Argonne NATIONAL LABORATORY

X-Ray optics simulations and current developments on software packages - I

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SyncLight 2015, the São Paulo School of Advanced Sciences (ESPCA) on Recent Developments in Synchrotron Radiation

U.S. DEPARTMENT OF ENERGY

Thanks and Slides

- ☑ Xianbo Shi - APS (XS)
- ☑ Manuel Sanchez del Rio- ESRF (MS)
- ☑ Oleg Chubar - NSLS-II (OC)

Rules:
Do not hesitate to interrupt to ask questions!
Just do it!

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Just do it!

No Ercan

Outline

- ☑Packages
- ☑SPECTRA
  - ☑ ID source
- ☑SHADOW
  - ☑ Simple focusing
  - ☑ High resolution soft x-ray monochromator
  - ☑ meV resolution hard x-ray monochromator
- ☑SRW- Wave propagation
  - ☑ Partial coherence

Design and Optimize a Beamline

- ☑ Source
  - ☑ Brightness
    - ☑ Flux
    - ☑ 2D Phase space
    - ☑ "Coherent modes"
  - ☑ Polarization
  - ☑ Bandwidth

- ☑ Experiment
  - ☑ Coherent Flux
  - ☑ Flux
  - ☑ Polarization
  - ☑ Spot Size
  - ☑ Angular divergence
  - ☑ Resolution

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Things to remember:
Cannot have all
Optics are not perfect

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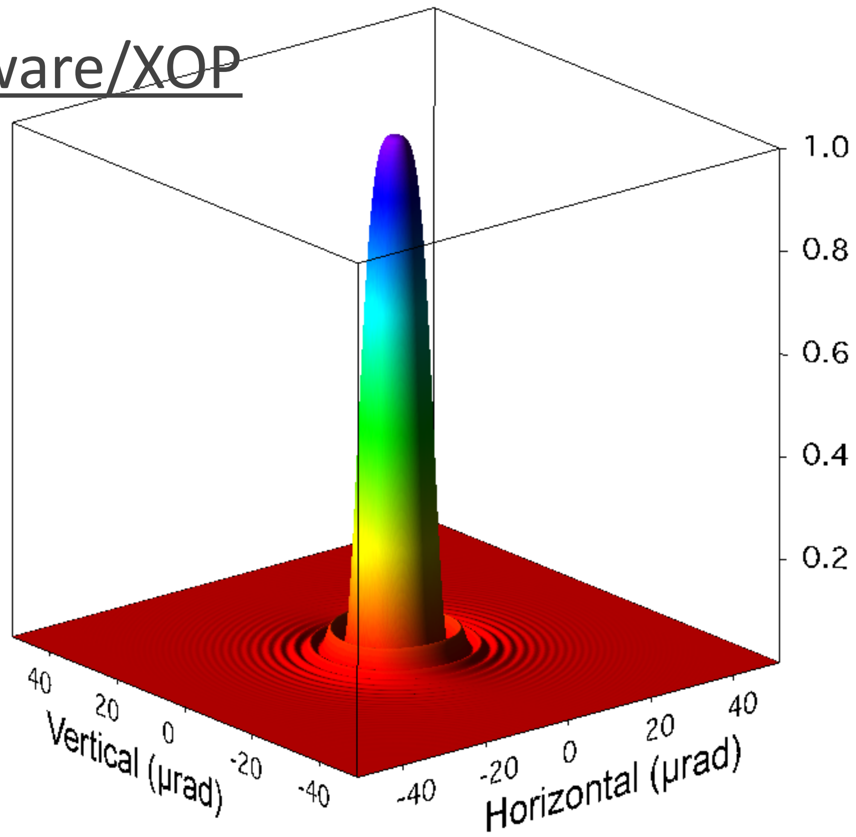
Things to remember:
Cannot have all
Optics are not perfect

