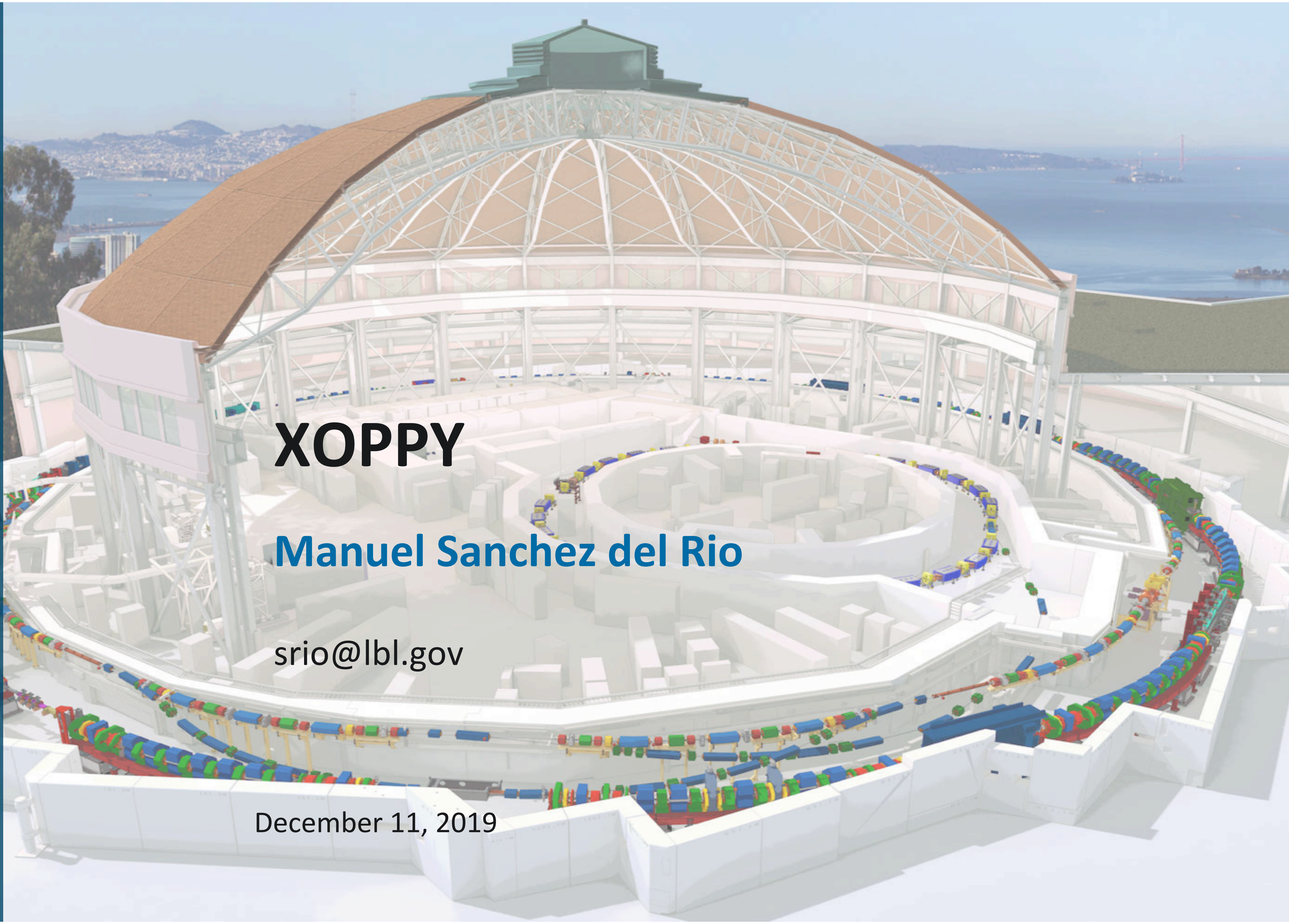

XOPPY

Manuel Sanchez del Rio

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December 11, 2019

utline

istory

utorial

xercises

- Sources: Flux and Power
- Examples

story

XOP

X-ray OPtics utilities

1997 – Manuel Sanchez del Rio & Roger J. Dejus

This code is a graphical user interface that performs calculations of radiation characteristics of X-ray sources and their intera
with matter, such as: insertion devices (undulator or wiggler) spectra and angular distributions, mirror and multilayer reflectiv
and crystal diffraction profiles [1].

XOP + python : XOPPY

Sanchez del Rio and Roger J. Dejus "XOP: a multiplatform graphical user interface for synchrotron radiation spectral and optics calculations", Proc. SPIE 3152, Materials, Manufacturing, and Measure
n Radiation Mirrors, (1 November 1997); https://doi.org/10.1117/12.295554.

OPPY in OASYS

SRW

XOPPY

WOFRY

https://github.com/oasys-kit/wofry

SHADOWOUI

SYNED

https://github.com/oasys-kit/syned

COMSYL

Orange

Utilities

OASYS = OrAnge SYncrotron Suite

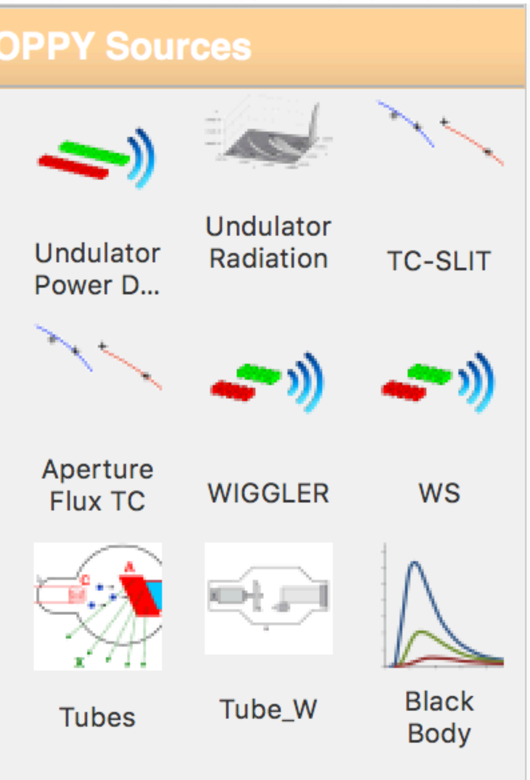
Luca Rebuffi (ANL) & Manuel Sánchez del Río (ESRF) [1].

