- Examples

THEORY MODEL

MAXWELL → WAVE → HELMHOLTZ

WAVE OPTICS

GEOMETRICAL OPTICS
λ->0

FRESNEL-KIRCHHOFF
…
FOURIER OPTICS

$$\vec{E} = \vec{e}\ e^{ik_0 S(r)}$$

$$\vec{H} = \vec{h}\ e^{ik_0 S(r)}$$

$$(\nabla S)^2 = n^2$$

$$\nabla S = n\ \vec{s}$$

$$\frac{d}{ds}\left(n\frac{d\vec{r}}{ds}\right) = \nabla n$$

$$\nabla n = 0 \Rightarrow \frac{d\vec{r}}{ds} = 0 \Rightarrow \vec{r} = s\vec{a} + \vec{b}$$

$$\vec{E}$$

Very simple solution: we can sample the beam in many rays

FULLY COHERENT OPTICS
e.g. SRW

FULLY INCOHERENT
e.g. SHADOW3

COHERENT FRACTION (?)

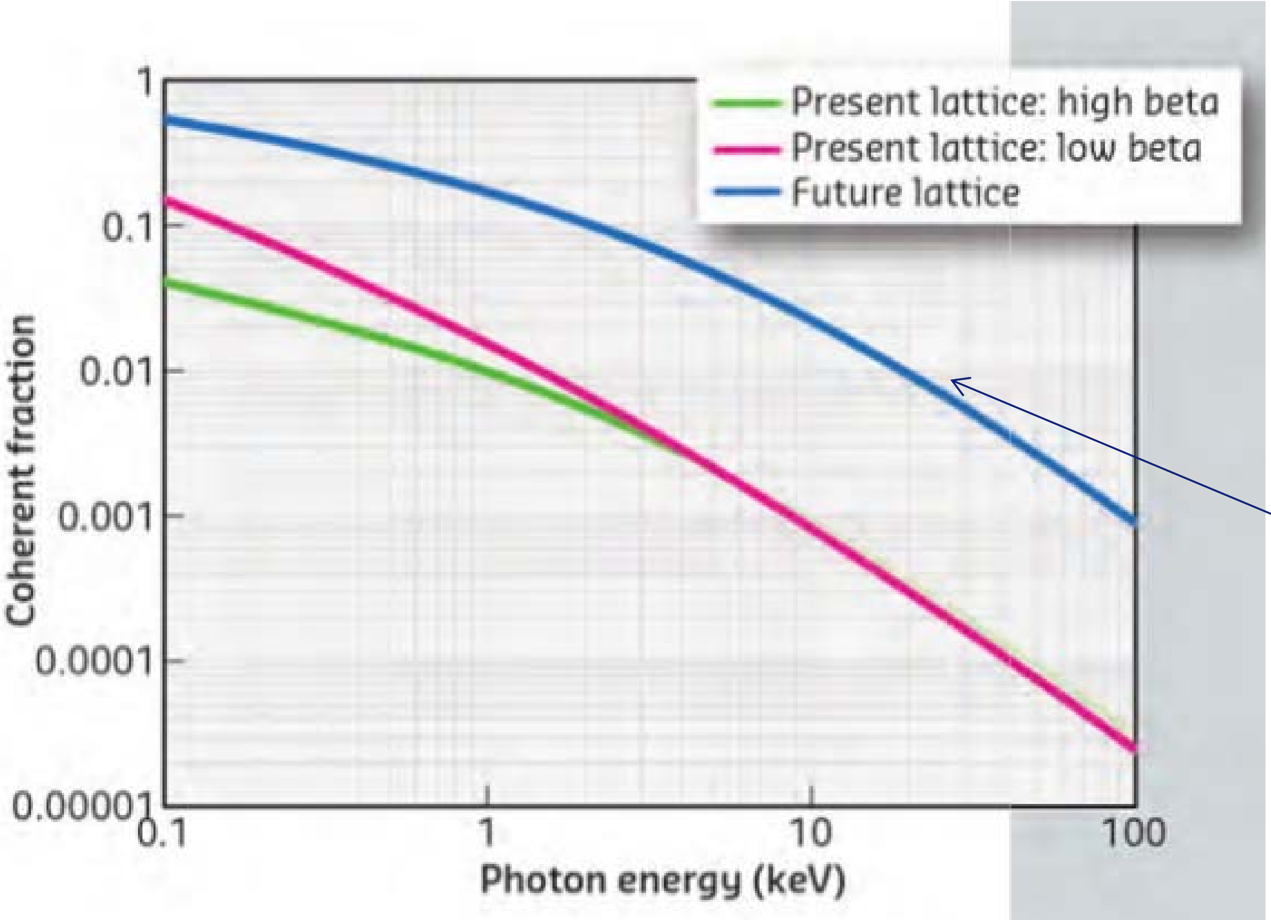


Figure 4.01: Comparison of the variation of the coherent fraction of X-ray emission with energy for the current insertion devices (low-β and high-β source points) and the proposed source.

Even with the new source, at 20 keV the emission is 99% incoherent =>

Optics simulations for incoherent beams cannot be neglected!!

THEORY MODEL

FULLY INCOHERENT

The HYBRID model:
apply concepts of wave optics to correct results of geometrical optics

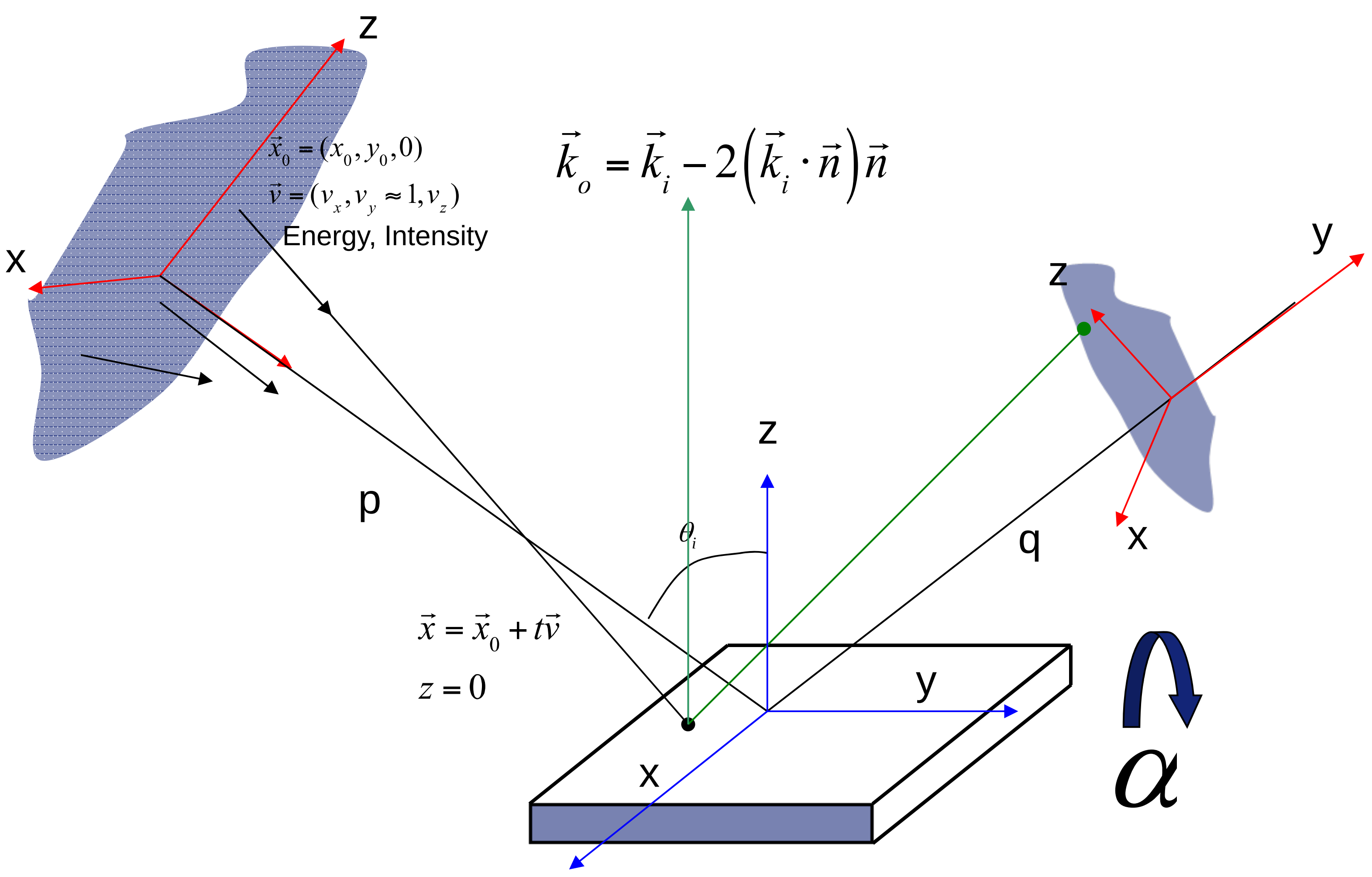
PARTIAL COHERENCE

- Combination of many waves
- Treated in a statistical way
- Full theory exists (Mandel & Wolf)
- Analytical model for Gaussian Beams

The multi e- model:
We know how to calculate and propagate a coherent wavefront (emitted by a single electron), so let the computer repeat it N times

FULLY COHERENT

Trace (the beamline)



A MODERN RAY-TRACING TOOL

RAY-TRACING ENGINE

SHADOW3

https://github.com/srio/shadow3

GUI AND DATA-FLUX ENGINE

orange
DATA MINING
FRUITFUL&FUN

http://orange.biolab.si

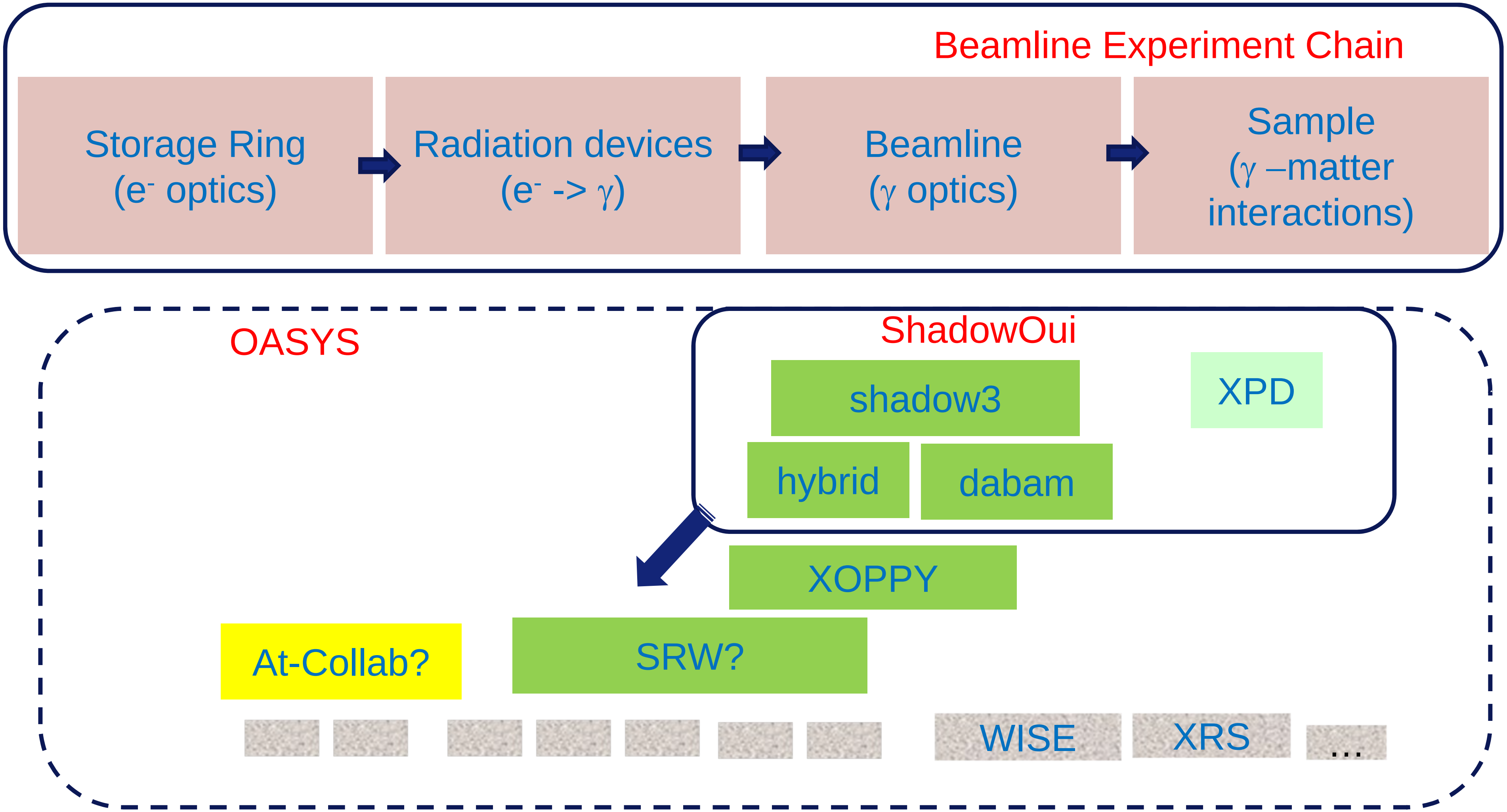
University of Ljubljana
Faculty of Computer and Information Science

COMBINING POWERFUL TOOLS TOGETHER

M. Sanchez del Rio, N. Canestrari, F. Jiang, F. Cerrina, "*SHADOW3*: a new version of the synchrotron X-ray optics modelling package", J. Synchrotron Rad. (2011), 18, 708–716

J. Demšar, B. Zupan, "Orange: From Experimental Machine Learning to Interactive Data Mining", White Paper (www.ailab.si/orange), Faculty of Computer and Information Science, University of Ljubljana(2004)

GOAL: VIRTUAL EXPERIMETS – SOFTWARE INTEGRATION



L Rebuffi

Graphical environment for optics (and more) simulations

- Python-based
- Module add-ons
- Packages that communicate

ShadowOui	XOPPY	X-ray server	WISE	crystal	Physical Optics	Accelerator tools
shadow3 xraylib pymca (silx)	xraylib silx	Stepanov codes	rough surface scattering	Stokes/muller	SRW? ?	pyAT

X-ray tubes

Radioactive sources / Excitation by radioactive decay

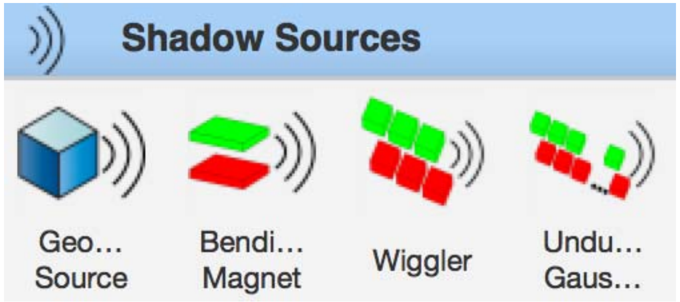
Synchrotron Bending Magnets

Synchrotron insertion devices (wigglers and undulators)

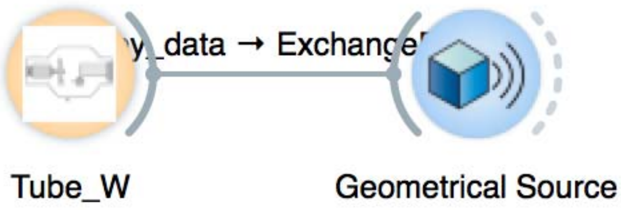
X-ray lasers

Others: Inverse Compton, Channelling

Pulsars/Quasars/Black holes etc.



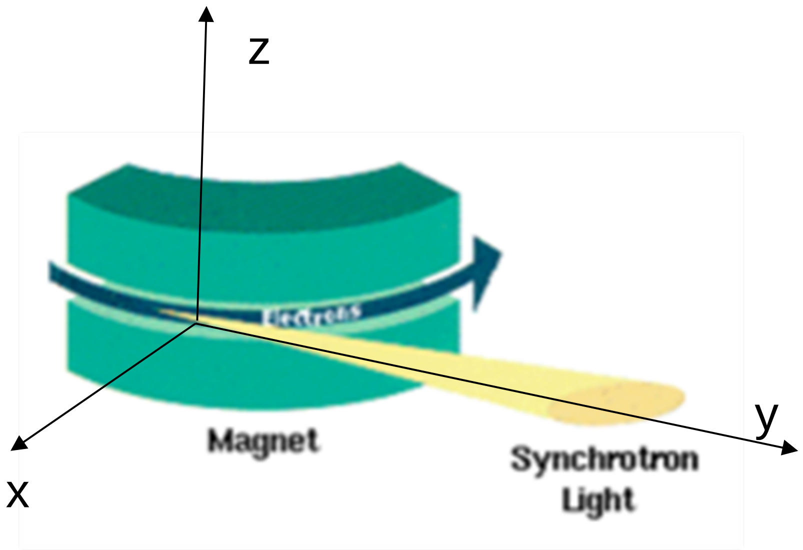
ShadowOui has tools to simulate synchrotron sources.