Life is a compromise

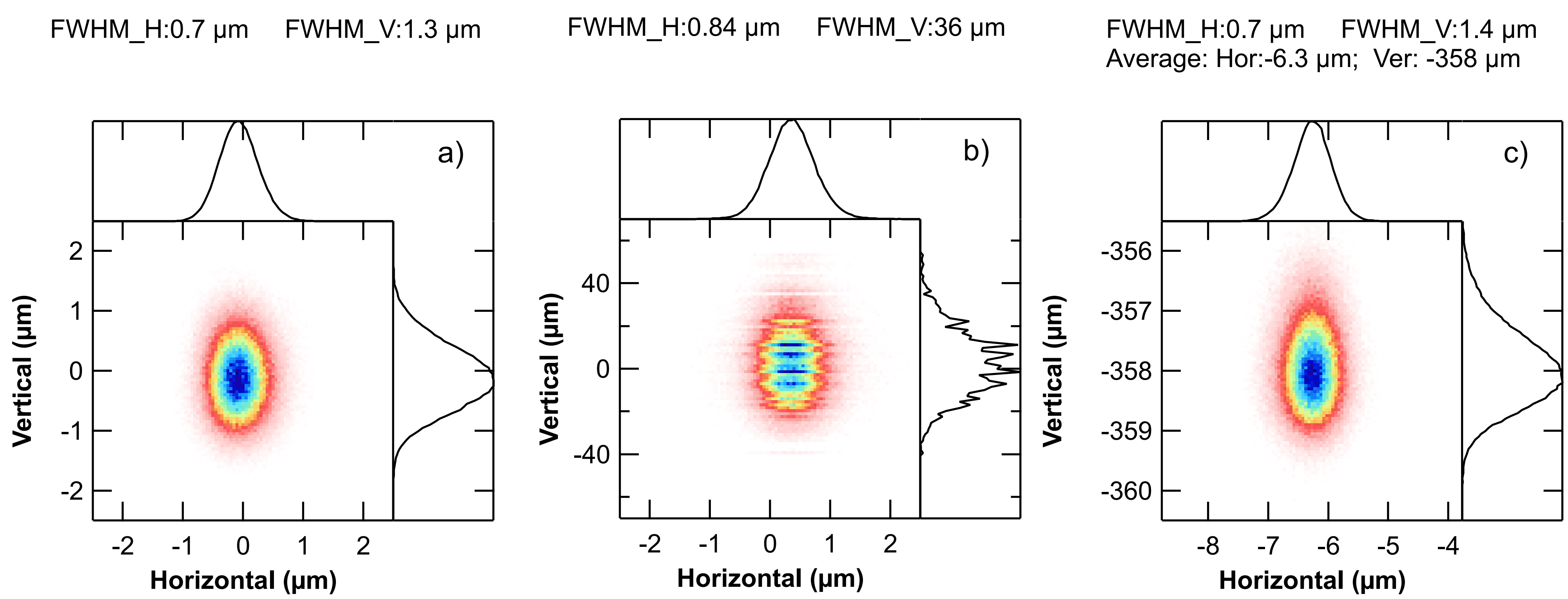
Source Codes: BM, Undulator, Wiggler

- Spectra: http://radiant.harima.riken.go.jp/spectra/
- SRW: https://github.com/ochubar/SRW
- XOP: https://www1.aps.anl.gov/Science/Scientific-Software/XOP
- Wave: http://www.helmholtz-berlin.de/forschung/oe/fg/nanometeroptik/methods/software_en.html#c157167
- XRT: http://pythonhosted.org//xrt/index.html
- Shadow: https://www1.aps.anl.gov/Science/Scientific-Software/XOP