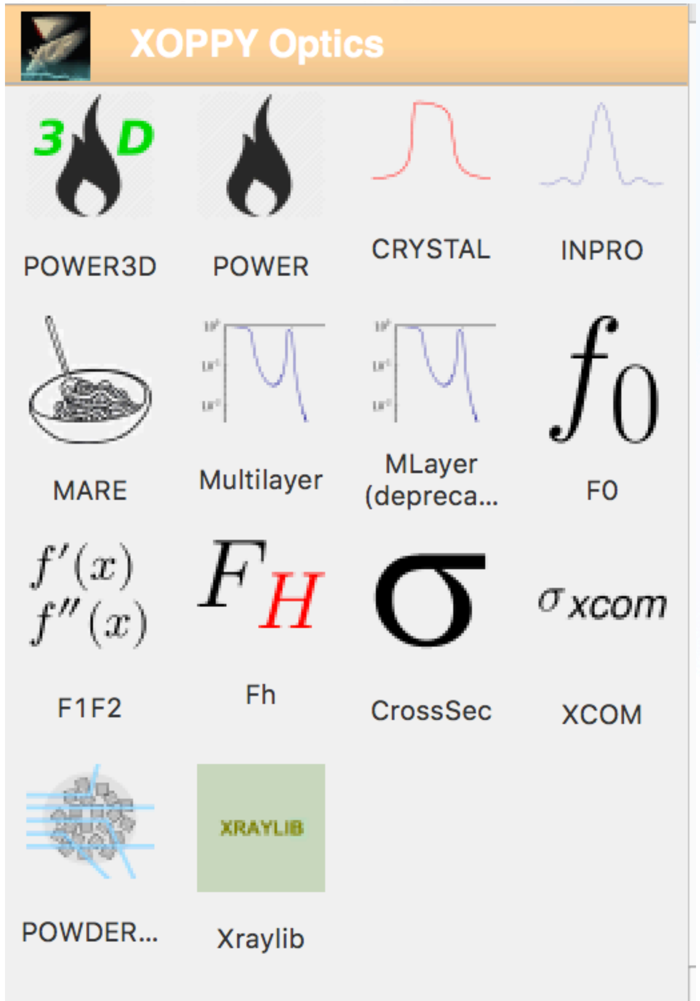
https://www.aps.anl.gov/Science/Scientific-Software/OASYS

https://github.com/oasys-kit

[1] L. Rebuffi, M. Sanchez del Rio, "OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for x-ray virtual experiments", Proc. SPIE 10388, 103880S (2017). DOI: 10.1117/12.2274263.

ckage


OPPY Sources
Undulator Power D...
Undulator Radiation
TC-SLIT
Aperture Flux TC
WIGGLER
WS
Tubes
Tube_W
Black Body


XOPPY Optics
POWER3D
POWER
CRYSTAL
INPRO
MARE
Multilayer
MLayer (depreca...
F0
F1F2
Fh
CrossSec
XCOM
POWDER...
XRAYLIB
Xraylib

plications

chrotron Sources

Bending Magnets, Wigglers : Spectral Flux and Power

Undulators:

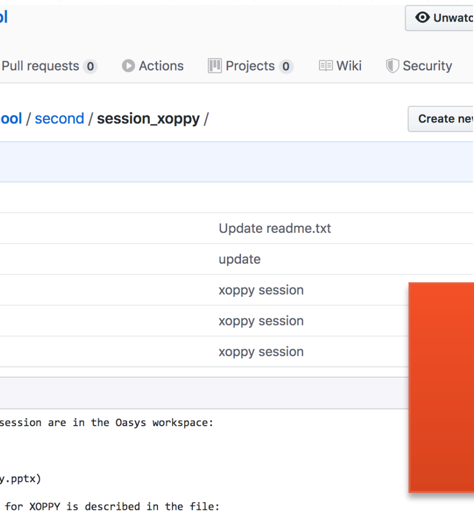
- Spectral Flux, Spectral Power W(E) + Elements (mirrors, filters)
- Power Density W(x,y)
- Radiation W(E,x,y) + Elements (Mirror, filters, apertures)
- Several calculation engines on the same interface (US, URGENT, SRW, py

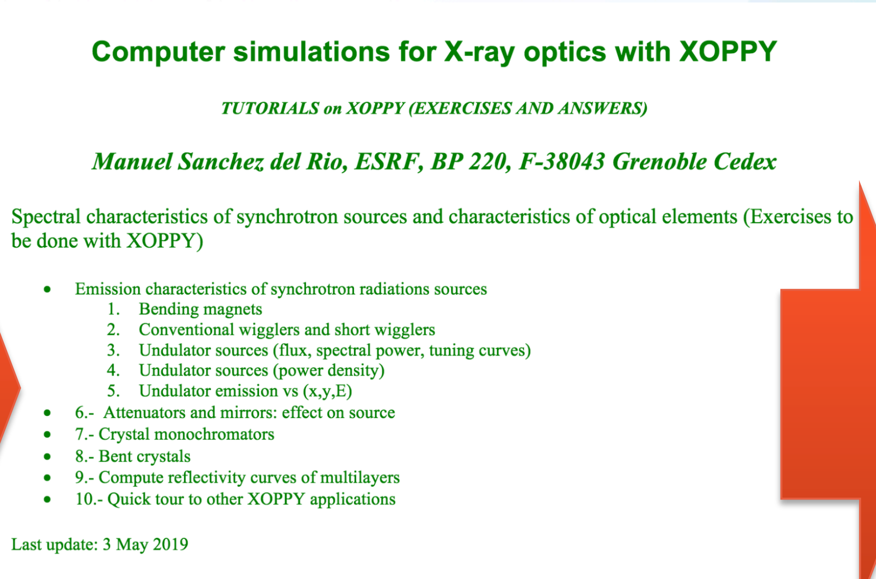
Optical elements reflectivity (crystals, mirrors, multilayers)

Miscellaneous applications

PPY Tutorial

http:/tinyurl.com/r5fq6pe





Computer simulations for X-ray optics with XOPPY

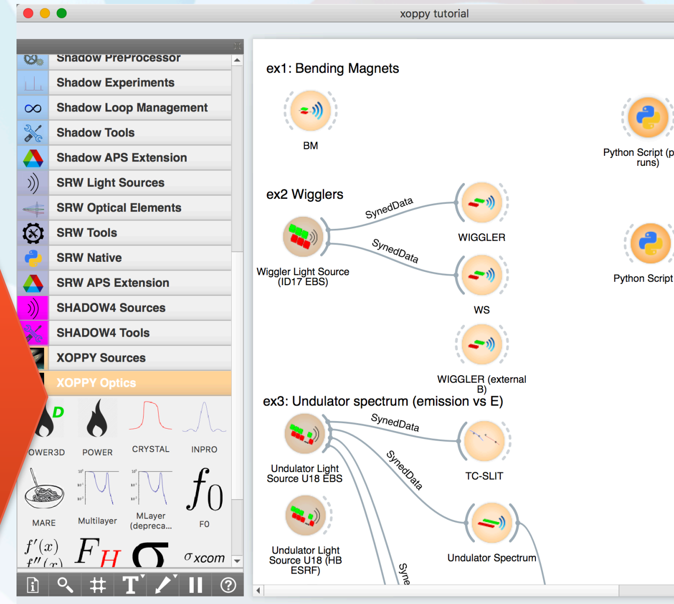
TUTORIALS on XOPPY (EXERCISES AND ANSWERS)