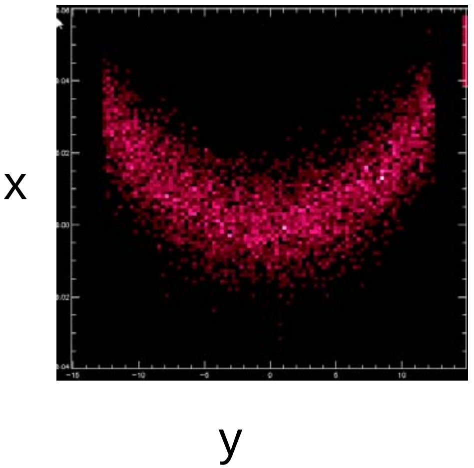
In addition a "Geometrical Source" can be used to approximate any source.

BM – INCOHERENT EMISSION ALONG THE TRAJECTORY

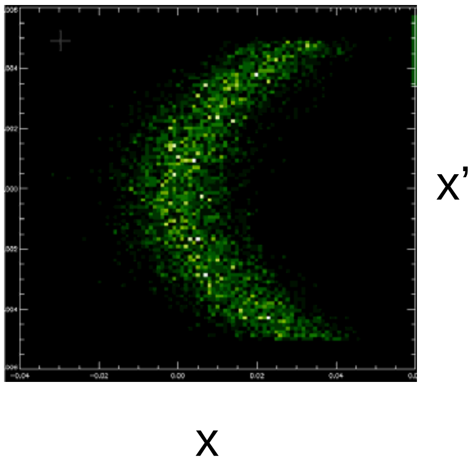
ex12_bendingmagnet.ows



Real Space (top)



Phase Space (H)



Monte Carlo (SHADOW)

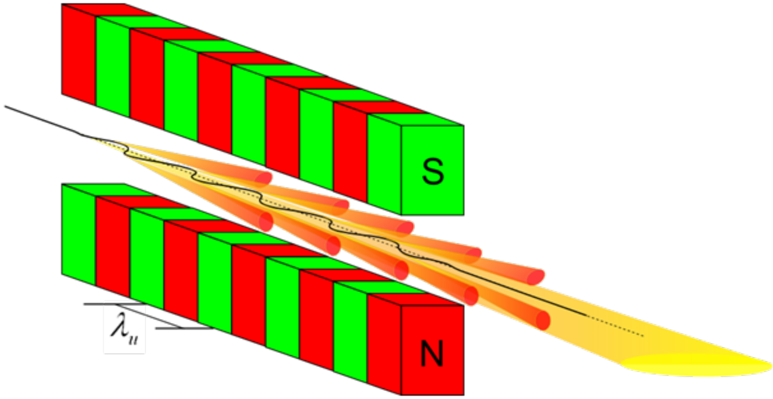
Energy (and polarisation) sampled from spectrum

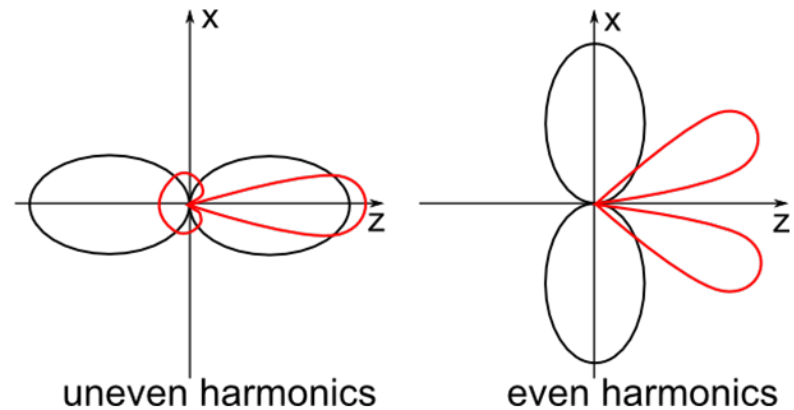
Geometry (along the arc,)

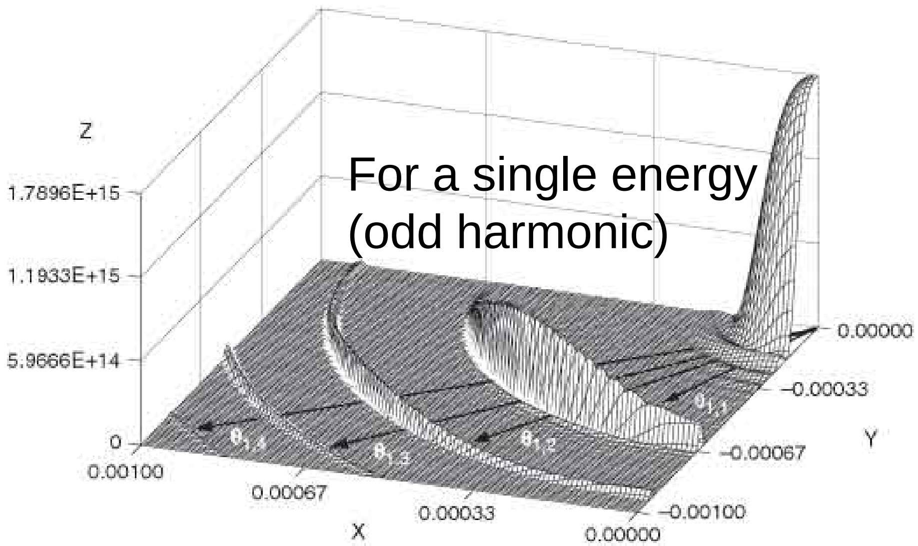
Angular Distribution for one electron

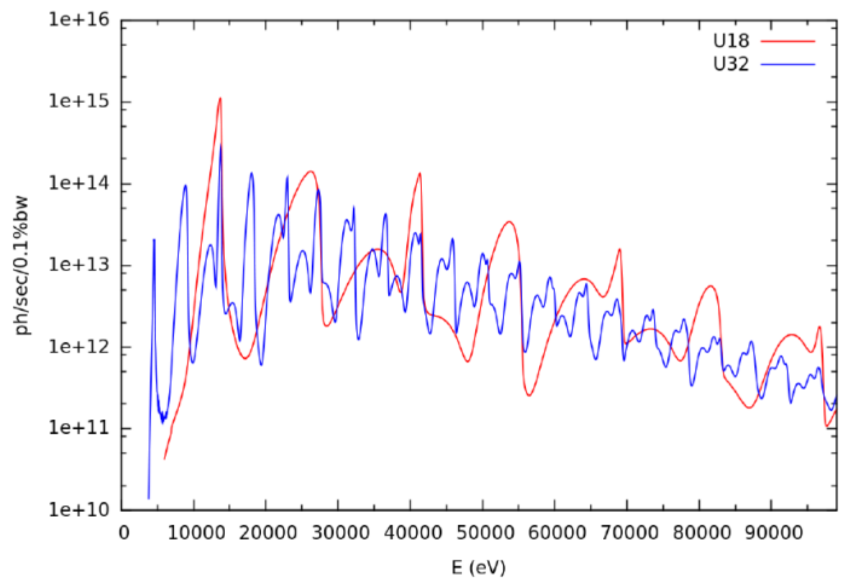
Convolution with electron beam (σ_x, σ_z, σ'_x, σ'_z)

UNDULATOR: MUCH MORE COMPLEX:
1E- EMISSION INTERFERS WITH ITSELF









Undulator

The FULL undulator is not yet available in ShadowOui, but it will be there very soon!

ONUKI & ELLEAUME UNDULATORS, WIGGLERS AND THEIR APPLICATIONS, CRC PRESS, 2002

below resonance

on resonance

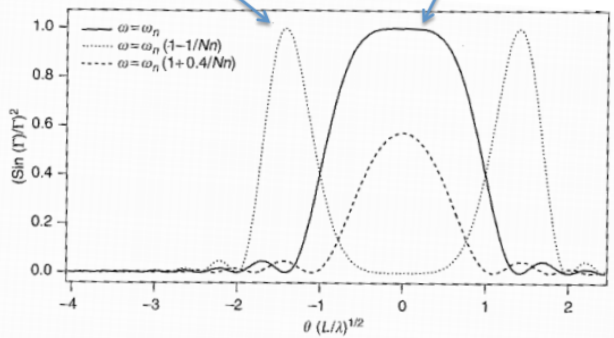


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2 + \theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1(0,0)$.

78 *P. Elleaume*

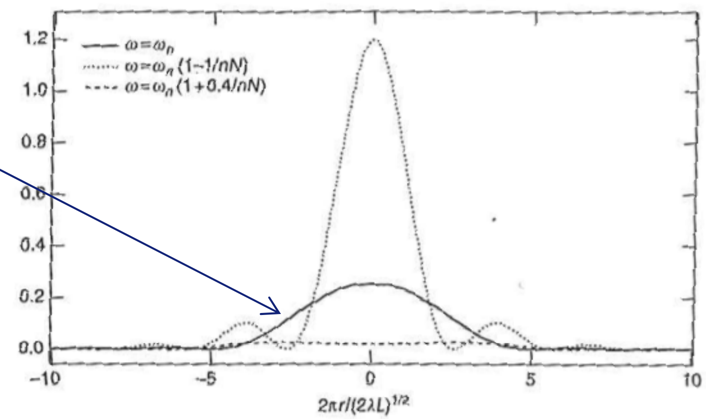


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0,0)$.

Even on resonance, beam is not fully Gaussian

But for resonance, can be reasonably approximated as Gaussian

$$\sigma_{r',photon} = 0.69\sqrt{\frac{\lambda}{L}}$$

$$\sigma_{r,photon} = \frac{2.704}{4\pi}\sqrt{\lambda L}$$

$$\Sigma_x^2 = \sigma_{x,elec}^2 + \sigma_{x,photon}^2 \qquad \Sigma_z^2 = \sigma_{z,elec}^2 + \sigma_{z,photon}^2$$

$$\Sigma_{x'}^2 = \sigma_{x',elec}^2 + \sigma_{x',photon}^2 \qquad \Sigma_{z'}^2 = \sigma_{z',elec}^2 + \sigma_{z',photon}^2$$

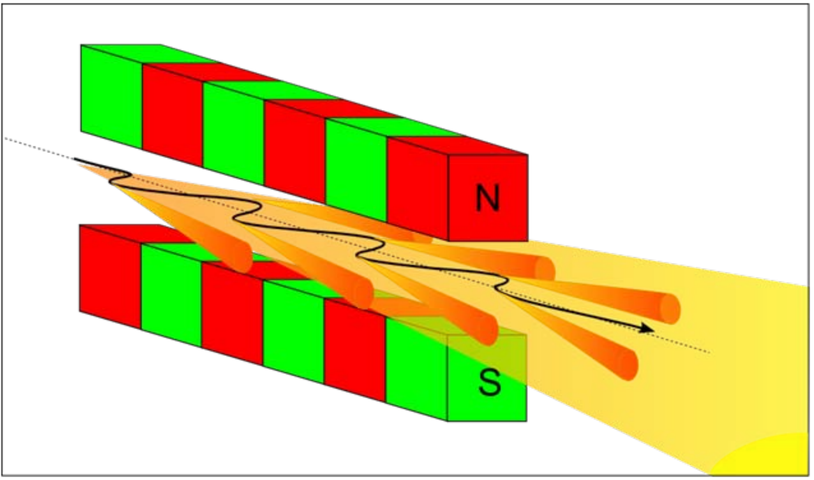
Undulator Gaussian

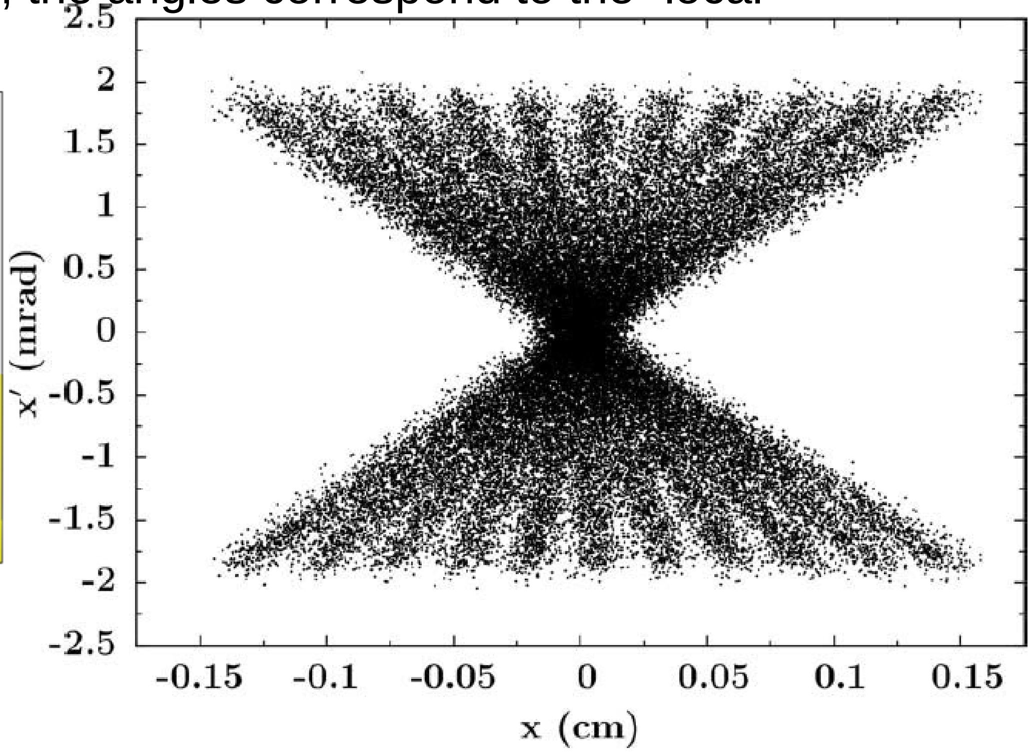
- THESE FORMULAS ARE VALID AT THE WAIST, AT THE UNDULATOR RESONANCE, AND SUPOSSING GAUSSIAN EMISSION OF PHOTONS)
- BY NOW IN ShadowOui WE APPROXIMATE UNDULATORS BY GEOMETRIC SOURCES WITH GAUSSIAN SIZES AND DIVERGENCES

WIGGLER: LIKE BM, BUT A BIT MORE COMPLEX

From magnetic field to trajectory, then:

- Photons emitted with axis tangent to the trajectory
- More photons where higher curvature
- At the emission point, the angles correspond to the "local" bending magnet





Wiggler

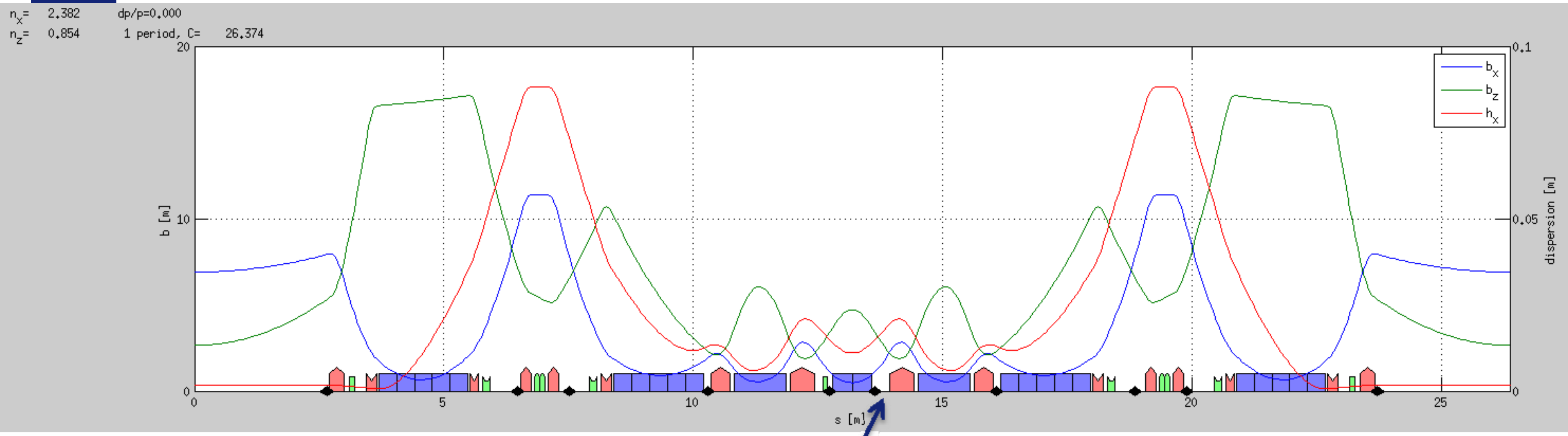
Figure 5
Plot of the horizontal phase space for a wiggler (ID17 at the ESRF) with 11 periods of 0.15 m length, K = 22.3 and electron beam energy of 6.04 GeV.

ex13_insertiondevices.ows

Practical case of Wiggler simulations:

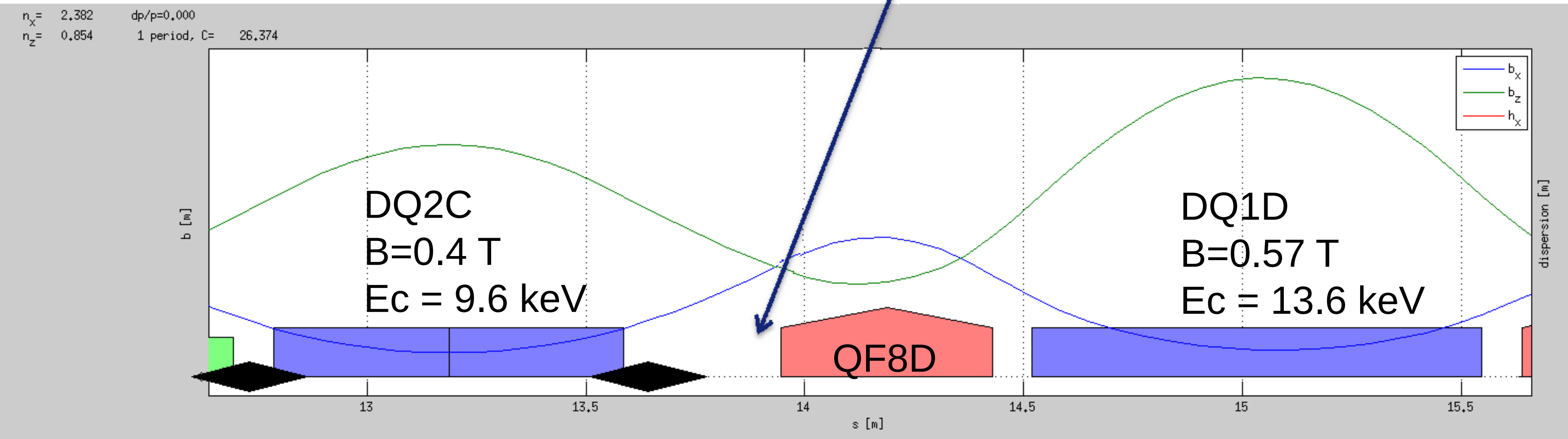
The new “Bending Magnet” beamlines at the EBS

 srio@esrf.eu



n_x= 2.382 dp/p=0.000
n_z= 0.854 1 period, C= 26.374
b [m]
dispersion [m]
s [m]
b_x
b_z
h_x

s_w =13.8379 m



n_x= 2.382 dp/p=0.000
n_z= 0.854 1 period, C= 26.374
b [m]
dispersion [m]
s [m]
b_x
b_z
h_x
DQ2C
B=0.4 T
Ec = 9.6 keV
DQ1D
B=0.57 T
Ec = 13.6 keV
QF8D

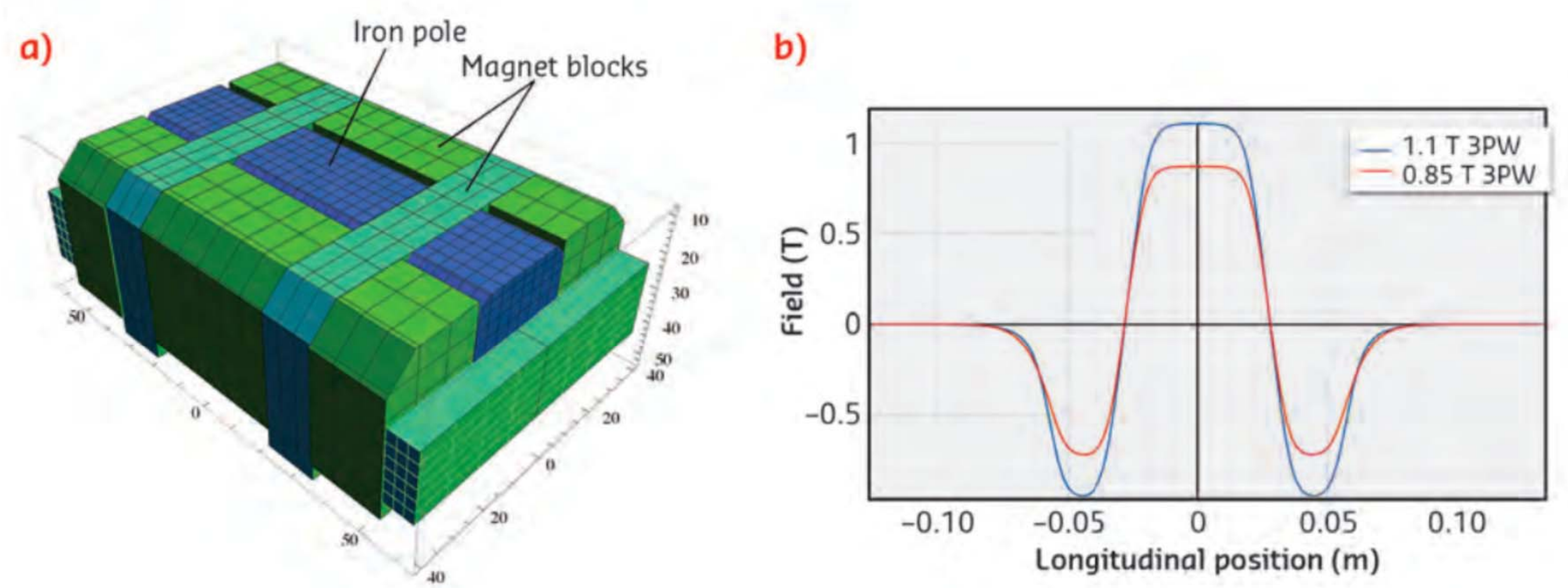
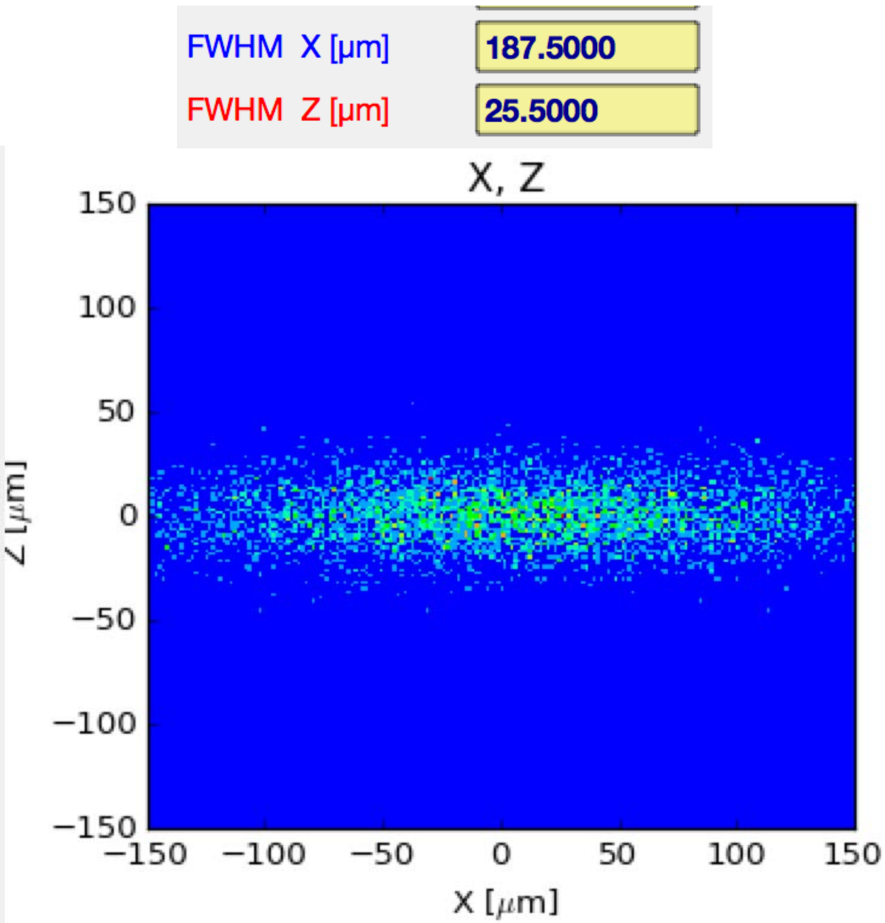


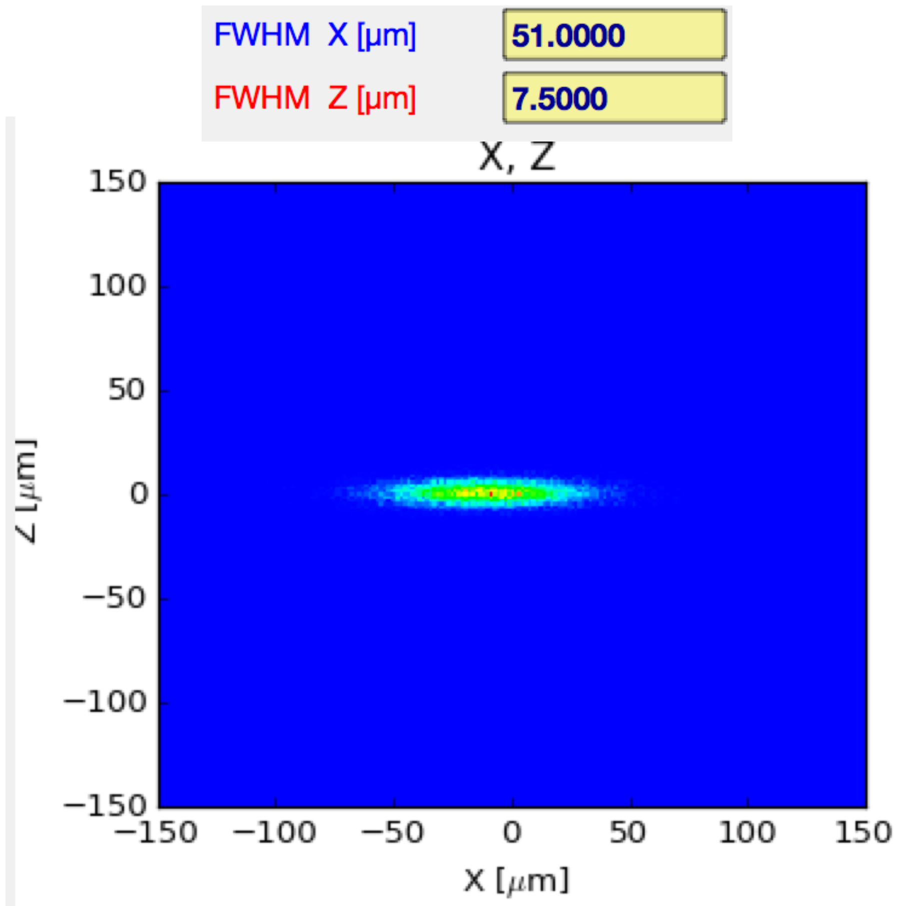
Figure 2.09: a) Magnetic structure of a typical three-pole wiggler (only one half represented for improved clarity) and b): Associated vertical field profile of the three-pole wiggler.

20 keV – 1:1 Ideal focusing

BM 3P

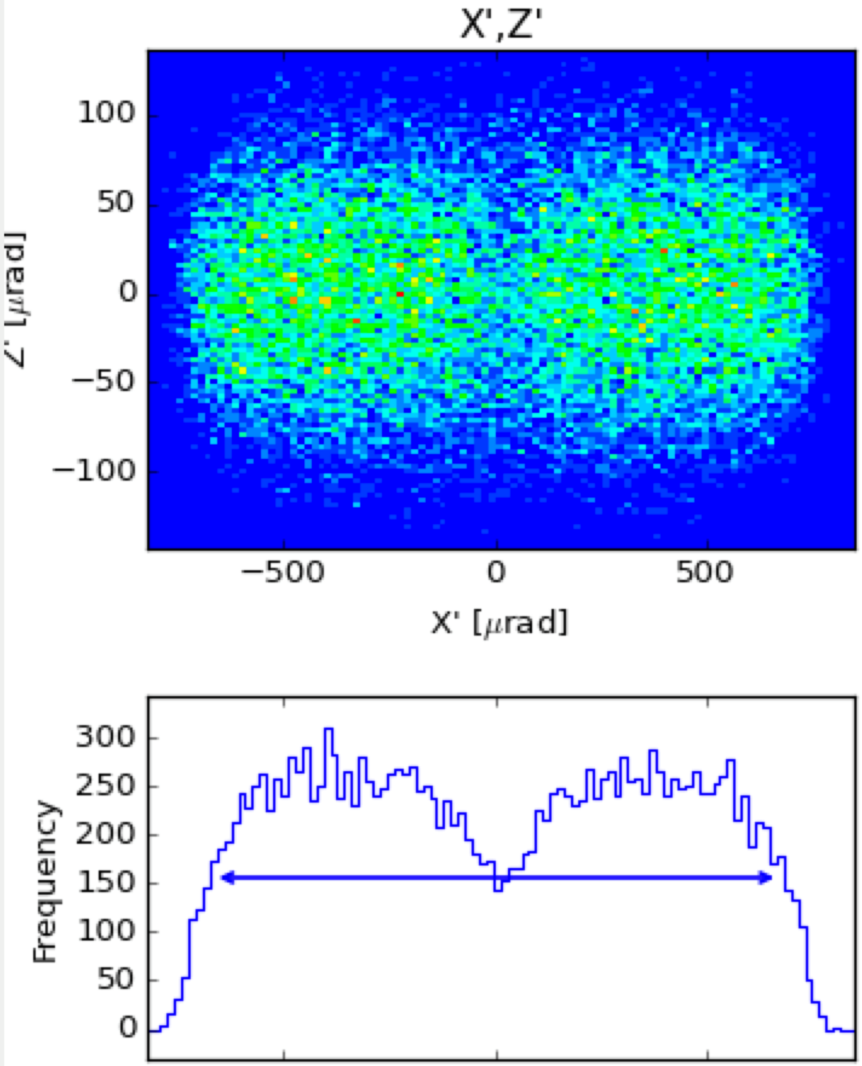
x12 Gain





Any solution produces a much more brilliant source than the present BMs

Emission 3P wiggler at 20 keV



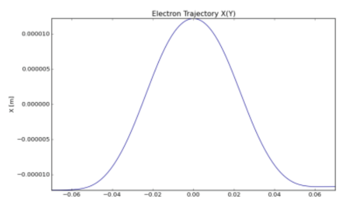
Accelerator Complexity

Beamline Performances?

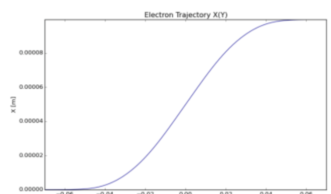
Effect of side BMs?