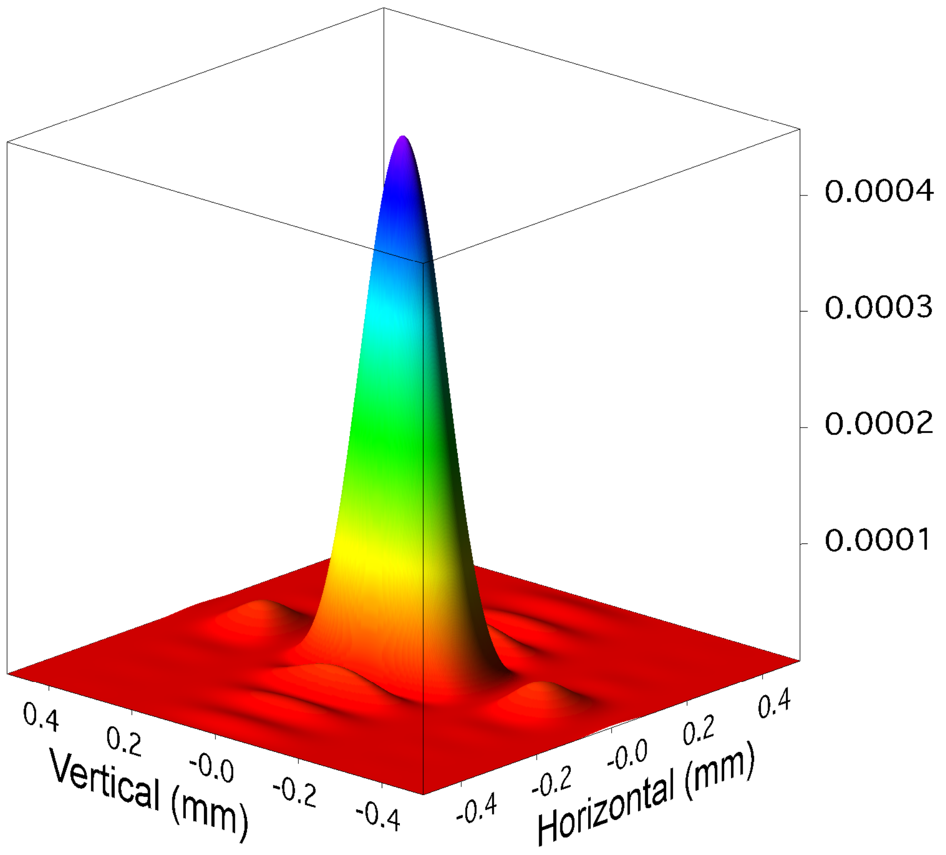
Ray Tracings: Geometrical

- Shadow: https://www1.aps.anl.gov/Science/Scientific-Software/XOP
- Ray: http://www.helmholtz-berlin.de/forschung/oe/fg/nanometeroptik/methods/software_en.html#c157167
- XRT: http://pythonhosted.org//xrt/index.html
- McXTrace: http://www.mcxtrace.org