Manuel Sanchez del Rio, ESRF, BP 220, F-38043 Grenoble Cedex

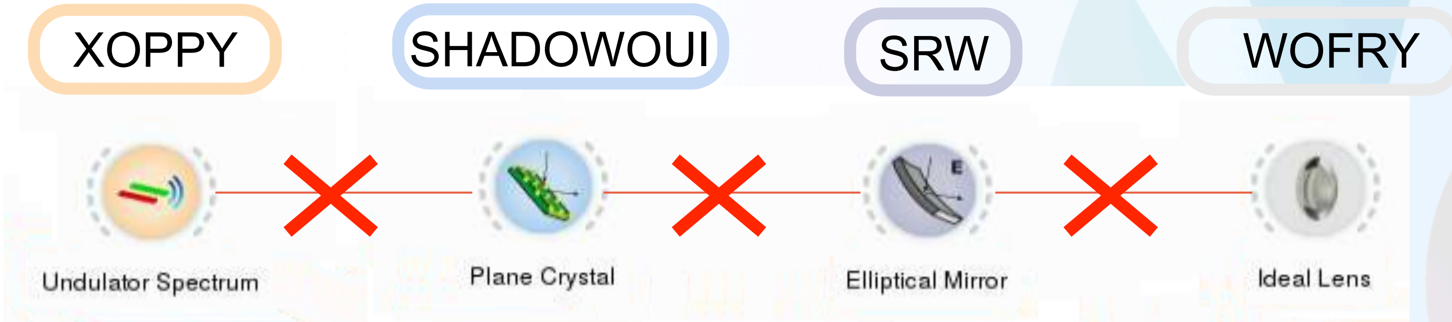
Spectral characteristics of synchrotron sources and characteristics of optical elements (Exercises to be done with XOPPY)

- Emission characteristics of synchrotron radiations sources
  1. Bending magnets
  2. Conventional wigglers and short wigglers
  3. Undulator sources (flux, spectral power, tuning curves)
  4. Undulator sources (power density)
  5. Undulator emission vs (x,y,E)
- 6.- Attenuators and mirrors: effect on source
- 7.- Crystal monochromators
- 8.- Bent crystals
- 9.- Compute reflectivity curves of multilayers
- 10.- Quick tour to other XOPPY applications

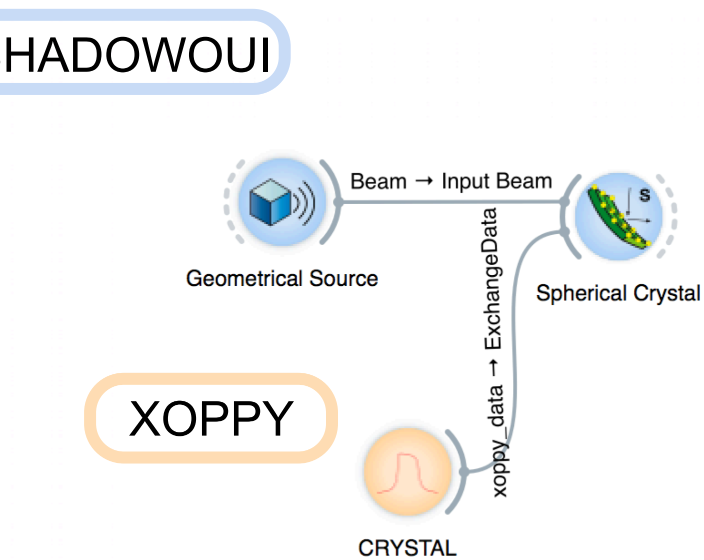
Last update: 3 May 2019

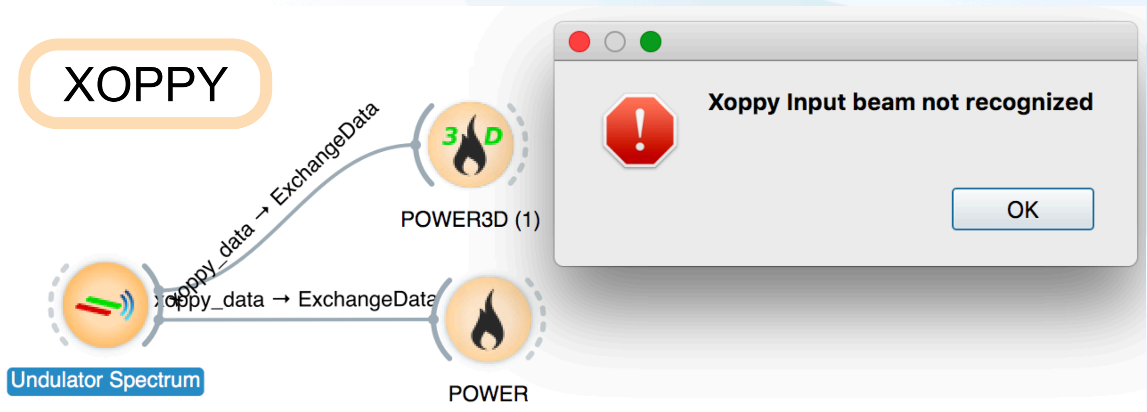


nnectivity & Interoperability



Hint: always keep an eye on the color code





ndulators: Power and spectral calculations

$$= \frac{eB_0\lambda_u}{2\pi mc} = 0.9337\,B_0(\mathrm{T})\lambda_u(\mathrm{cm})$$