0 Poles

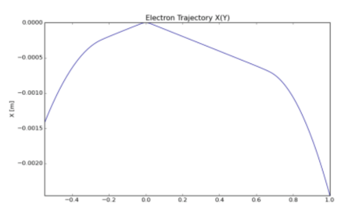
3 Poles

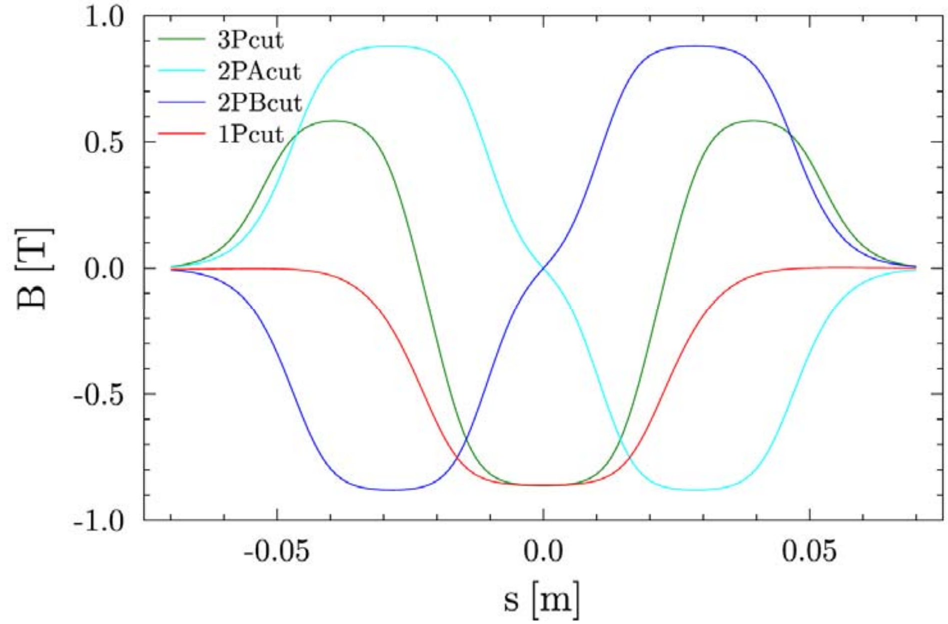


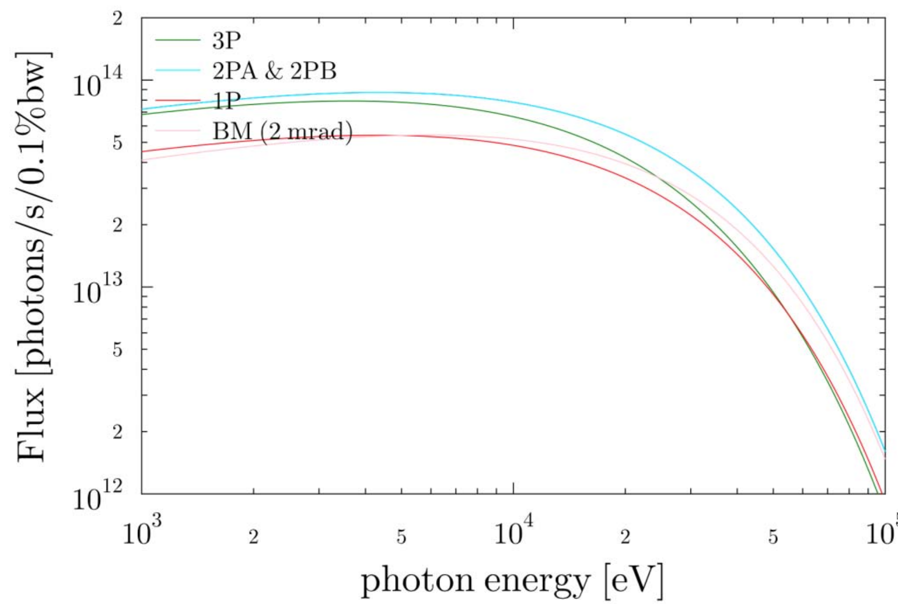
2 Poles



1 Pole

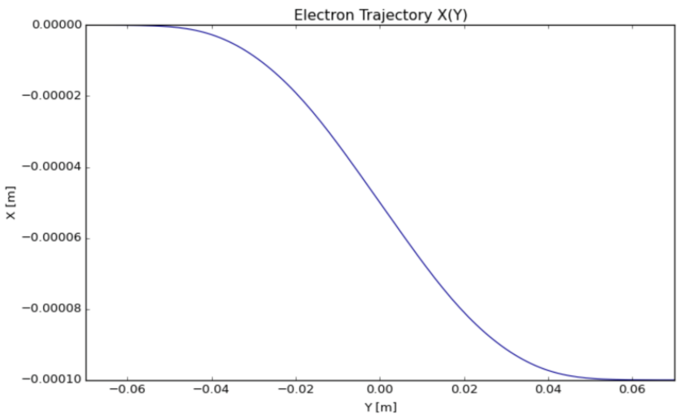


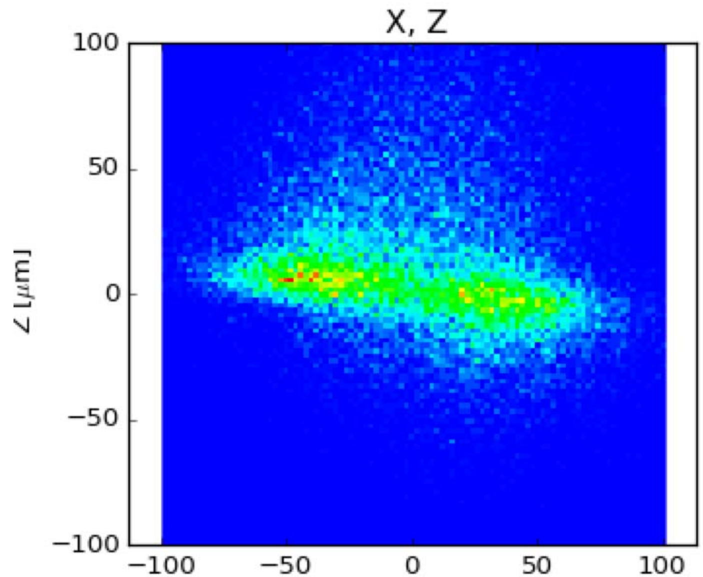


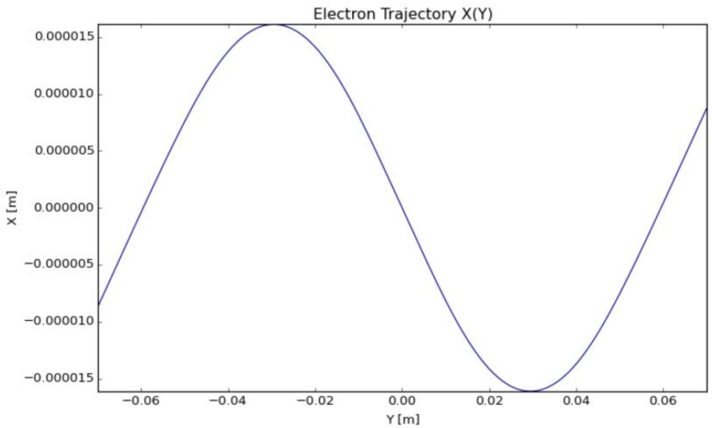


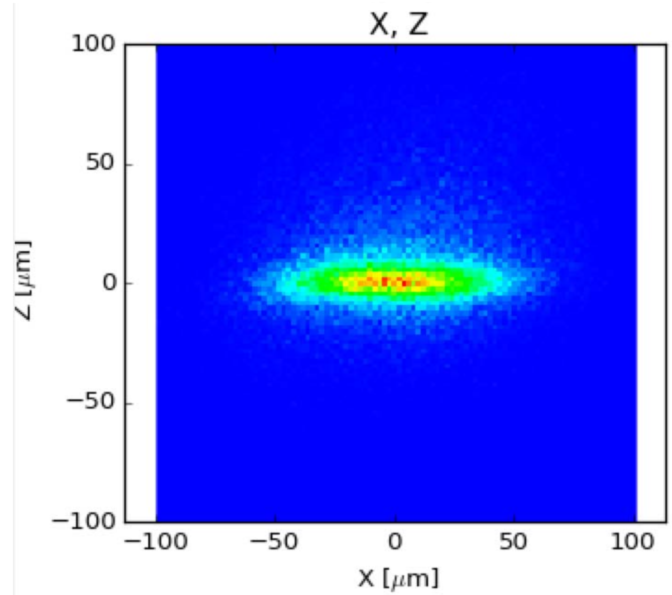
2PBcut – 20 keV – alignment

Trajectory 1:1 focusing (Toroid)



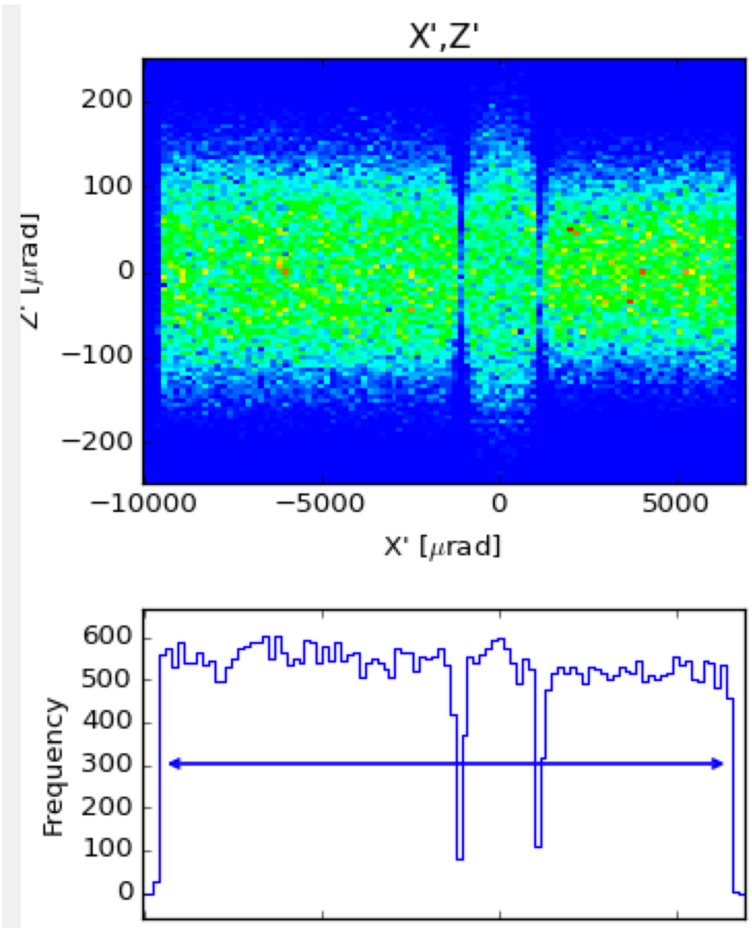


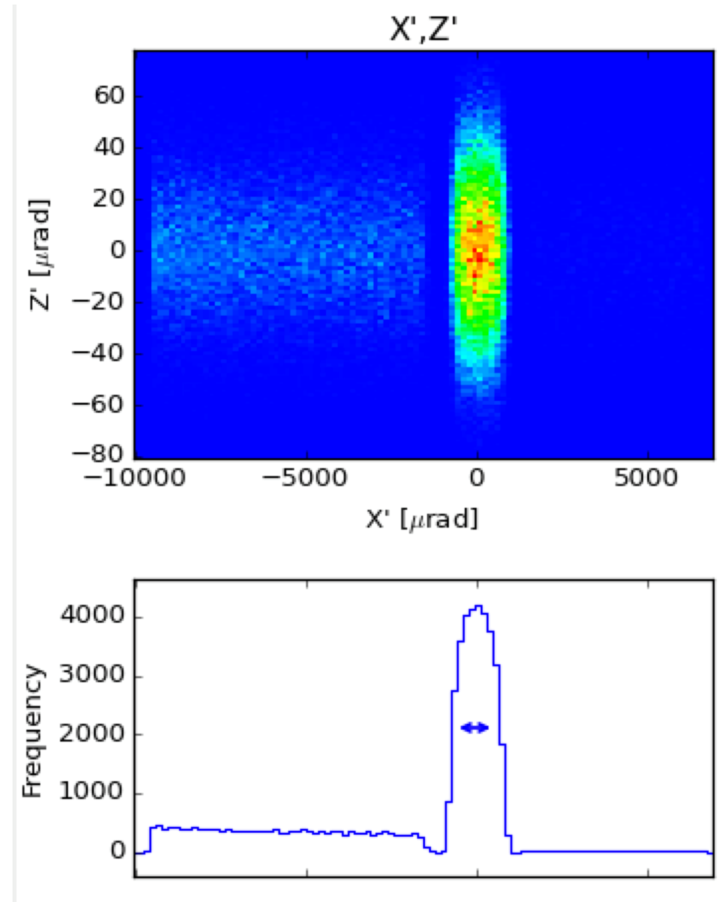




1P Divergences

5keV   80 keV





ROLES

- Transport the beam (vacuum)
- Shape the beam (slits)
- Focus (or collimate) (focusing elements: mirrors, lenses)
- Filtering (high pass: attenuators/filters, low pass: mirrors)
- Monochromatizing (crystals, multilayers)

Passive

Slits

Attenuators

Reflective optics

Mirrors

Refractive Optics

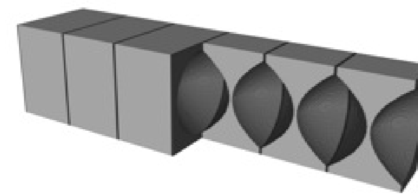
Lenses

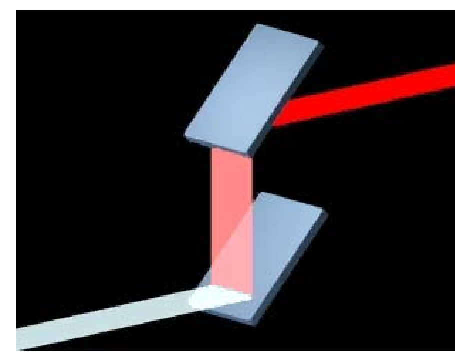
Diffractive optics

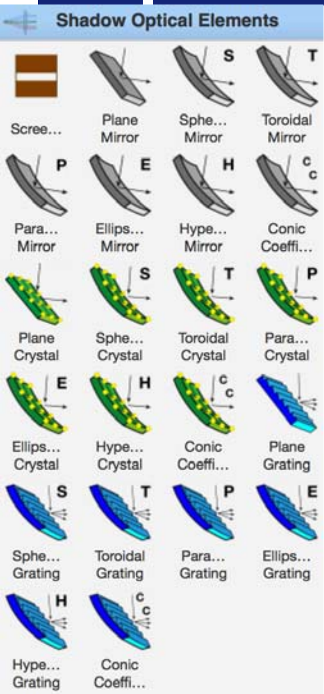
(Gratings)

Multilayers

Crystals







For each optical element we need:

Geometrical model: how the direction of the rays are changed:

reflected (mirrors)

refracted (lenses)

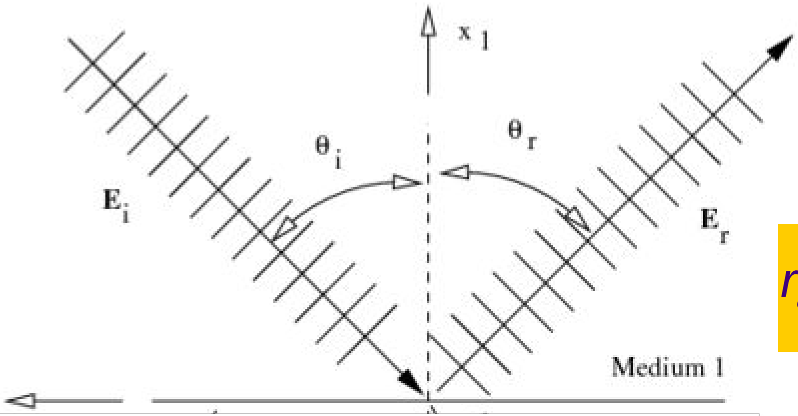
diffracted (gratings and crystals)

Physical model: how the ray intensity (in fact electric fields) decreases because of the interaction

- Structures along the surface =>playing with the direction
- Structures in depth => playing with the reflectivity

MIRRORS

GEOMETRICAL MODEL

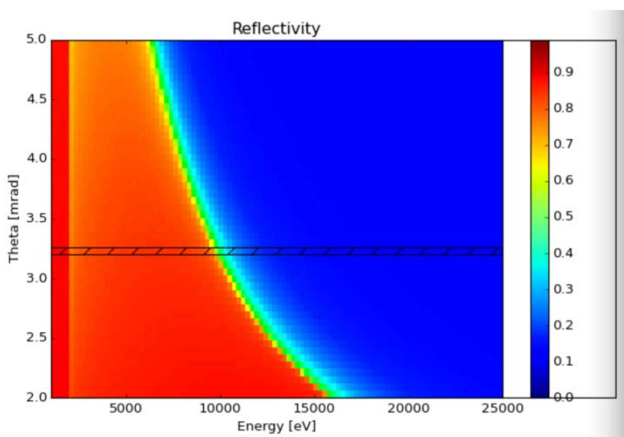


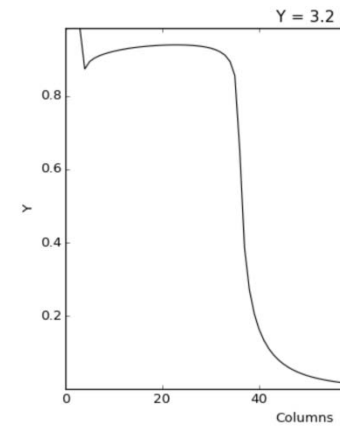
$$\vec{k}_o = \vec{k}_i - 2\left(\vec{k}_i \cdot \vec{n}\right)\vec{n}$$

PHYSICAL MODEL

Fresnel equations give the reflectivity as a function of angle and photon energy. As a consequence, one gets the critical angle:

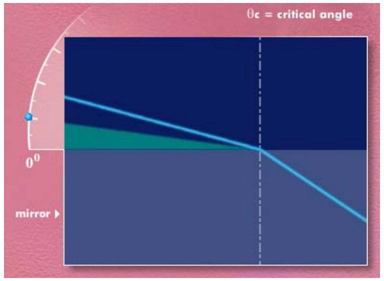
$$r_\sigma = \frac{n_1 \sin\theta_1 - n_2 \sin\theta_2}{n_1 \sin\theta_1 + n_2 \sin\theta_2}; \quad r_\pi = \frac{n_1 \sin\theta_2 - n_2 \sin\theta_1}{n_1 \sin\theta_2 + n_2 \sin\theta_1}$$

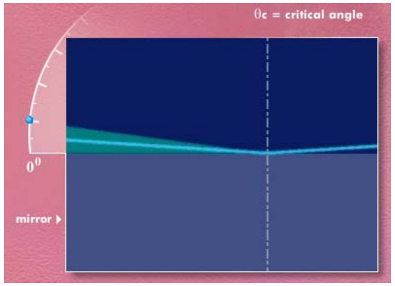




MIRRORS

ex15_aberration.ows ex16_kb.ows





$$\theta_c = \sqrt{2\delta}$$

- Total reflection: very grazing angles (~mrad):
    - Long mirrors
    - High aberration (shape is very important)
    - Surface finish
        - Slope errors: ~ urad
        - Roughness: ~A
- Mirror combinations (e.g. KB)