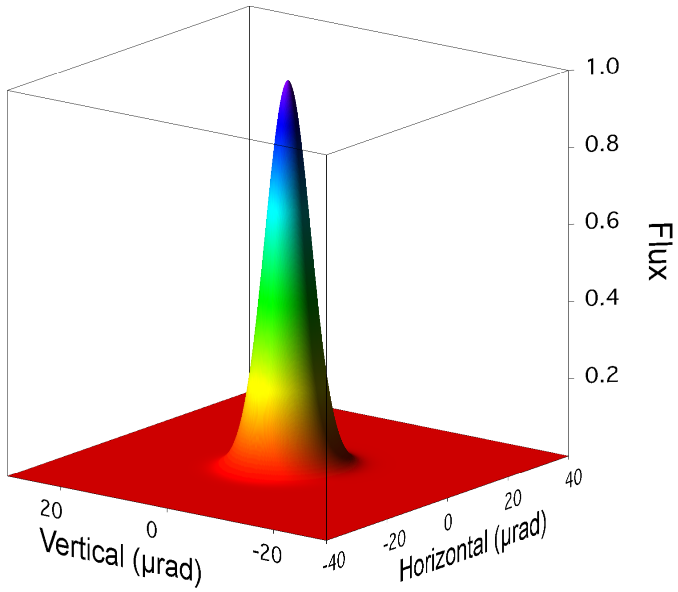
Wave Propagation: Diffraction

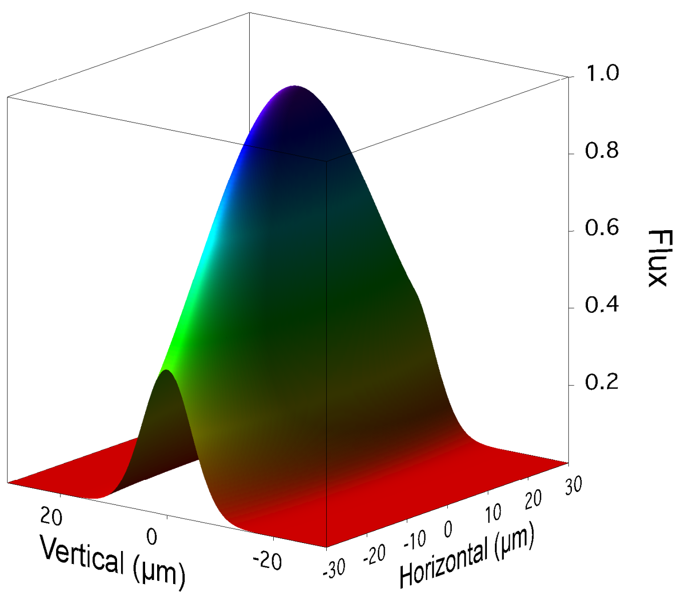
- SRW: https://github.com/ochubar/SRW
- Phase: http://www.helmholtz-berlin.de/forschung/oe/fg/nanometeroptik/methods/software_en.html#c157167
- XRT: http://pythonhosted.org//xrt/index.html
- Shadow + Hybrid: https://www1.aps.anl.gov/Science/Scientific-Software/XOP