$$\lambda = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right)$$

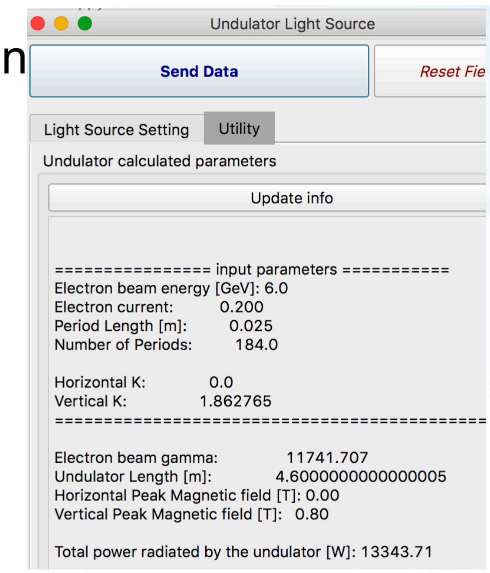
$$\gamma m_e c^2$$

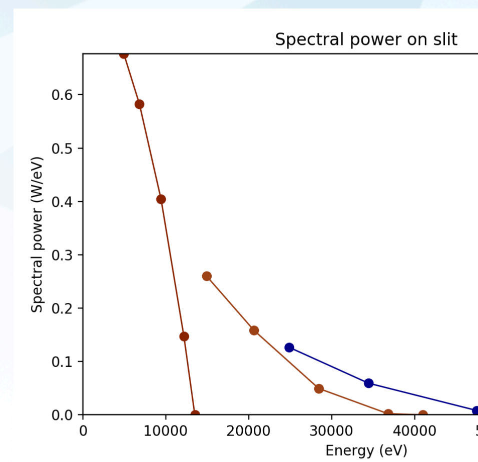
$m_e c^2 = 0.51$ MeV

$$Power[kW] \approx 0.633 \cdot B^2\,[T] \cdot E^2[GeV] \cdot I[A] \cdot L[m]$$

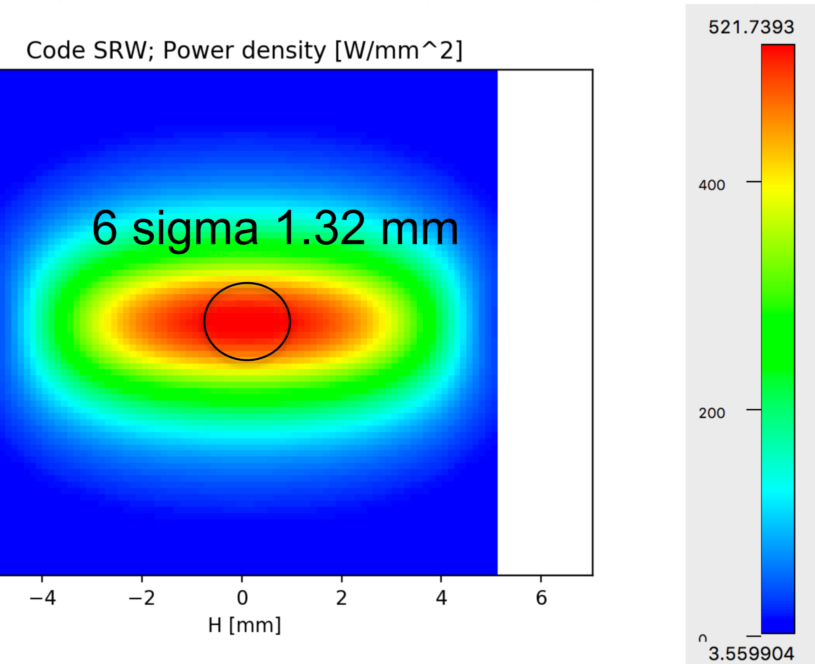
$$\frac{Power}{Solid\ Angle}[W/mrad^2] \approx 10.84 \cdot B\,[T] \cdot E^4[GeV] \cdot I[A] \cdot L[m] \cdot N \cdot G(K)$$

um power is obtained at highest K (or B) correspondin
minimum photon energy
ectral range covered by undulator is shown by the
Curves.

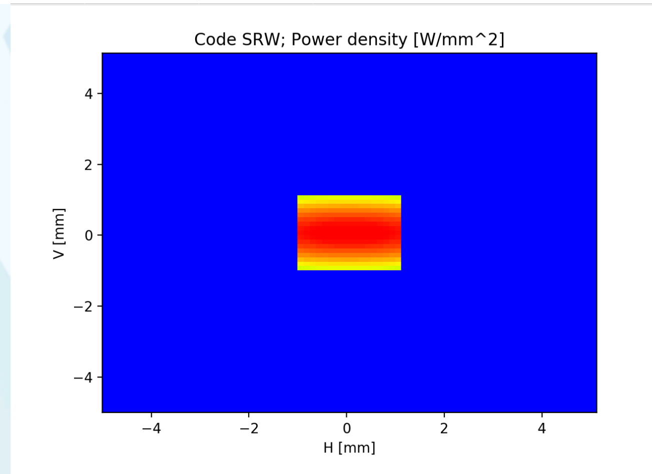




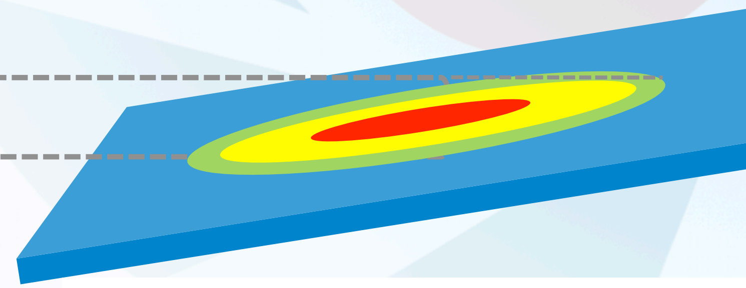
wer density (Power vs X and Y)



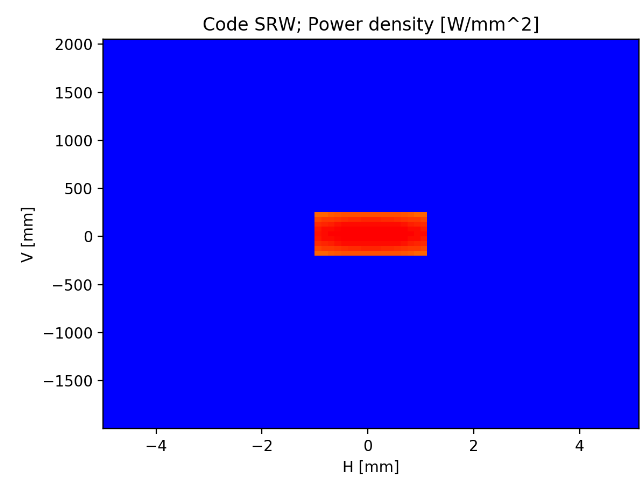
Mask
2x2 mm @ 25.4,=m
Or
2.1x2.1 @ 28m



Mirror:
400mm
2.1mm (mask)



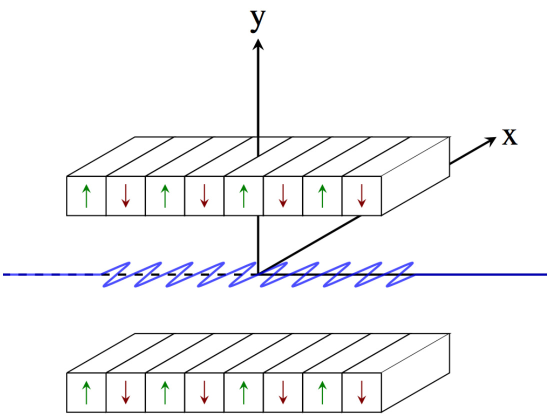
culate on aperture large enough to accept all the radiation
ect “modify slit” to calculate power on smaller slit and to calculate
ver density on mirror surface

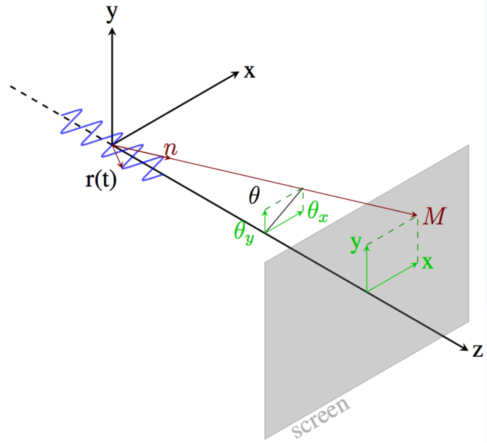


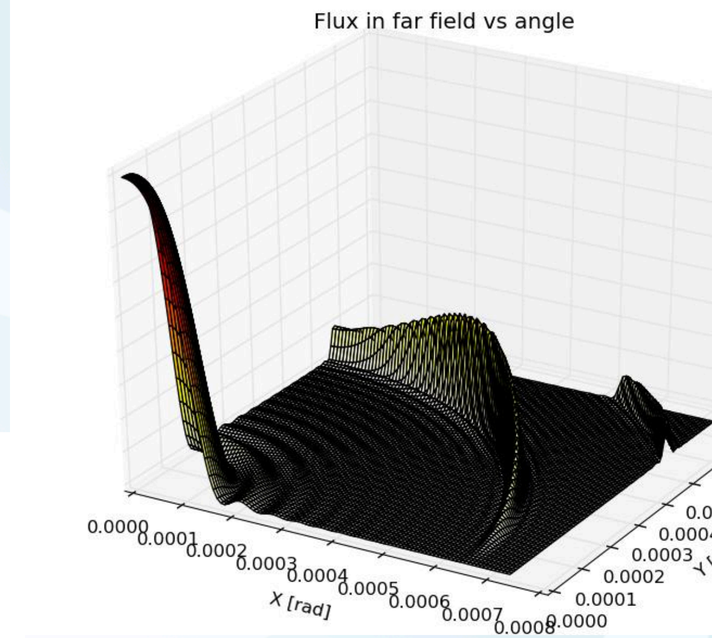
KELEY LAB | ALS-U

ux and Spectral Power

Undulator emission, after classical electrodynamics (e.g., Jackson, etc)