Waviness

Height Profile Simulator

DABAM Height Profile

Kirkpatrick-Baez Mirror

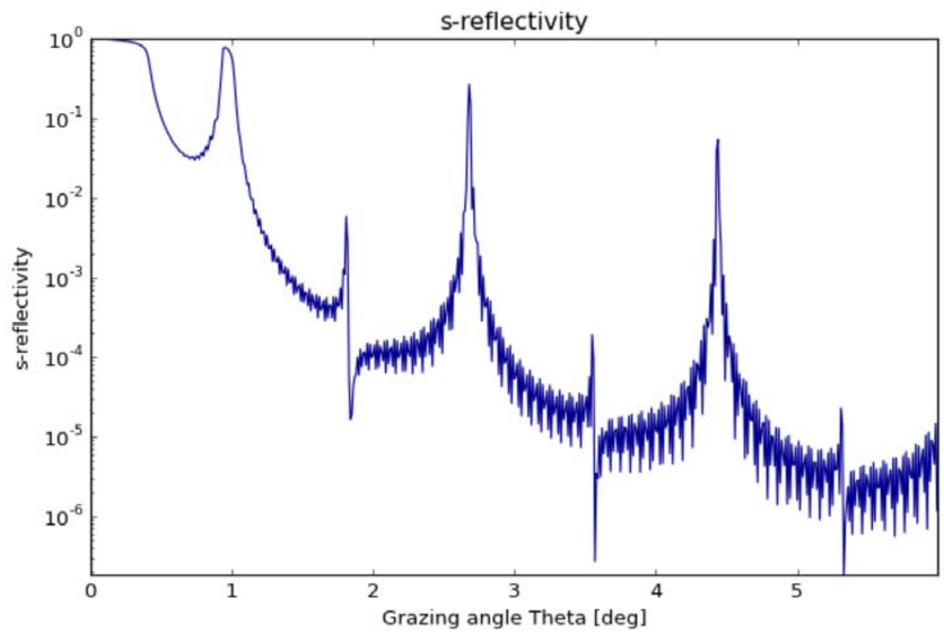
MULTILAYER *MIRRORS* (PHYSICAL MODEL)

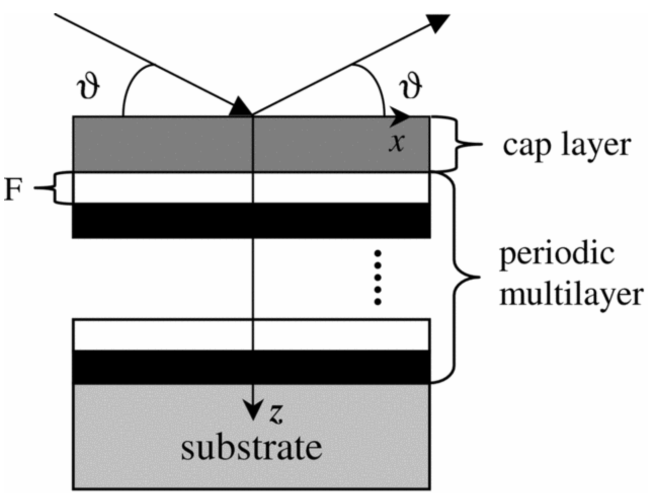
PHYSICAL REVIEW VOLUME 95, NUMBER 2 JULY 15, 1954

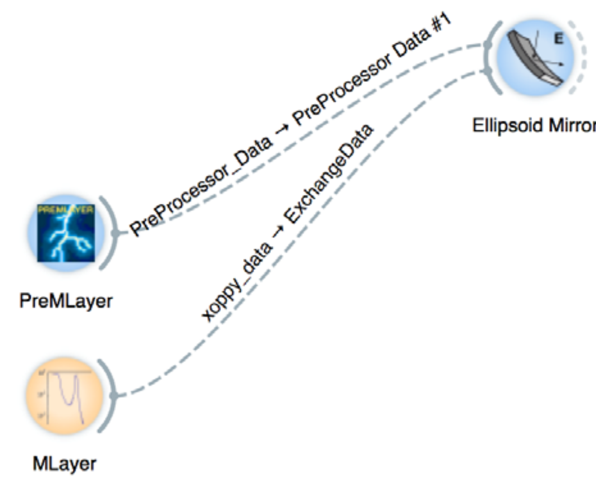
Surface Studies of Solids by Total Reflection of X-Rays*

L. G. PARRATT
Cornell University, Ithaca, New York
(Received March 22, 1954)

- no reflection from the back of the substrate
- compute recurrently the reflectivity of each layer from bottom (substrate) to top





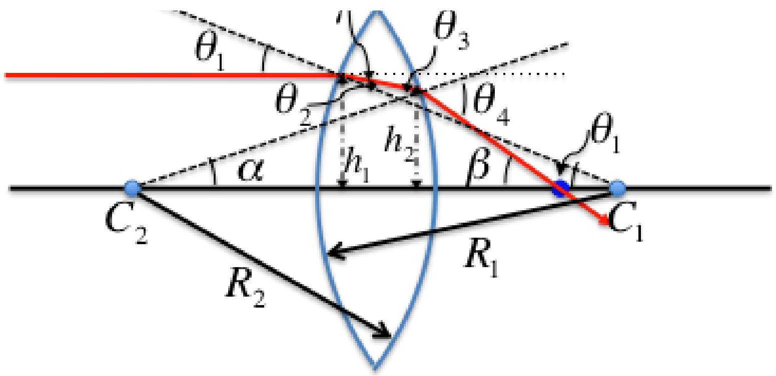


LENSE = TWO INTERFACES

GEOMETRICAL MODEL

Law of Refraction (Snell's Law)

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$



Focusing
Absorption
Chromatic aberrations
Geometrical aberrations:

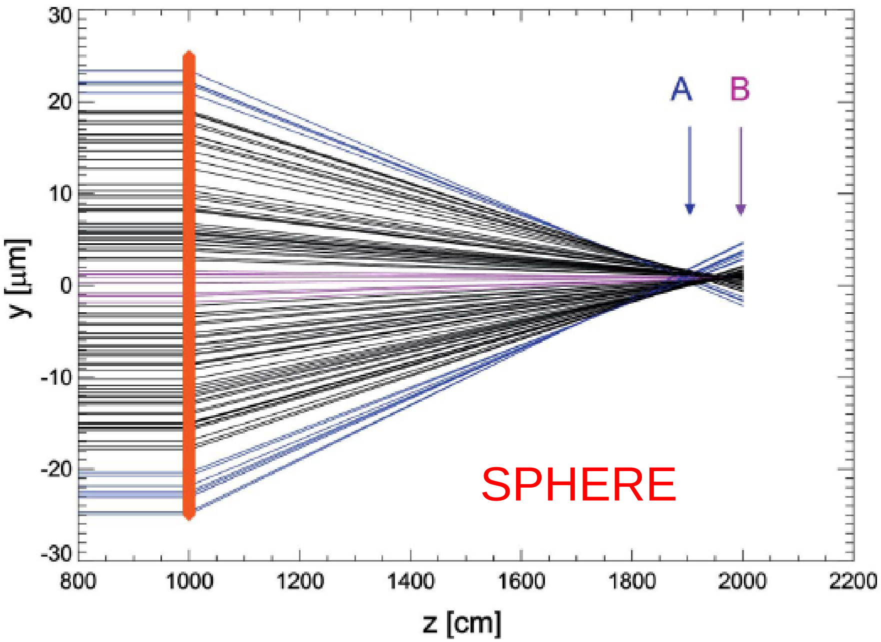
- Which is the best shape?
- Cylindrical => Lots of aberrations
- Parabolic => Much less aberrations (but non-zero)
- Elliptical => collimated beam to convergent beam
- Hyperbolic => convergent beam to collimated beam

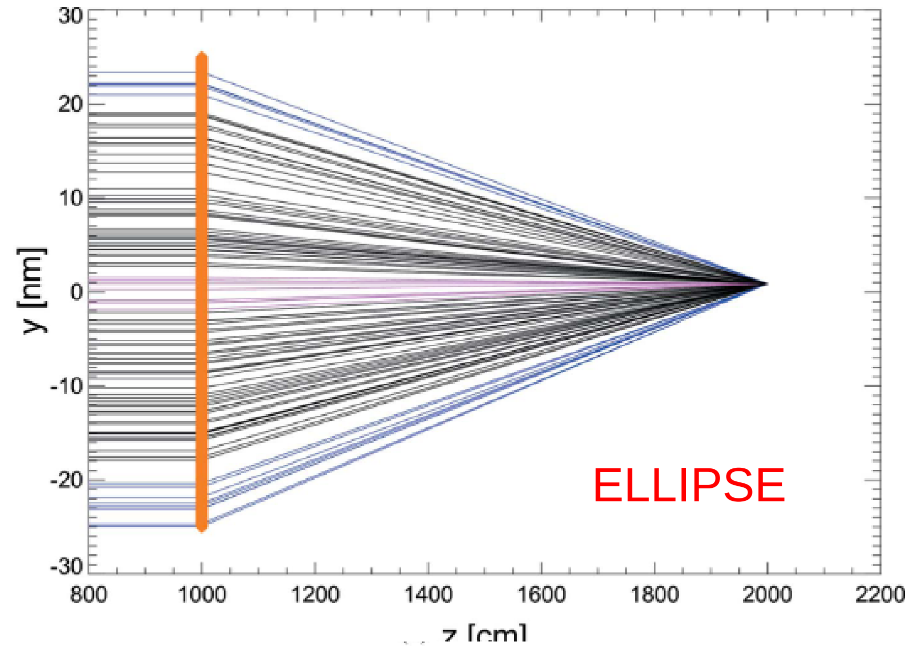
PHYSICAL MODEL

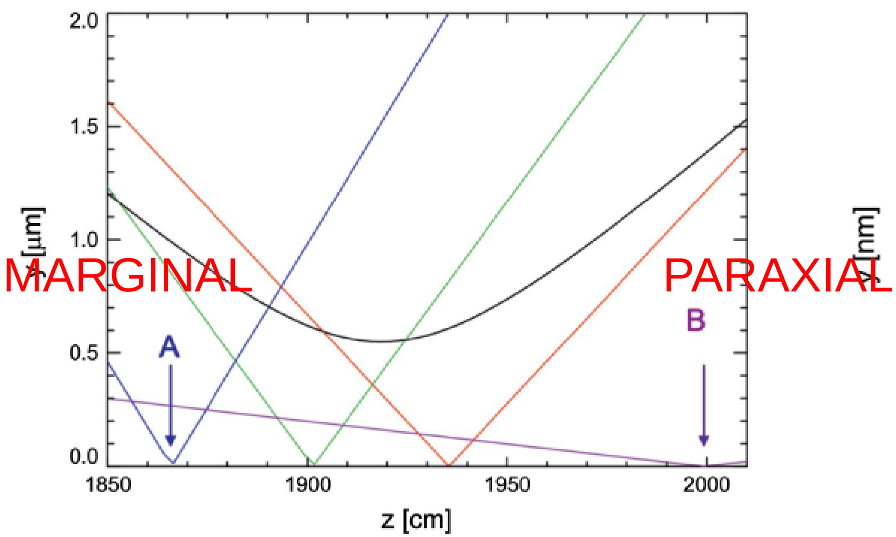
absorption in media

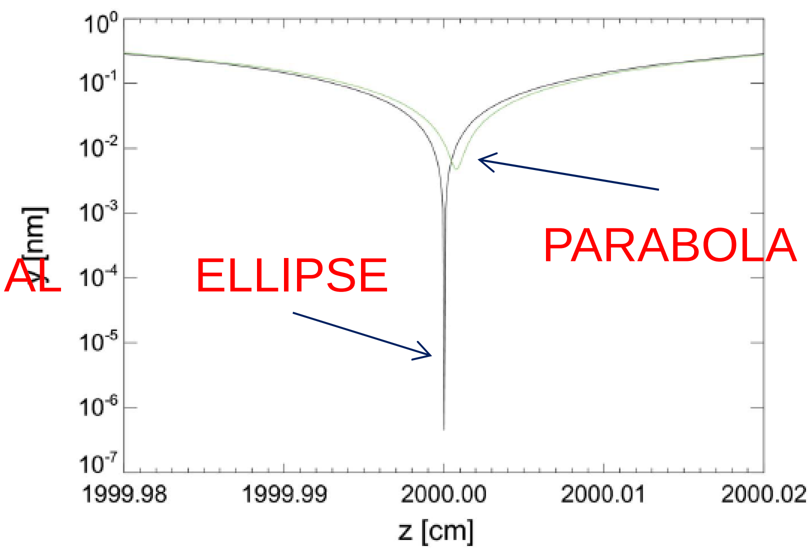
$$I/I_0 = \exp(-\mu\ t)$$

IDEAL INTERFACE SHAPE FOR FOCUSING A COLLIMATED BEAM



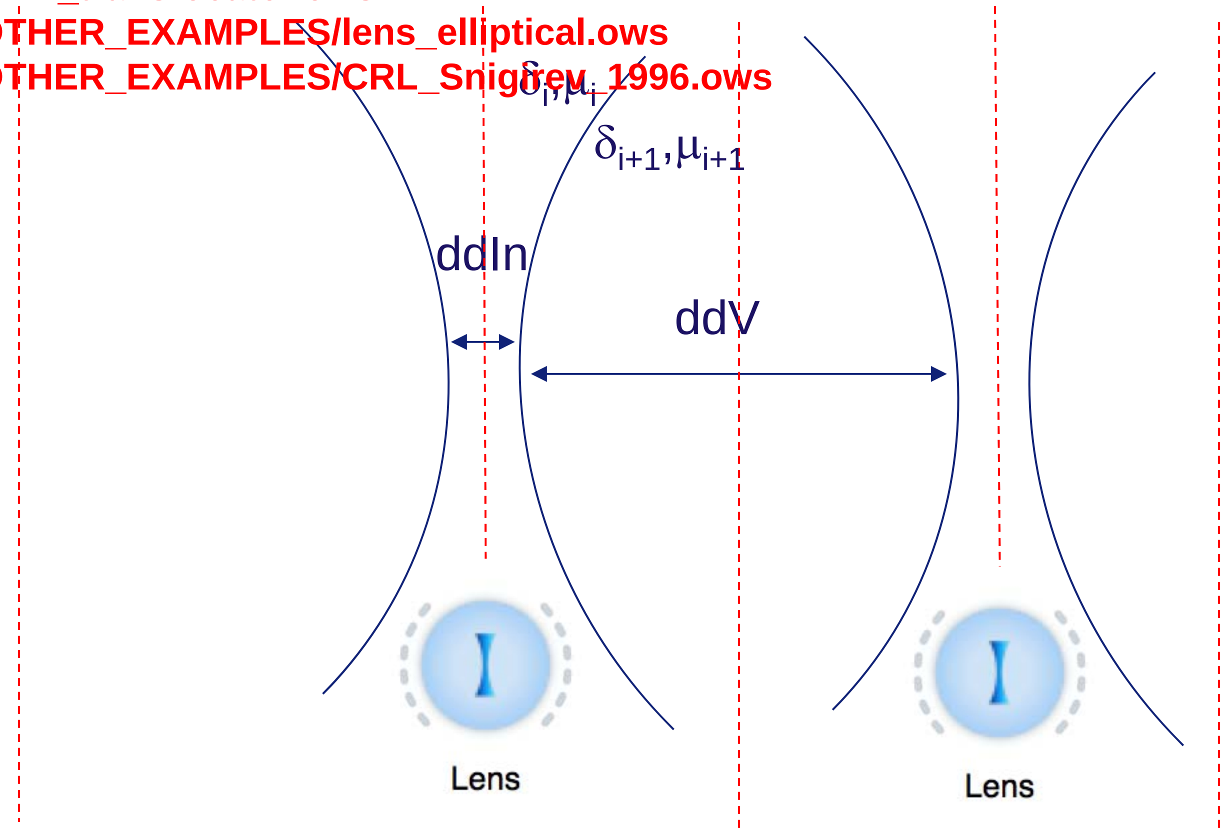






FULL RAY TRACING WITH SHADOWOUI: STACK OF INTERFACES

ex24_transfocator.ows
OTHER_EXAMPLES/lens_elliptical.ows
OTHER_EXAMPLES/CRL_Snigirev_1996.ows




```
OE surface in form of conic equation:
    c[1]*X^2 + c[2]*Y^2 + c[3]*Z^2 +
    c[4]*X*Y + c[5]*Y*Z + c[6]*X*Z  +
    c[7]*X + c[8]*Y + c[9]*Z + c[10] = 0
 with
 c[1] =   0.0000000000000000
 c[2] =   1.0000000000000000
 c[3] =   0.0000000000000000
 c[4] =   0.0000000000000000
 c[5] =  -0.0000000000000000
 c[6] =   0.0000000000000000
 c[7] =   0.0000000000000000
 c[8] =   0.0000000000000000
 c[9] = -0.10000000000000001
 c[10] =   0.0000000000000000
       ...
```

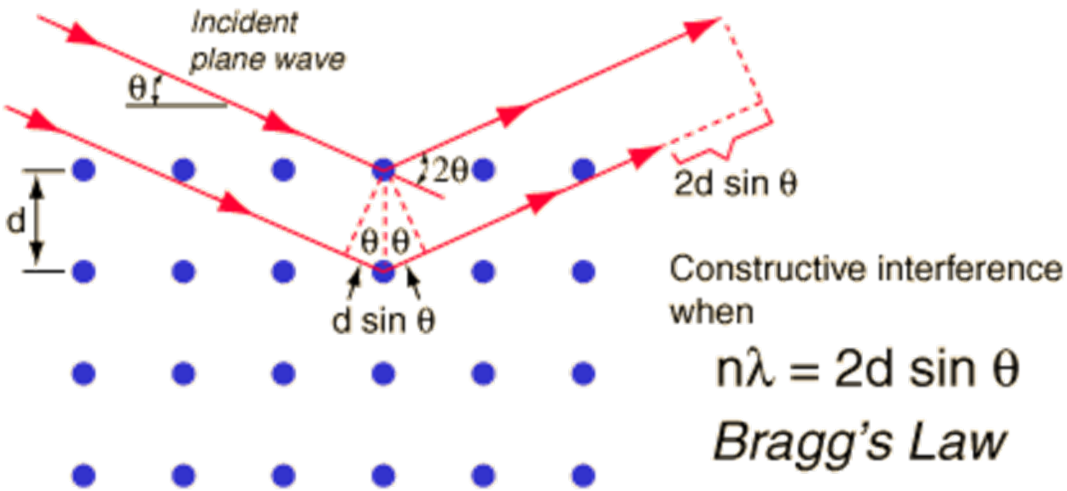
CRL = *n* identical Lenses

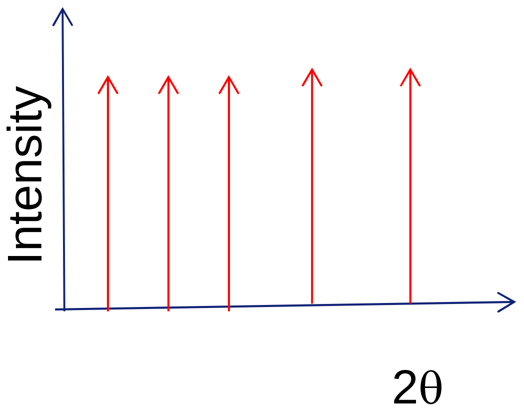
TRANSFOCATOR = *m* different CRLs

A result of COHERENT (RAYLEIGH) scattering of the X-rays on the elements of a periodic structure (e.g., atoms).