SPECTRA: APS-U ID:3.3 cm, 2.4 m long @10keV

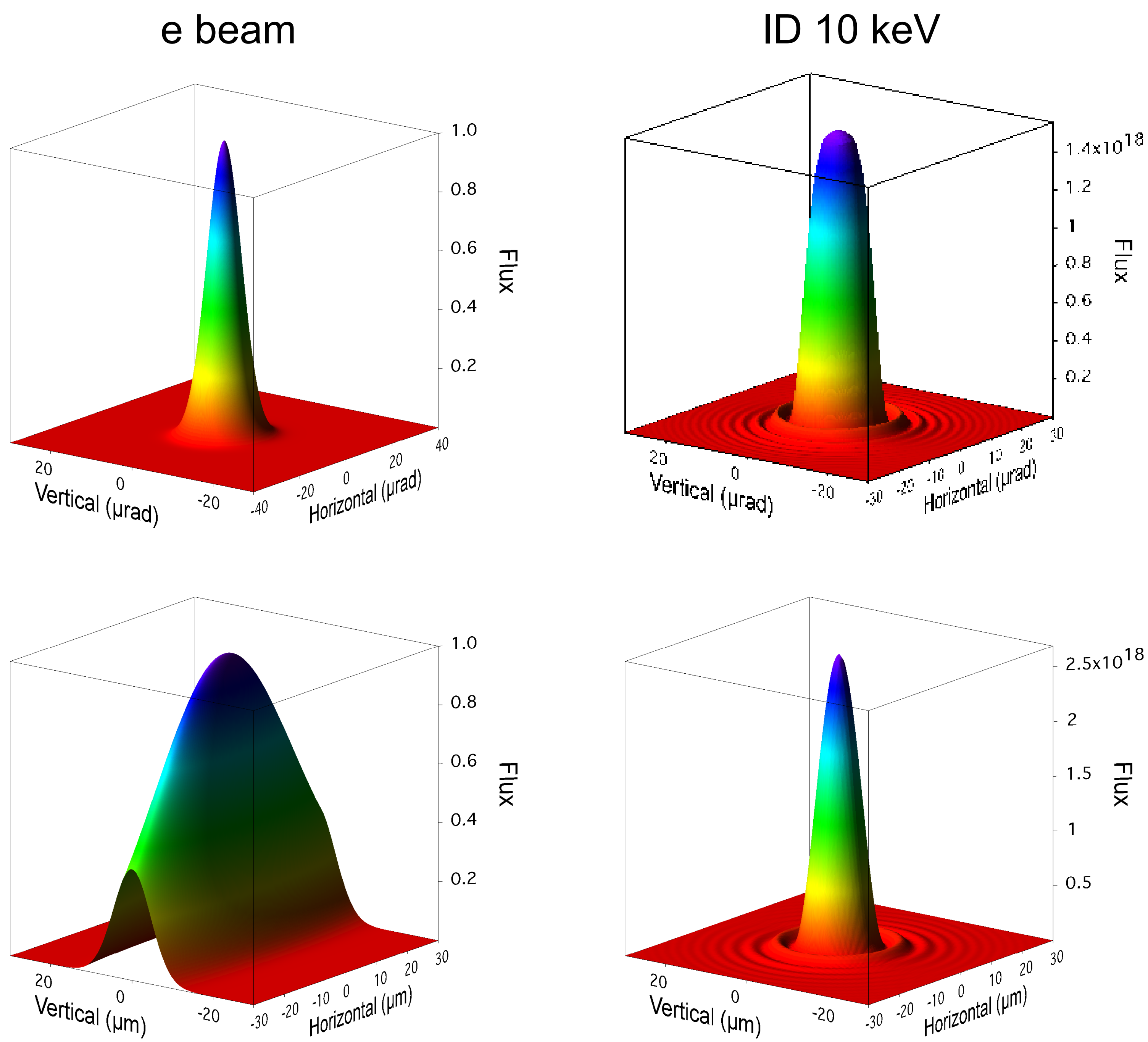
e beam





SPECTRA: APS-U ID:3.3 cm, 2.4 m long @10keV

Single e emission



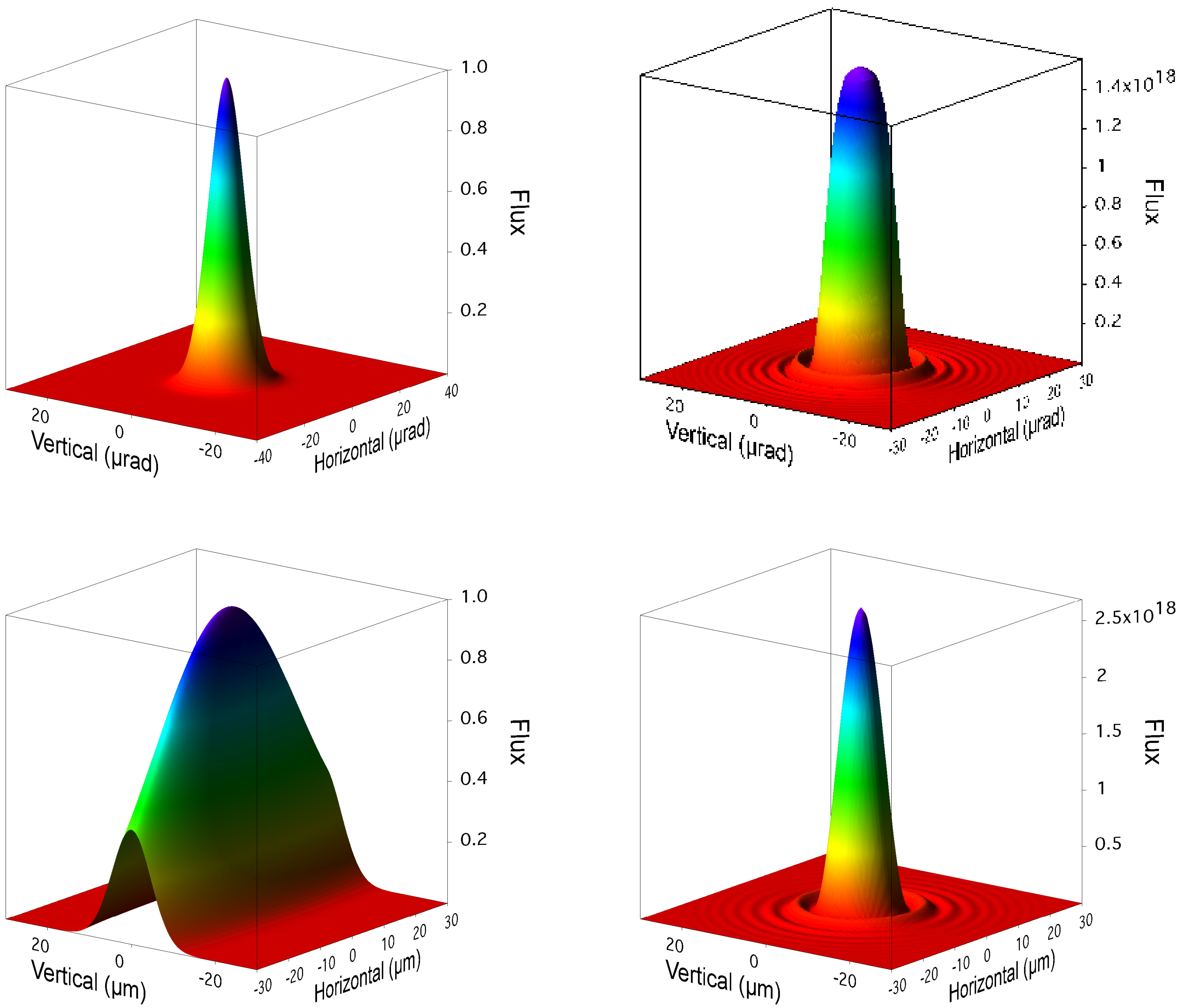