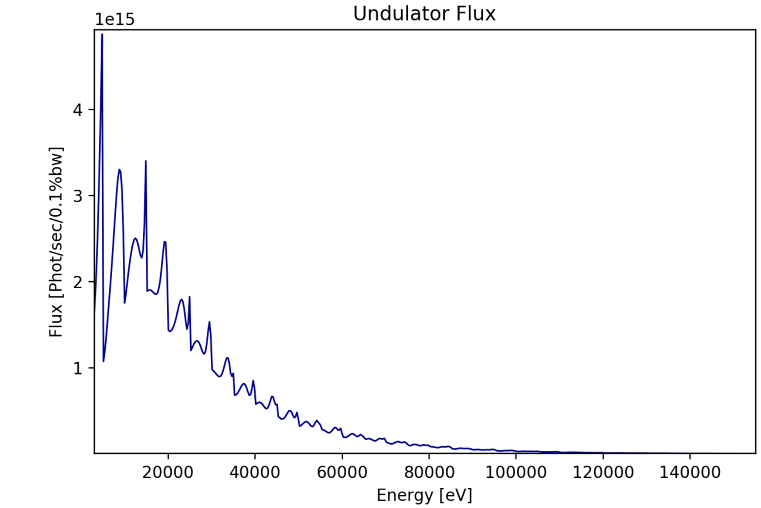


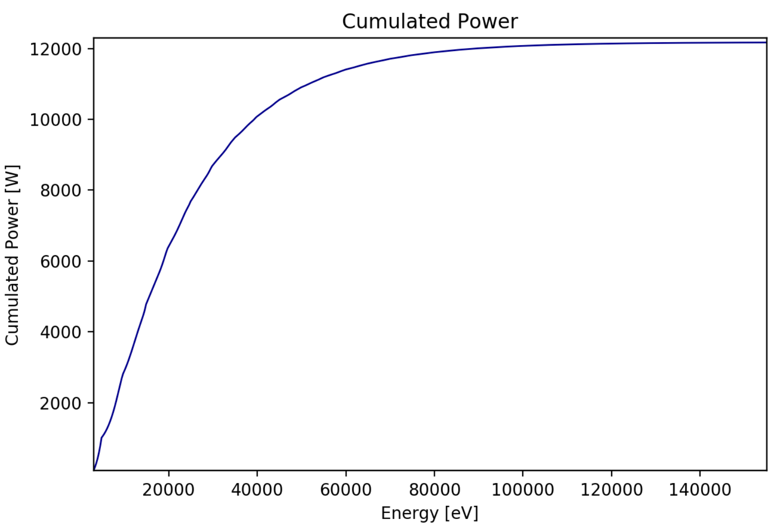


$$\frac{eI}{8\pi^2 c\epsilon_0 h}10^{-9}\left|\int_{-\infty}^{\infty}\left[\frac{n\times\left[(n-\beta)\times\dot{\beta}\right]}{(1-\beta\cdot n)^2}+\frac{c}{\gamma^2 R}\frac{(n-\beta)}{(1-\beta\cdot n)^2}\right]e^{i\omega(t'+R(t')/c)}dt'\right|^2$$

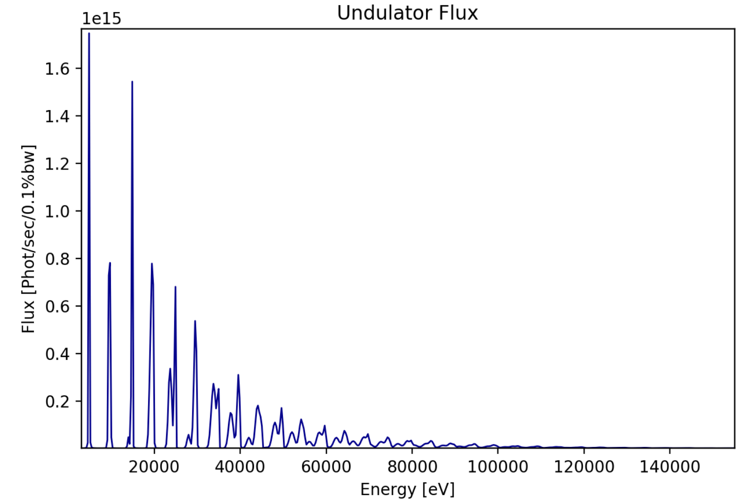
ux and Spectral Power

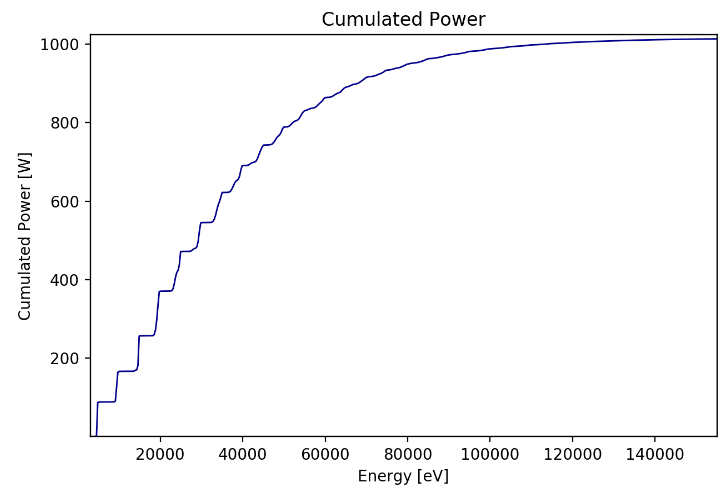
Open Slit (10 x 10 mm^2)





Slit (2.1 x 1 mm^2)