Although σ_R is small compared to other processes, the effect is the basis of X-ray diffraction.

The (small) scattering is enhanced by the periodic distribution of the scatterers (atoms)



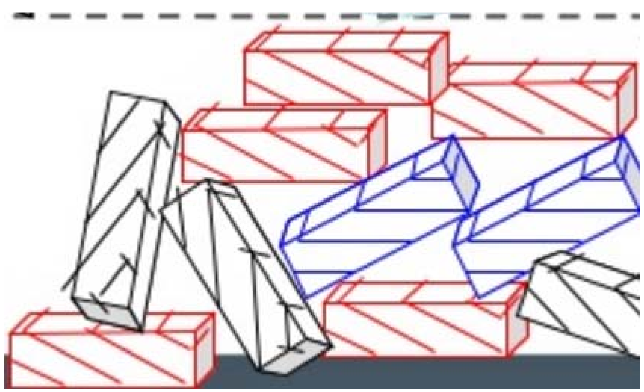


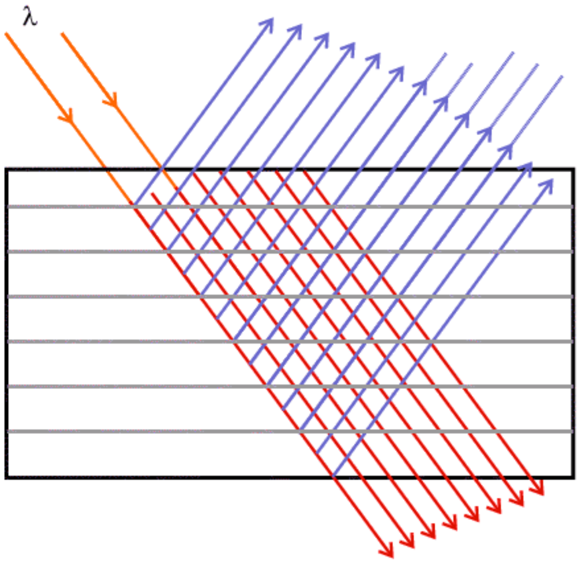
The diffraction of X-rays by very small crystals has been described by Laue's **kinematic theory**.

It supposes that oscillators in the crystal are only under the influence of the incident wave, neglecting the interaction between oscillators.

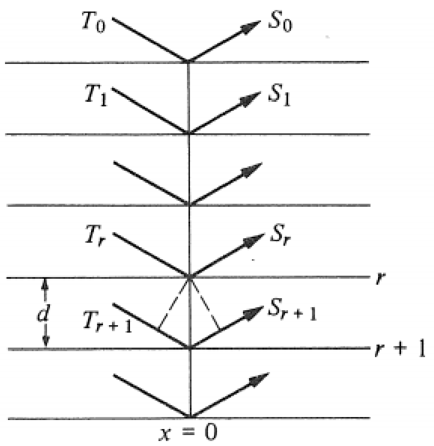
It can be applied to small crystals, like in powder diffraction.

For large crystals, the kinematical theory is no longer valid. This case is treated by the **dynamical theory** which includes multiple scattering of the radiation emitted by the oscillators and its interaction with the incident wave.





DARWIN TREATMENT OF DYNAMICAL THEORY (1914) – THE DARWIN WIDTH

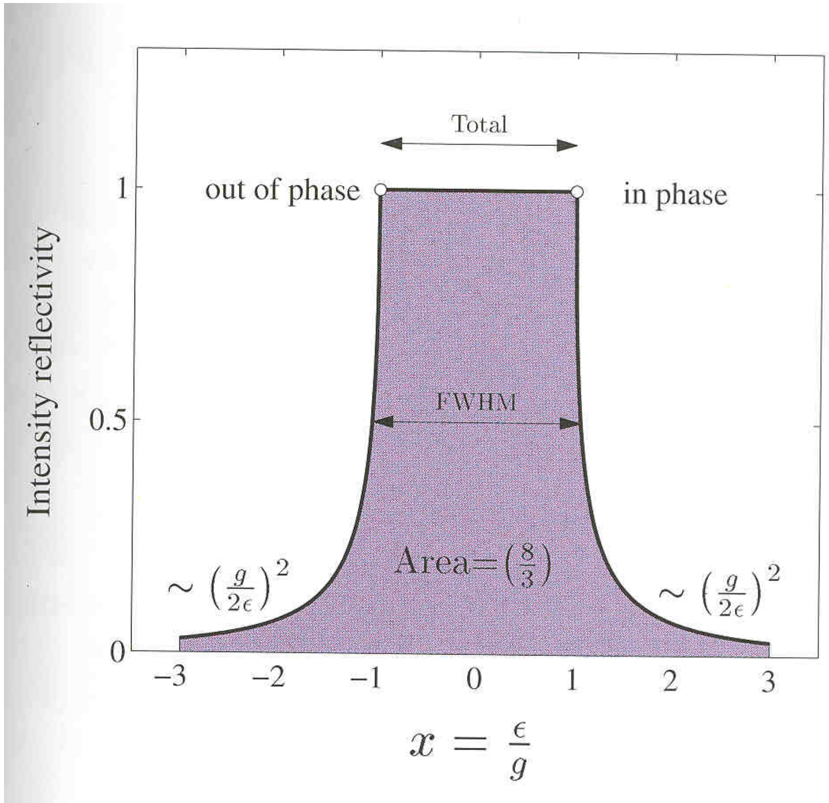


$$S_r = \frac{T_r - (1 - h + iq_0)T_{r-1}e^{-i\phi}}{iqe^{-i2\phi}}.$$

$$R(x) = \begin{cases} \left(x - \sqrt{x^2 - 1}\right)^2 & \text{for } x \geq 1 \\ 1 & \text{for } |x| \leq 1 \\ \left(x + \sqrt{x^2 - 1}\right)^2 & \text{for } x \leq -1 \end{cases}$$

$$(\Delta\theta)_D = 2\left|\frac{P|\Psi_H|}{(|b|)^{1/2}\sin(2\theta_B)}\right|$$

$$\Psi_H = \frac{-r_0\lambda^2}{\pi v_c}F_H, \quad r_0 = \frac{e^2}{mc^2}$$



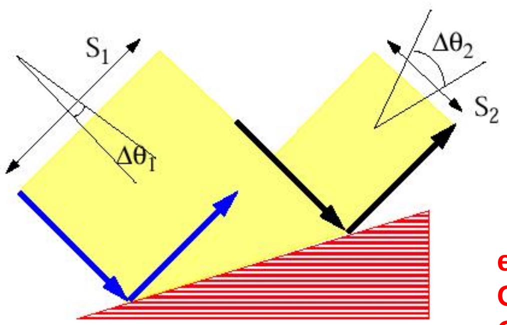
Geometrical model

Guarantees that the Liouville's theorem is fulfilled

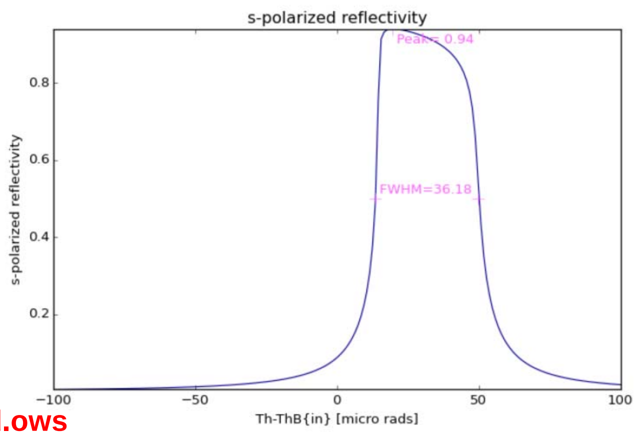
$$S_1 \Delta\theta_1 = S_2 \Delta\theta_2$$

Physical model

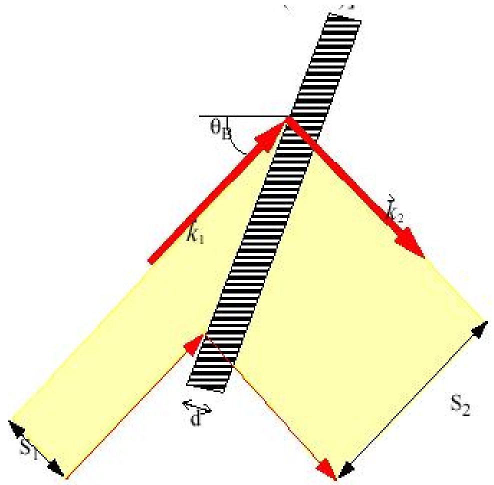
Crystal reflectivity is given by the Dynamical Theory of Diffraction (Zachariasen formalism)



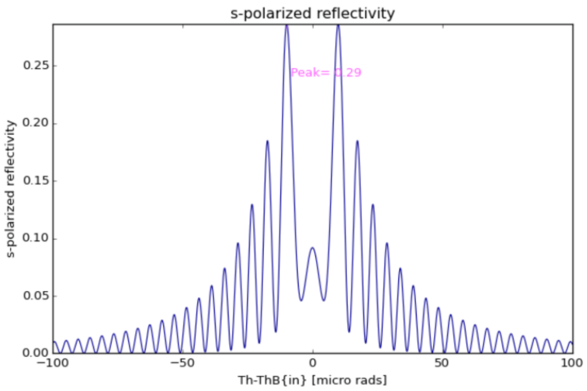
BRAGG or reflection



ex17_sagittalfocusing.ows
OTHER_EXAMPLES/crystal_analyzer_diced.ows
OTHER_EXAMPLES/crystal_asymmetric_backscattering.ows



LAUE or transmission



ex23_crystal_laue.ows

Playing with shape and geometry in crystal

- Factors that affect the energy resolution
- Sagittal focusing
- Bent crystal analyzers (ID26)

Dispersive crystals: some consequences

- Visibility of coherent patters
- Laue focusing
- Rainbow spectrometers

$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \Delta\theta_0 \cot\theta_0 \approx \sqrt{\omega_D^2 + \left[\left|\frac{p}{R\sin\theta_1} - 1\right|\Delta_{src} + \frac{s_1}{p}\right]^2}\,\cot\theta_0$$

Source size s_1

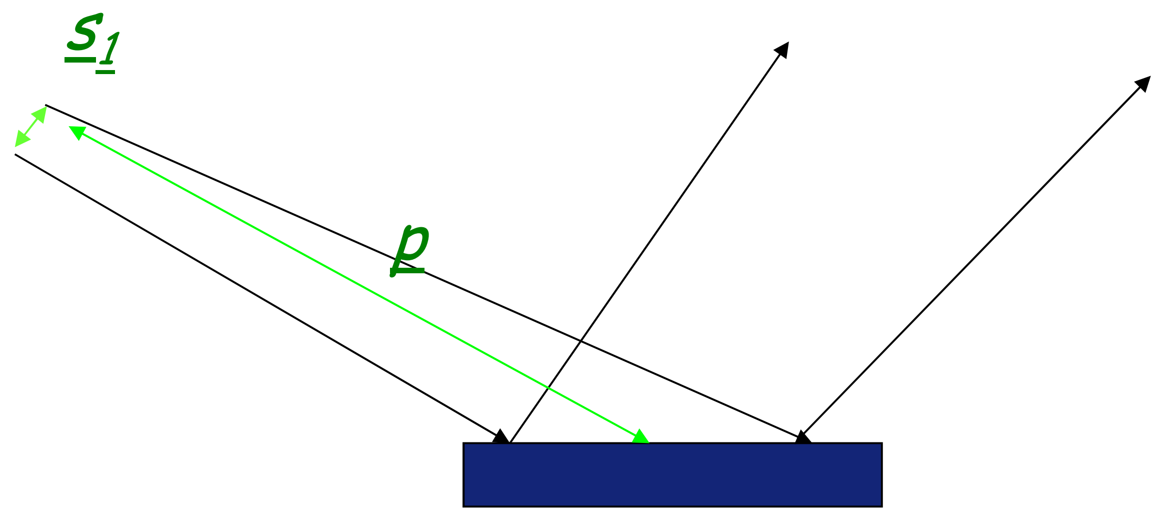
Source divergence Δ_{src}->

Slits, collimation or antiparalel (++)

Geometrical term (curvature R)

Darwin width ω_D-> Intrinsic resolution

Bragg's angle dependency cotθ_0



$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \Delta\theta_0 \cot\theta_0 \approx \sqrt{\omega_D^2 + \left[\left|\frac{p}{R\sin\theta_1} - 1\right|\Delta_{src} + \frac{s_1}{p}\right]^2}\cot\theta_0$$

Source size s_1

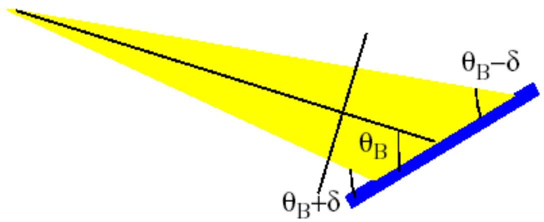
Source divergence Δ_{src}->

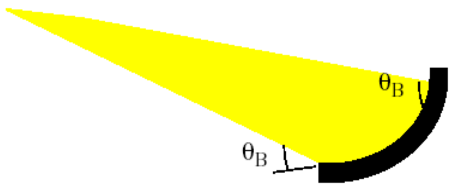
Slits, collimation or antiparalel (++)

Geometrical term (curvature R)

Darwin width ω_D-> Intrinsic resolution

Bragg's angle dependency cotθ_0





System	I_1	I_2	ΔE_1 [eV]	ΔE_2 [eV]
flat-flat	413 ±14	307 ±12	8.92 ±0.55	8.71 ±0.6 9
Rowland(1:1)-flat	414 ±25	65 ±9	1.44 ±0.06	1.23 ±0.2 4
Rowland(concave+convex)	399 ±12	296 ±10	1.44 ±0.07	1.32 ±0.0 6
Out-Rowland(1:3)-flat	408 ±18	36 ±3	8.2 ±0.9	2.1 ±0.5

$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \Delta\theta_0 \cot\theta_0 \approx \sqrt{\omega_D^2 + \left[\left|\frac{p}{R\sin\theta_1} - 1\right|\Delta_{src} + \frac{s_1}{p}\right]^2} \cot\theta_0$$