2.5 10^{14} p/s/0.1%

SPECTRA: APS-U ID:3.3 cm, 2.4 m long @10keV

Single e emission

e beam

ID 10 keV



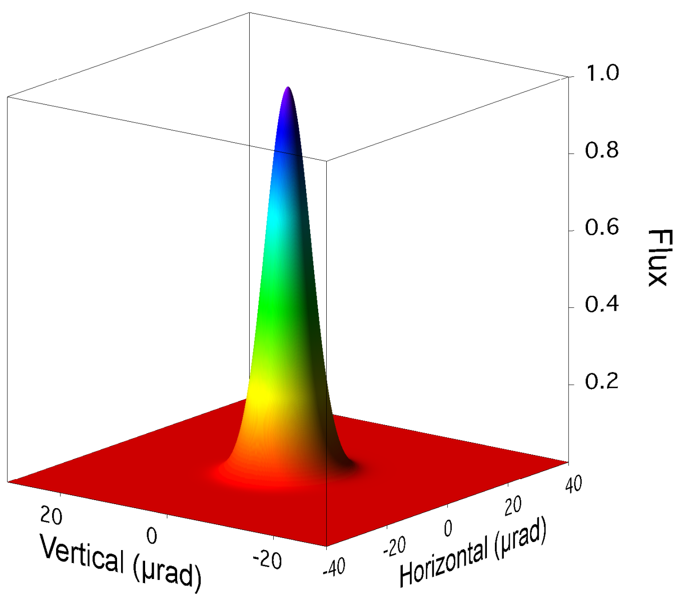
Convolution @ Source .
@ Sample?