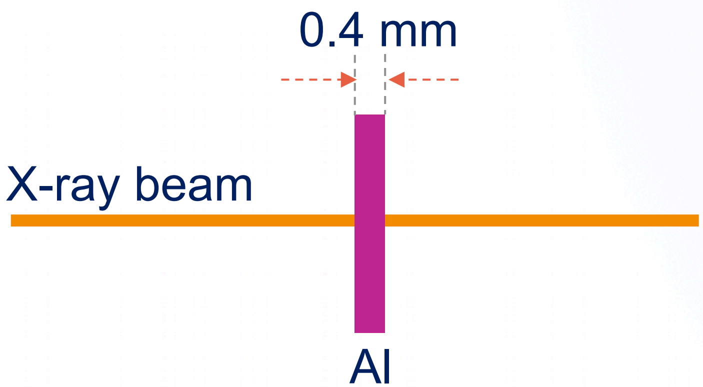


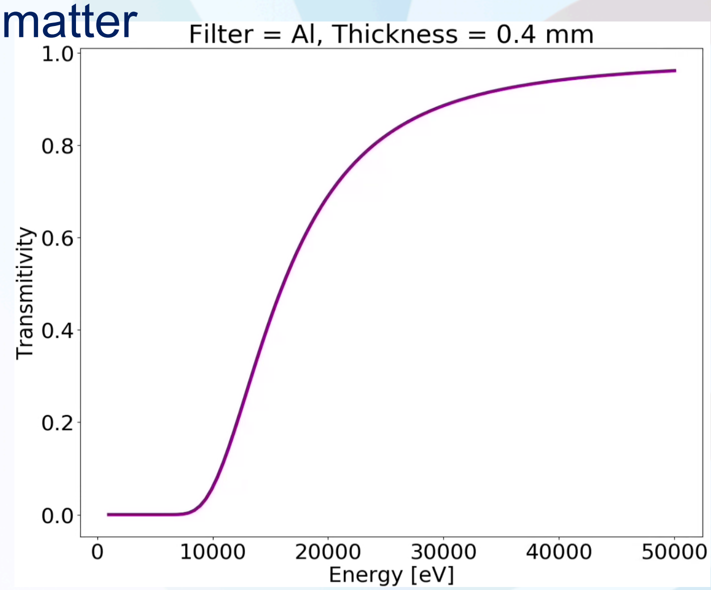


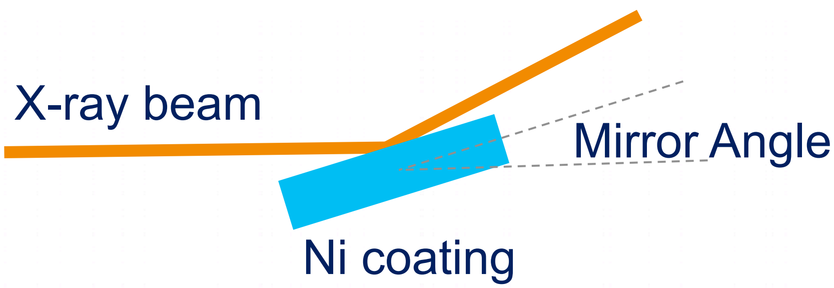
ectral response of mirrors and attenuators (filters)

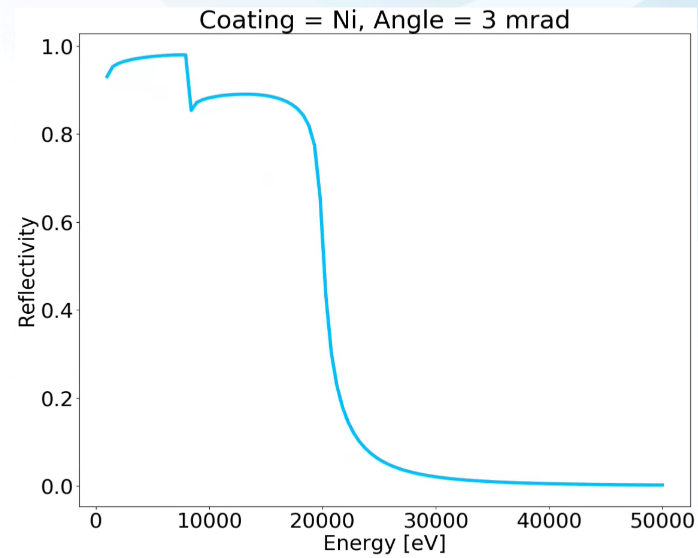
XOPPY

Interaction of radiation with matter





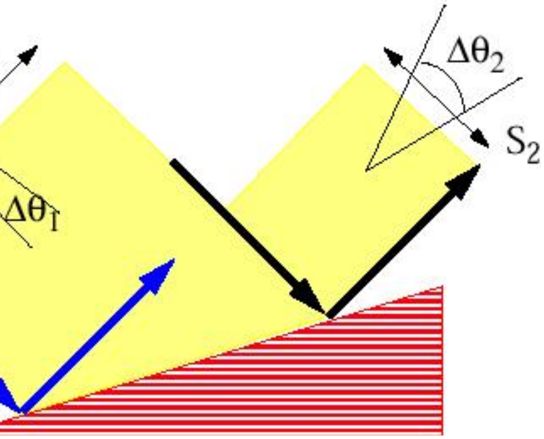




ystals: Zachariasen treatment for plane crystals

BRAGG or reflection

LAUE or transmission



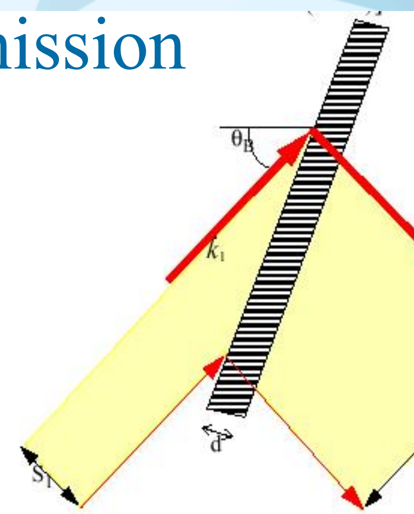
$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{-z \pm (qP^2 + z^2)^{1/2}}{P\Psi_{\overline{H}}}$$

$$c_1 = \exp(-i\varphi_1 T), \quad c_2 = \exp(-i\varphi_2 T),$$

$$\varphi_1 = -\frac{2\pi k^0 \delta'_0}{} \quad \varphi_2 = -\frac{2\pi k^0 \delta''_0}{},$$

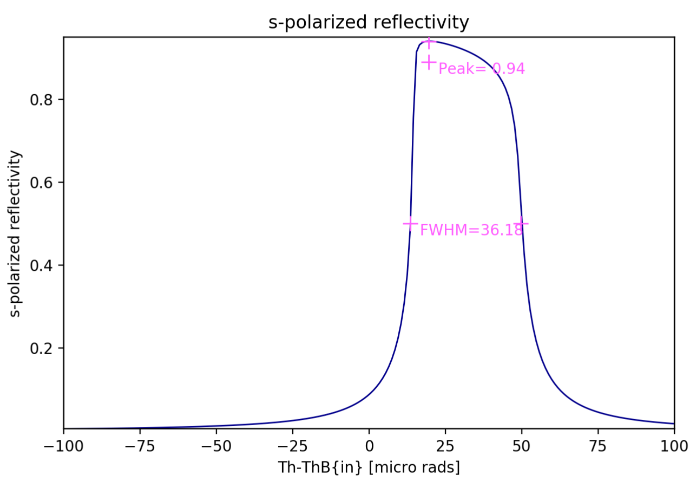
$$\begin{pmatrix} \delta'_0 \\ \delta''_0 \end{pmatrix} = \frac{1}{2}\left[\Psi_0 - z \pm (qP^2 + z^2)^{1/2}\right]$$