Source size s_1

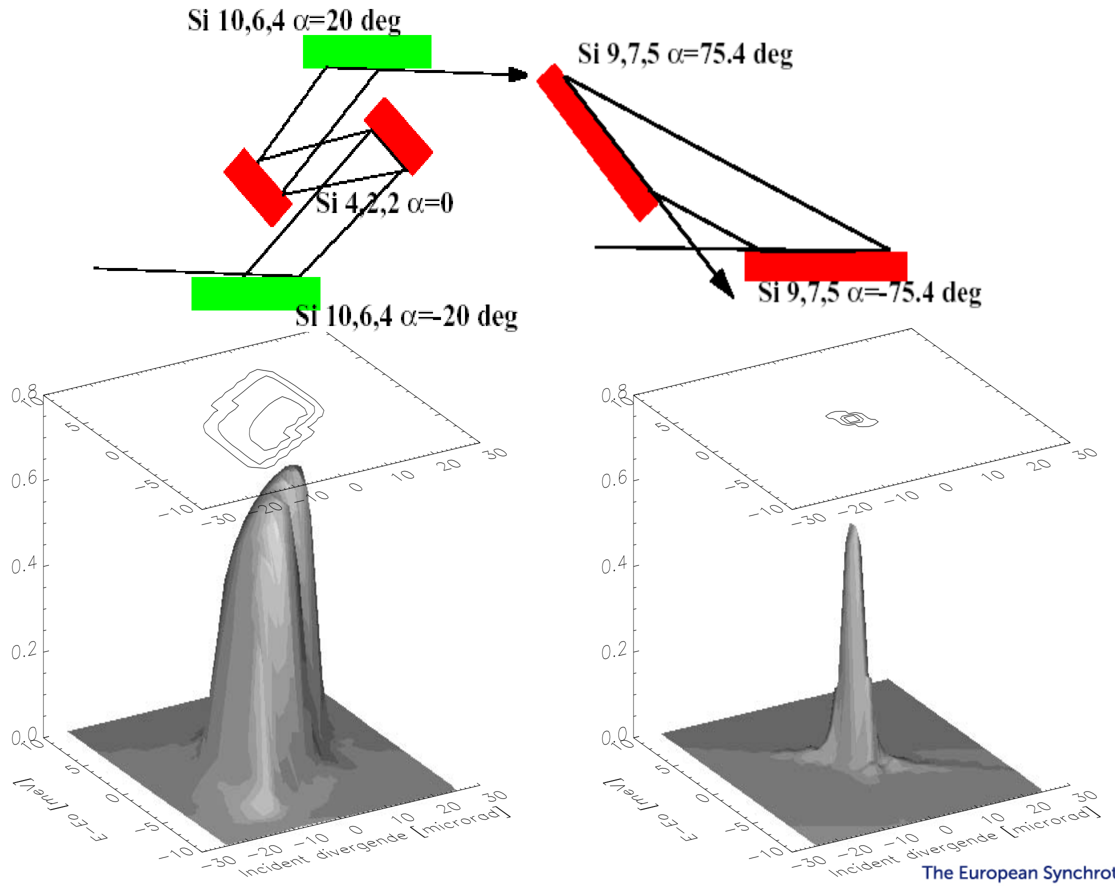
Source divergence Δ_{src}->

Slits, collimation or antiparalel (++) ←

Geometrical term (curvature R)

Darwin width ω_D-> Intrinsic resolution ←

Bragg's angle dependency $\cot\theta_0$



$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \Delta\theta_0 \cot\theta_0 \approx \sqrt{\omega_D^2 + \left[\left|\frac{p}{R\sin\theta_1} - 1\right|\Delta_{src} + \frac{s_1}{p}\right]^2} \cot\theta_0$$

Source size s_1

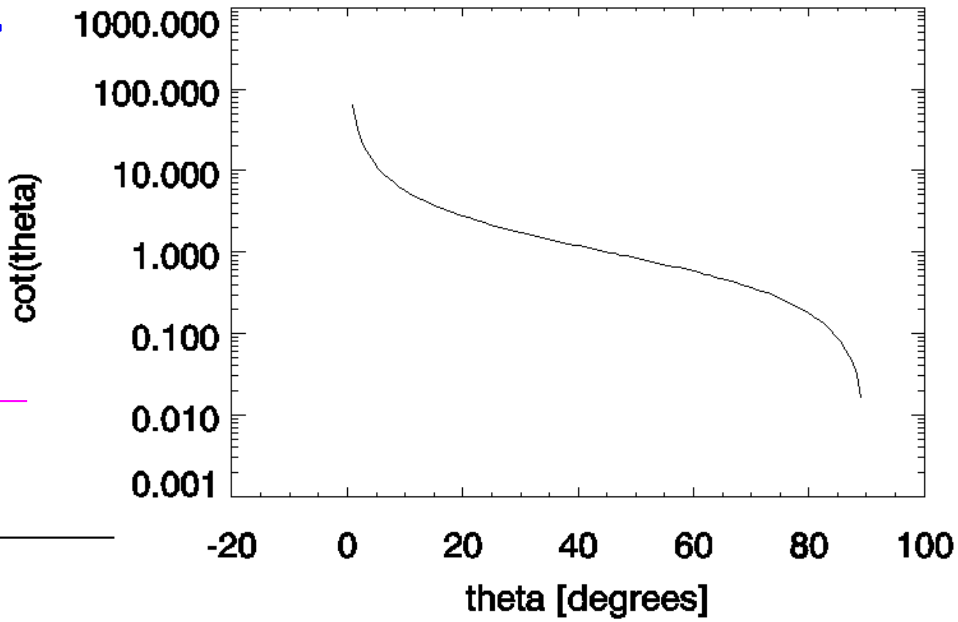
Source divergence Δ_{src}->

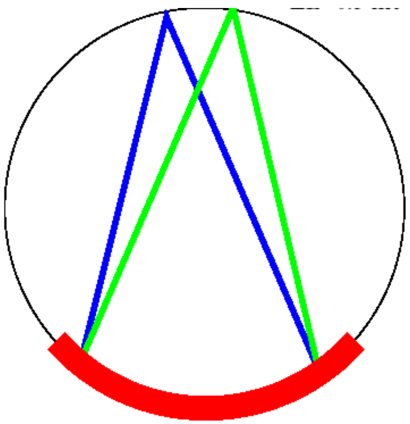
Slits, collimation or antiparalel (++)

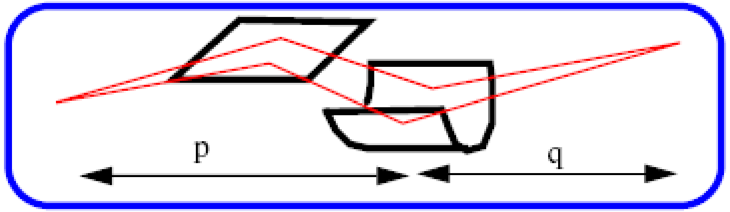
Geometrical term (curvature *R*)

Darwin width ω_D-> Intrinsic resolution

Bragg's angle dependency $\cot\theta_0$

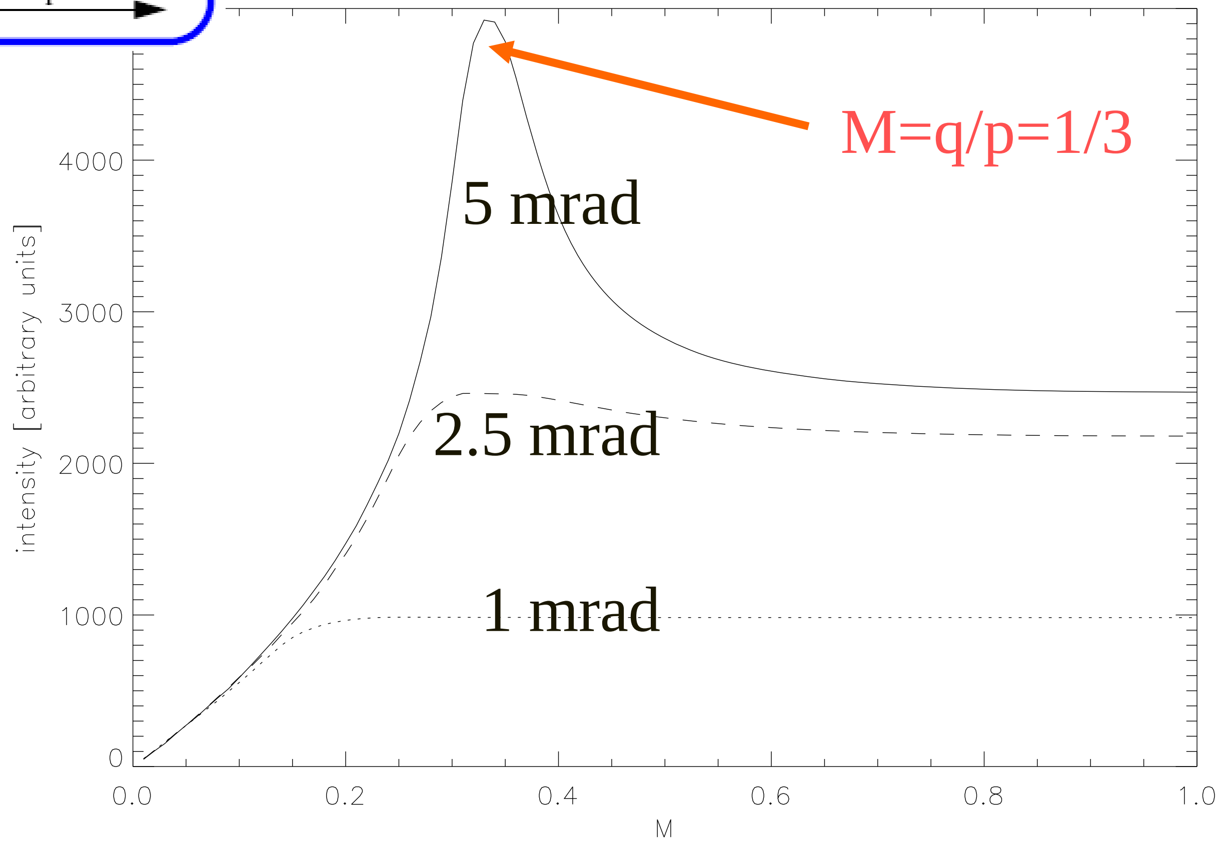






Shape effects:
- **Anticlastic curvature**
- **Cylindrical vs**
- **Conic (Ice&Sparks, JOSA A11 (1994) 1265)**

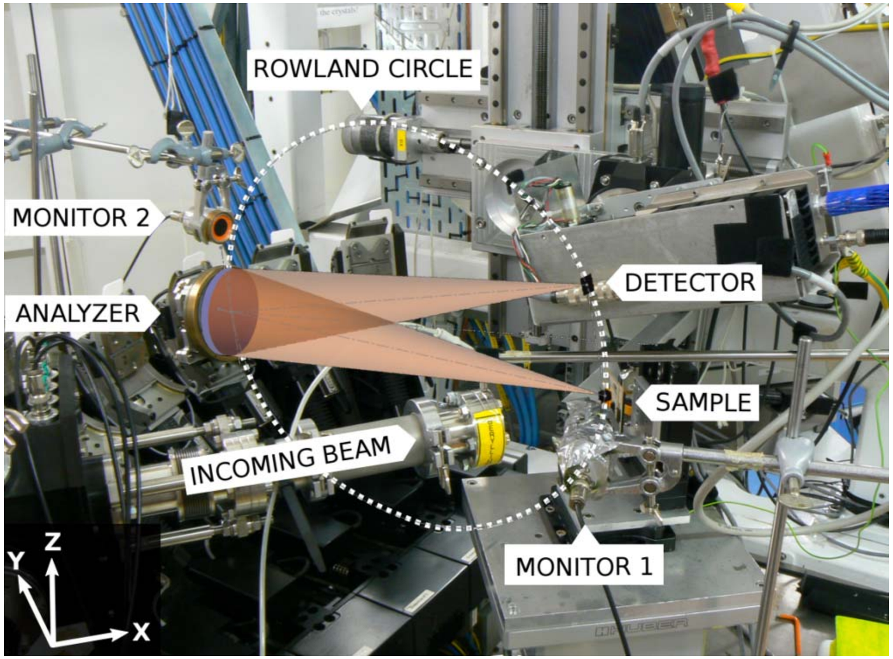
Beam transmission vs angular divergence

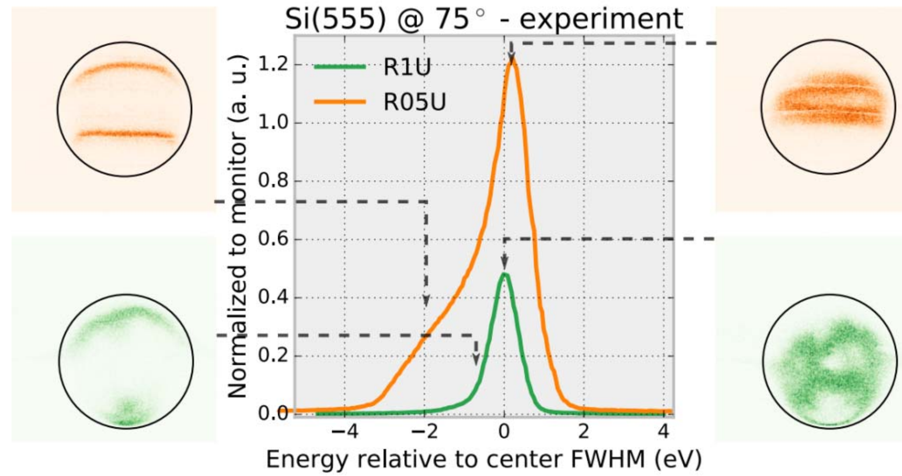


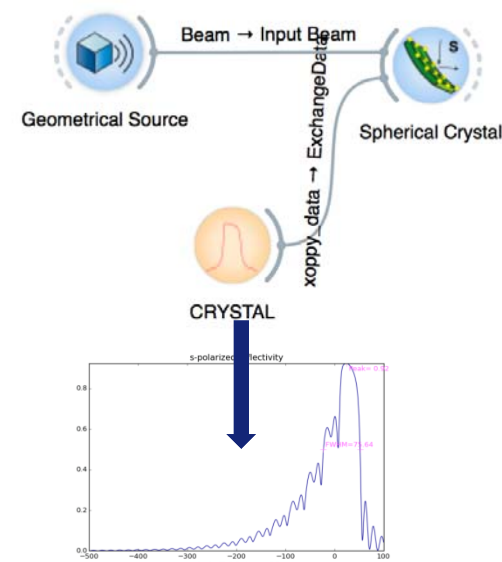
Intensity (in arbitrary units) versus magnification factor M for monochromatic (E=20 keV) point source placed at 30 m from the sagittaly bent crystal. We clearly observe the maximum of the transmission at M=0.33, as predicted by the theory (C. J. Sparks, Jr. and B. S. Borie Nuclear Instruments and Methods, 172, 237-242 (1980)).

See: ex18b_sagittalfocusing.ws

SPHERICALLY BENT CRYSTAL ANALYZERS OF 0.5 M RADIUS (M ROVEZZI)







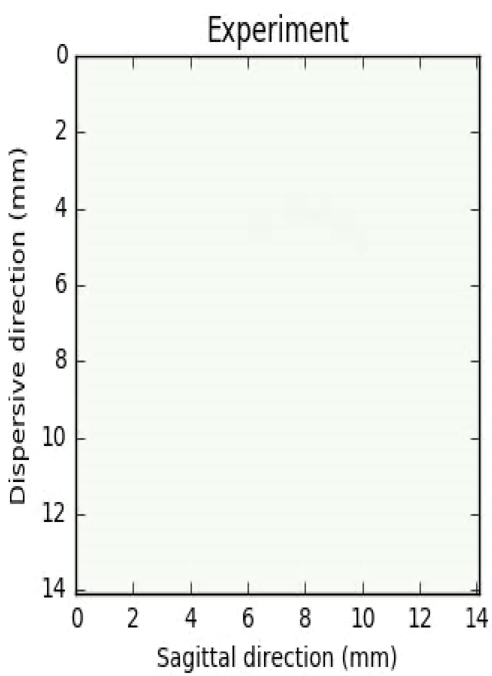
Experiment vs ray tracing study.