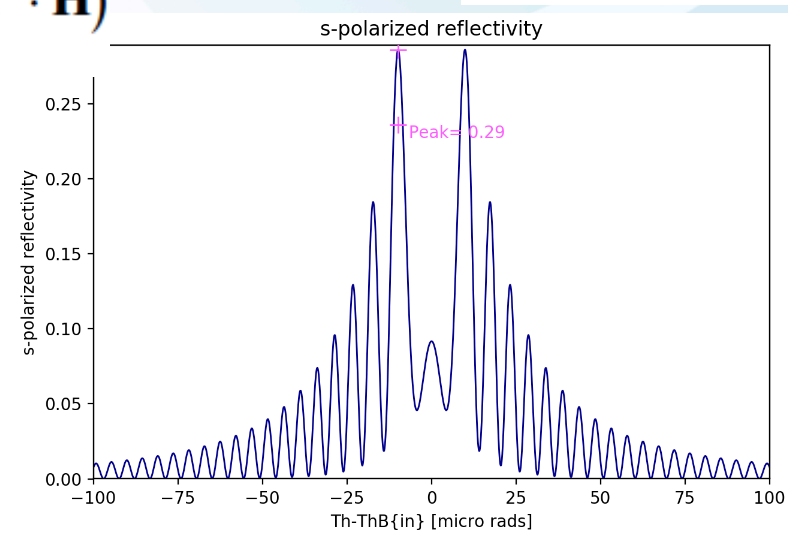
$$\alpha_Z = \frac{1}{|\mathbf{k}^0|^2}\left(|\mathbf{H}|^2 + 2\mathbf{k}^0 \cdot \mathbf{H}\right)$$



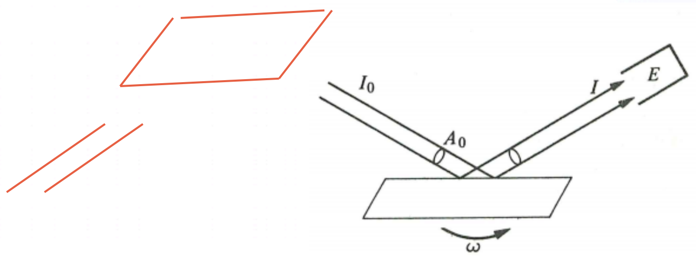
$$) \equiv \frac{1}{|b|}\frac{I^H}{I^0} = \frac{1}{|b|}\left|\frac{x_1x_2(c_1 - c_2)}{c_2x_2 - c_1x_1}\right|^2.$$

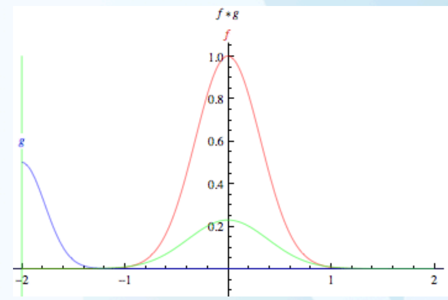
$$r^{\mathrm{Laue}}(\alpha_Z) \equiv \frac{1}{|b|}\frac{I^H}{I^0} = \frac{1}{|b|}\left|x_1\right.$$



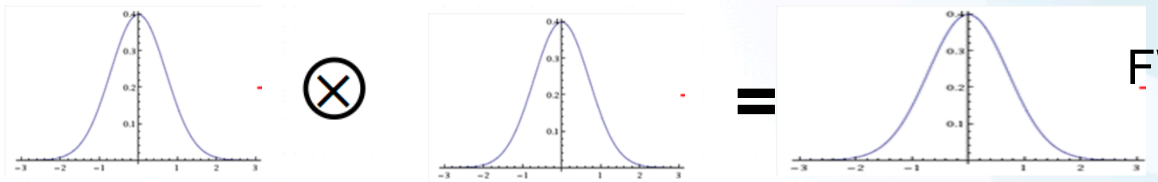


tals: Rocking curves

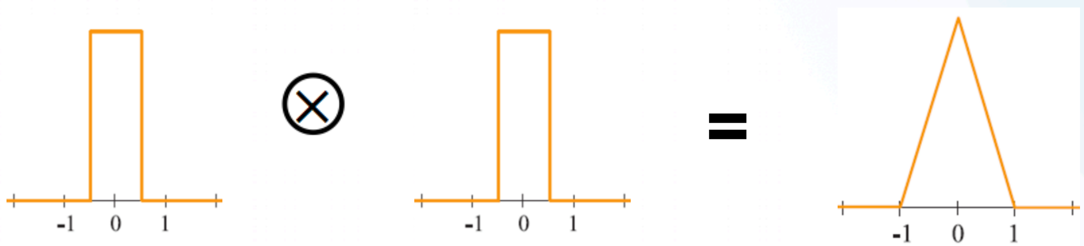




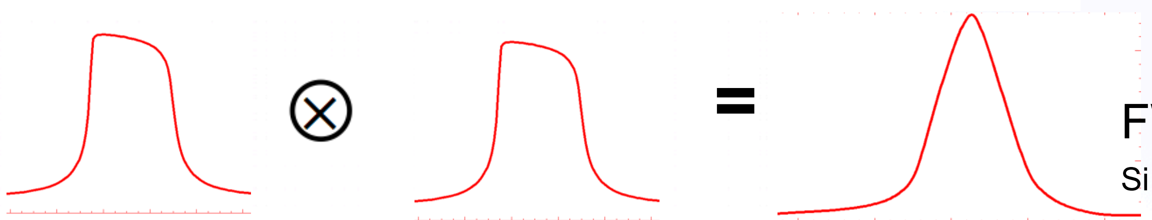
The rocking curve is the **CONVOLUTION** of the two diffraction profiles.



$\mathrm{FWHM}_R = 1.4\ \mathrm{FWHM}_1$



$\mathrm{FWHM}_R = 1\ \mathrm{FWHM}_1$

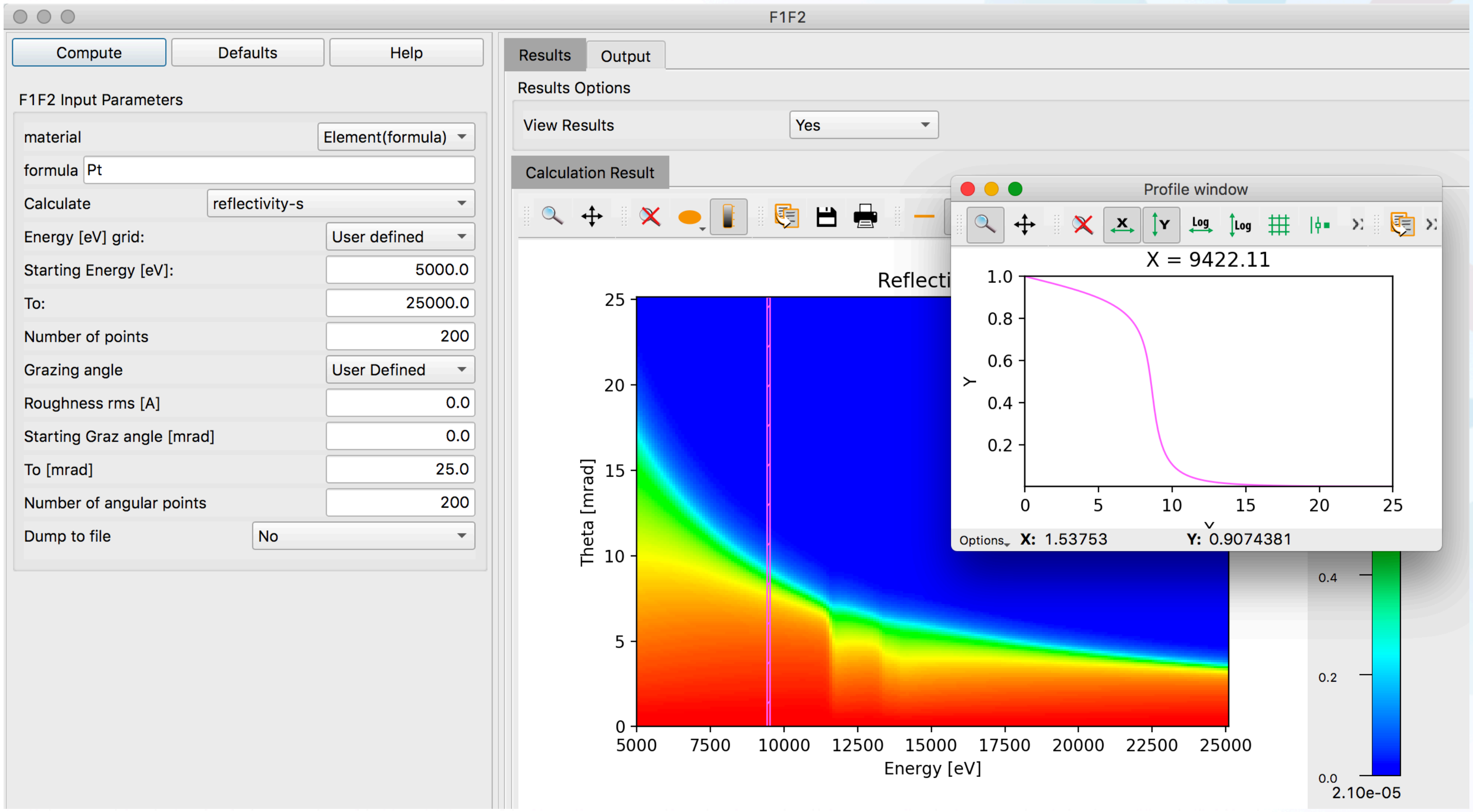


$\mathrm{FWHM}_R \sim 1.5\ \mathrm{FWHM}_1$

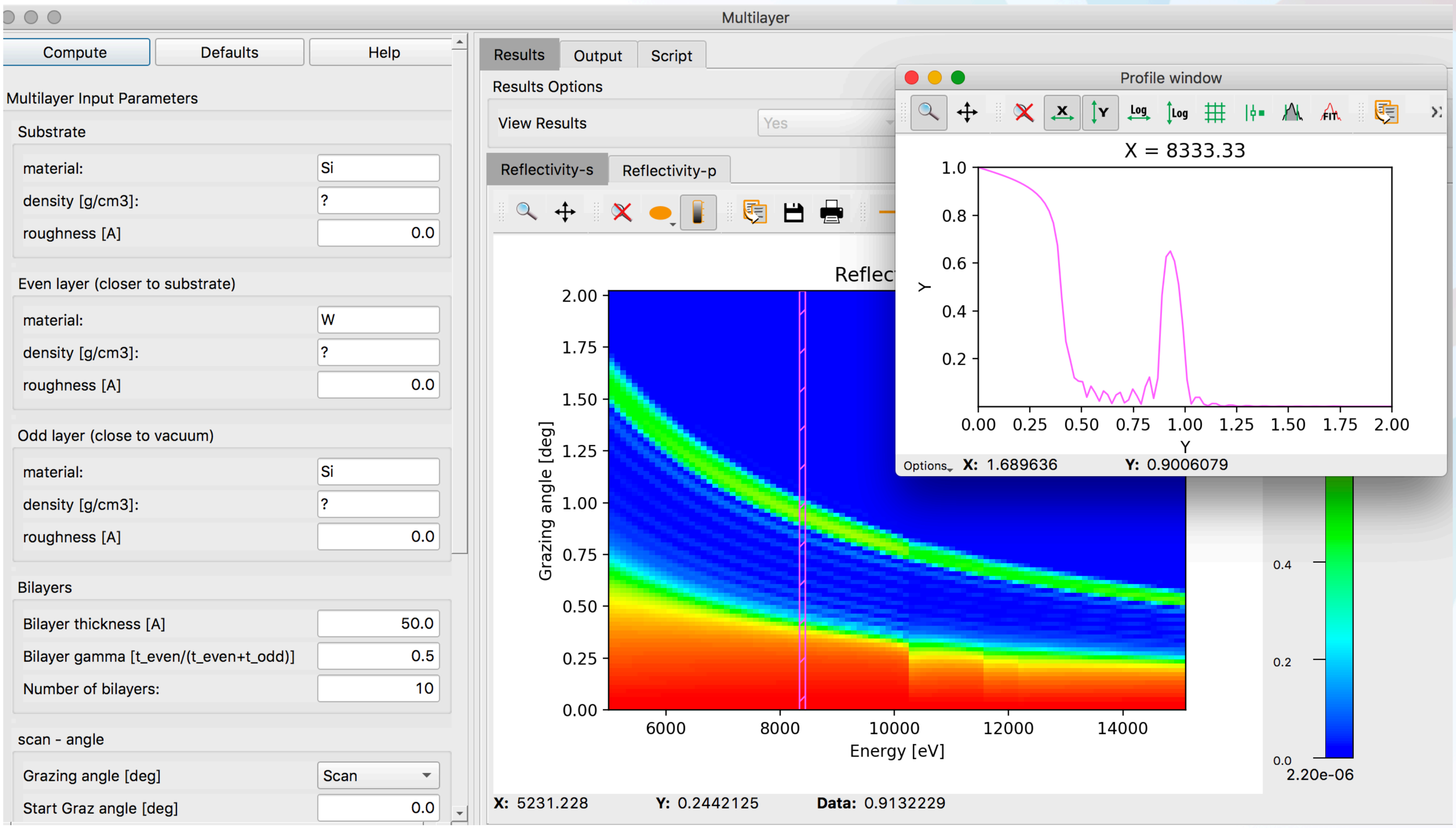
Si111 8 keV

For a full discussion about rocking curves see: Masiello *et al.* J. Appl. Crystall. 47, 1304-1314 (2014)

irror reflectivity F1F2



ultilayer reflectivity



ultiple Bragg Diffraction

Simultaneous multiple diffraction occurs when the incident wave finds several sets of planes satisfying the Bragg law.

- They were first discovered by Renninger (1937) so they are called Renninger reflections of detour reflections (umweganregung).
- Kinematical theory (Cole, Acta Cryst.15 138 (1962); Rossmanith PSILAM; XOP/ MARE)
- Beyond kinematical theory (Colella, Acta Cryst. A30, 413 (1974); Shen; Stepanov http://x-server.gmca.aps.anl.gov)