All details in the paper:

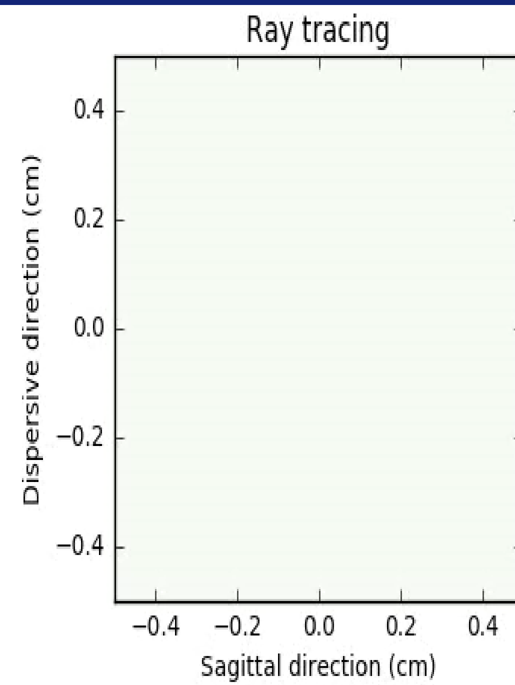
M. Rovezzi et al., arXiv:1609.08894 (2016)

http://arxiv.org/abs/1609.08894

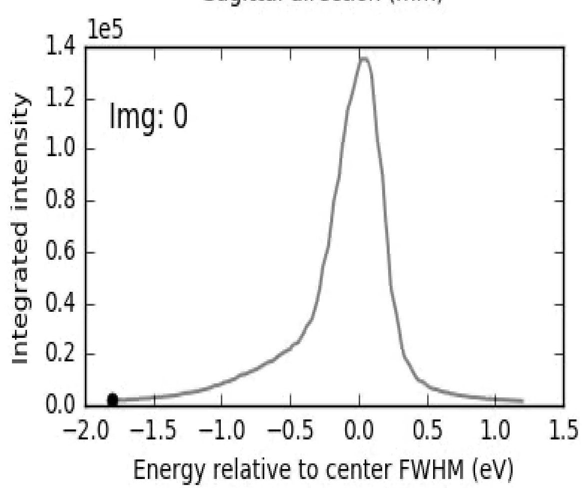
SBCA 1 M AT 75°



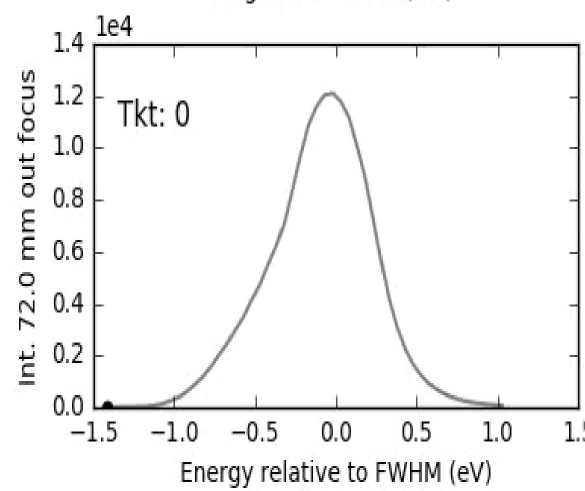
Experiment
Dispersive direction (mm)
0
2
4
6
8
10
12
14
0 2 4 6 8 10 12 14
Sagittal direction (mm)



Ray tracing
Dispersive direction (cm)
0.4
0.2
0.0
−0.2
−0.4
−0.4 −0.2 0.0 0.2 0.4
Sagittal direction (cm)

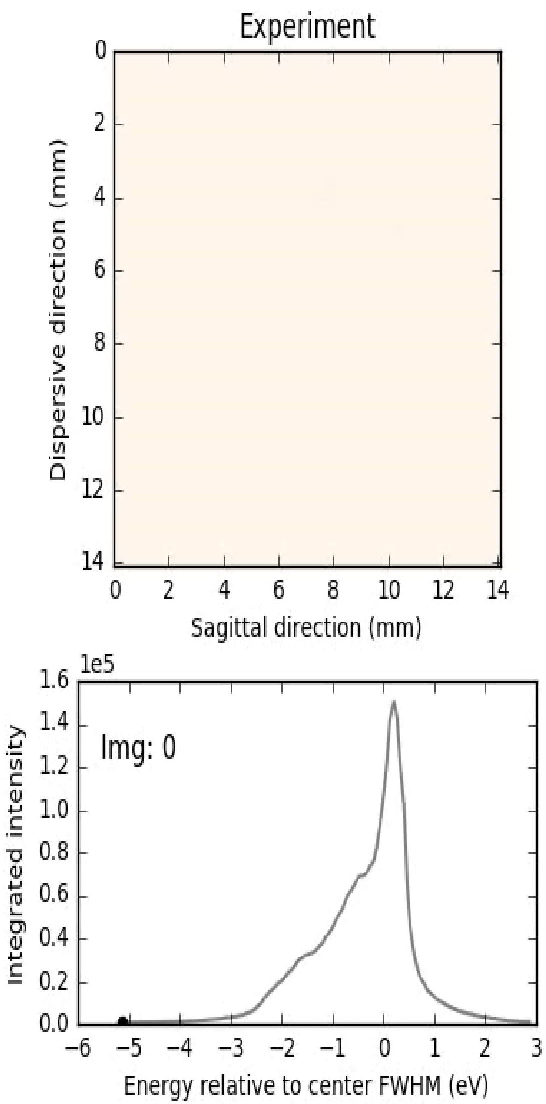


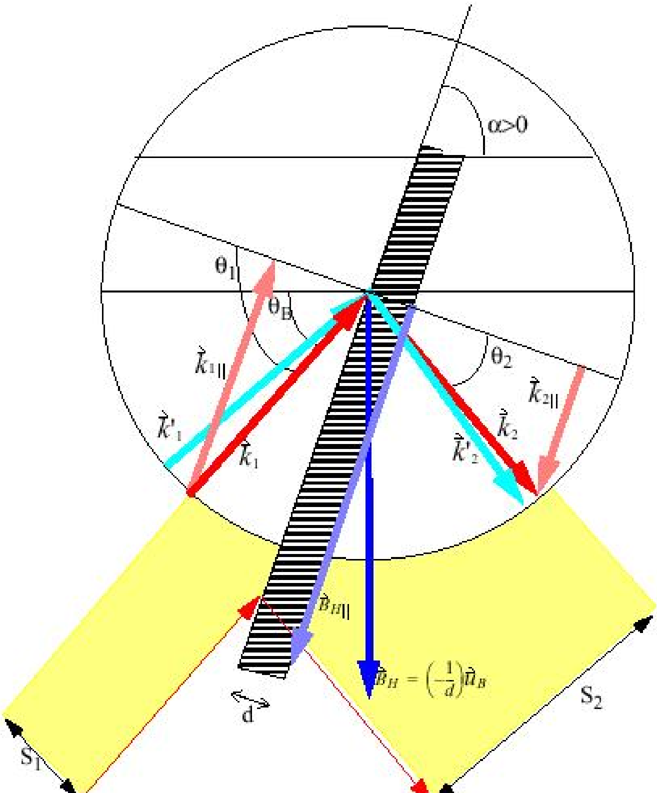
1e5
Integrated intensity
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Img: 0
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5
Energy relative to center FWHM (eV)



1e4
Int. 72.0 mm out focus
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Tkt: 0
−1.5 −1.0 −0.5 0.0 0.5 1.0 1.5
Energy relative to FWHM (eV)

SBCA 0.5 M AT 75°





The change in the direction of any monochromatic beam (not necessarily satisfying the diffraction condition or Laue equation) diffracted by a crystal (Laue or Bragg) can be calculated using (i) elastic scattering in the diffraction process:

$$|\mathbf{k}^0| = |\mathbf{k}^H| = \frac{1}{\lambda}, \quad (2)$$

with $\mathbf{k}^{0,H} = (1/\lambda)\mathbf{V}^{0,H}$ and $\mathbf{V}$ a unita and (ii) the boundary conditions at the crystal sur

$$\mathbf{k}_{\parallel}^{H} = \mathbf{k}_{\parallel}^{0} + \mathbf{H}_{\parallel}, \quad (3)$$

$$-|\sin\theta_2| = |\sin\theta_1| - \frac{\lambda}{d}\sin\alpha$$

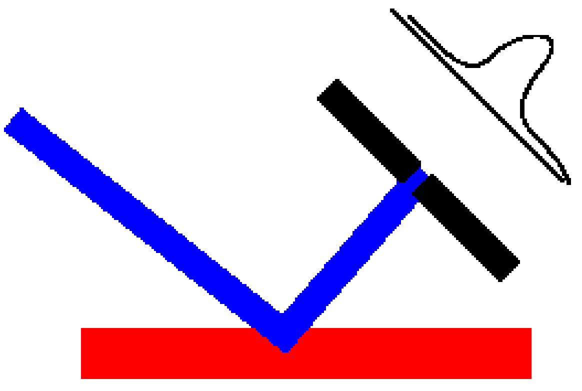
A crystal behaves like a grating or prism, except the Bragg Symmetric crystal that behaves like a mirror.

$$\frac{d}{\sin\alpha} = \frac{d_{Grating}}{m}$$

- **Asymmetric Bragg & every Laue** crystals are **dispersive elements** (X-rays with different energies will exit in different directions)
- **Bragg symmetric** crystals are **non-dispersive**

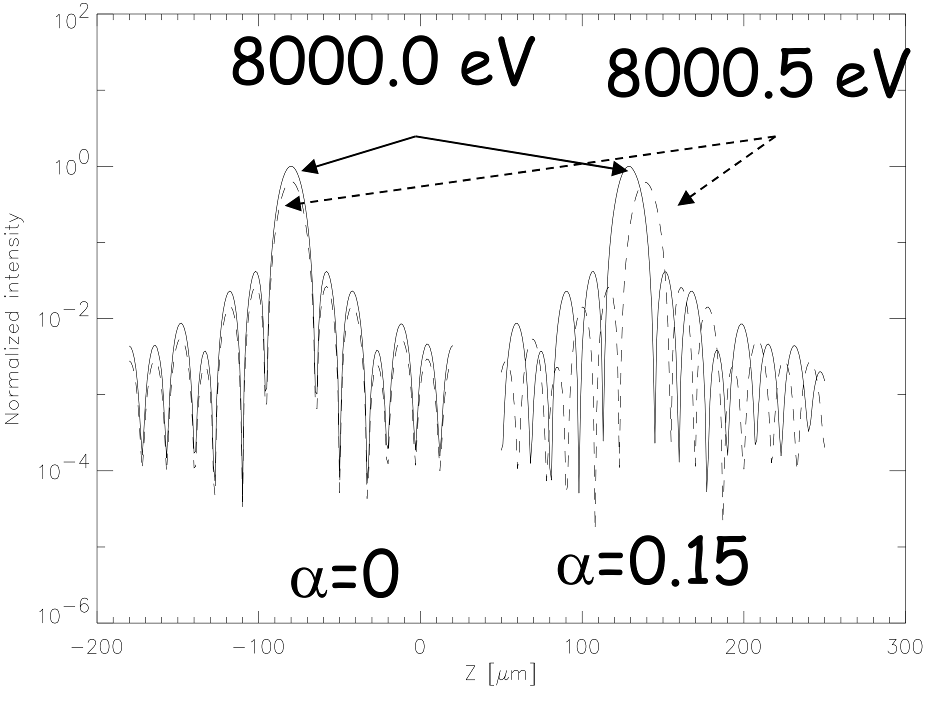
They modify the divergence of the beam. It must be taken into account when combined with other focusing elements

Dispersive crystals reduce visibility of diffraction patterns by coherent light

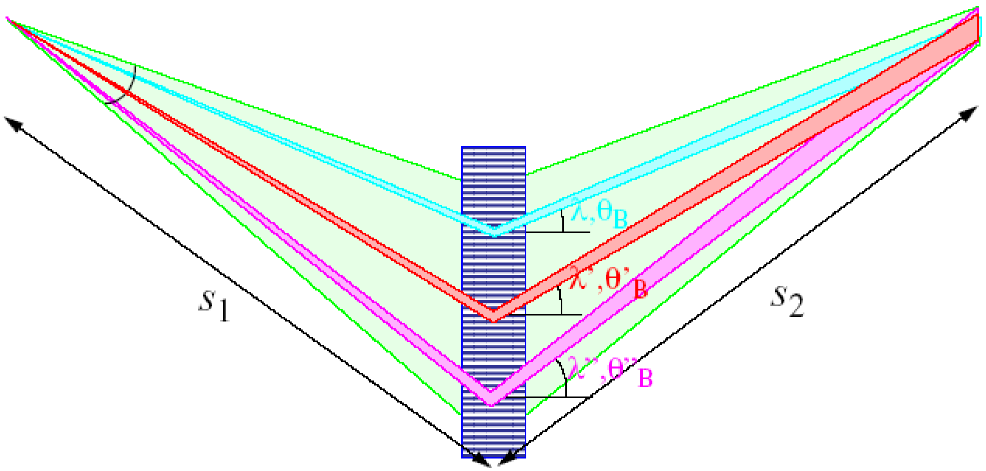


Si 111, α=0, α=0.15 deg

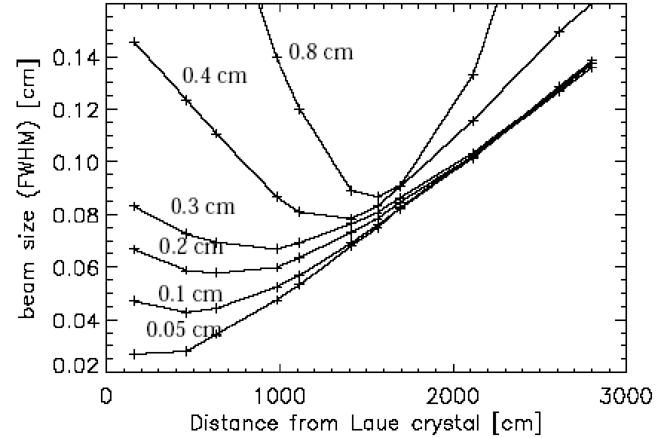
8 keV, ΔE~ 1 eV



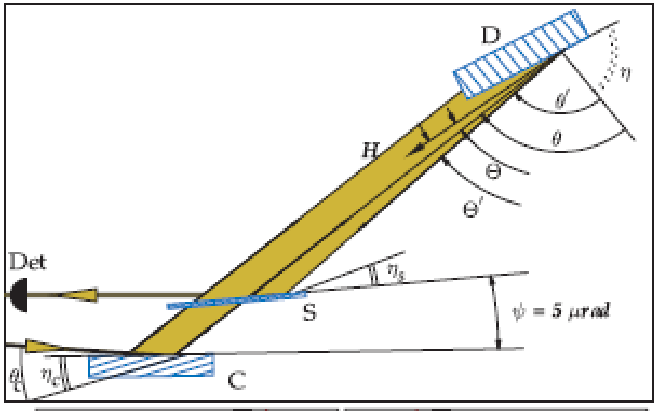
“Polychromatic focusing” with flat Laue crystals is fake focusing



M. Sanchez del Rio et al, Rev Sci Instrum, 66 (11) 5148- 5152, Nov 1995



Extreme asymmetry (backscattering) produces a rainbow effect Shvyd'ko 2006 PRL 97, 235502



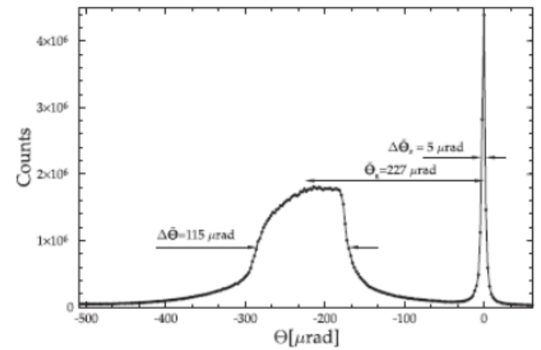
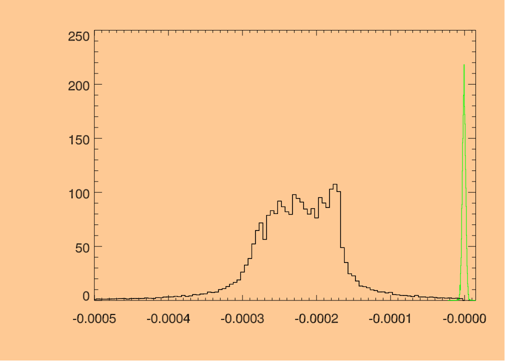
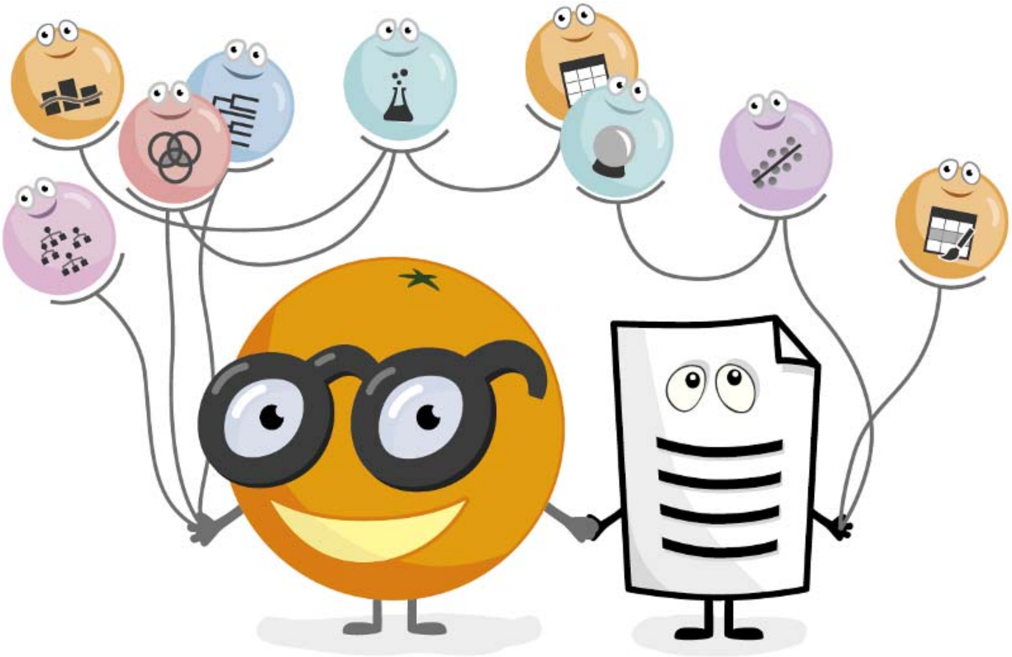


FIG. 4. Bragg reflectivity from crystal D of 9.1315 keV x rays, exactly backwards, as a function of the angle of incidence $\Theta = \pi/2 - \theta$ to the reflecting atomic planes.



See you in the practical session to model your beamline like you were playing video games!!



Thanks!