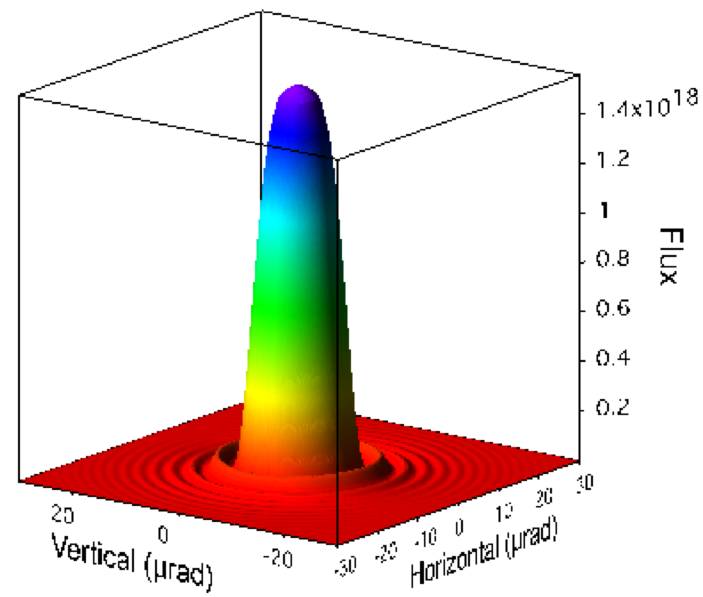
2.5 10^{14} p/s/0.1%

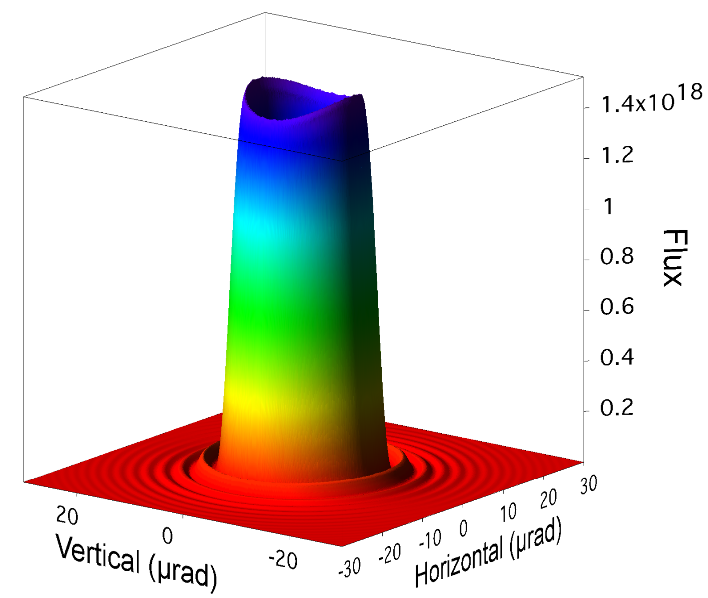
SPECTRA: APS-U ID:3.3 cm, 2.4 m long @10keV

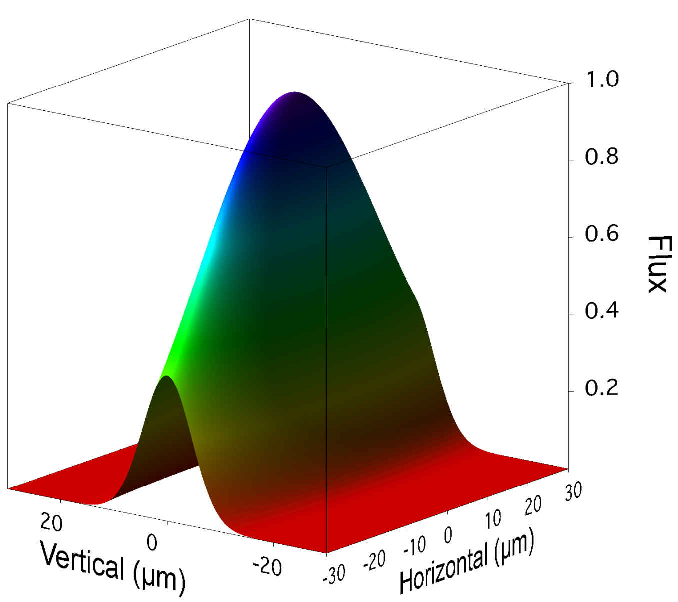
Single e emission

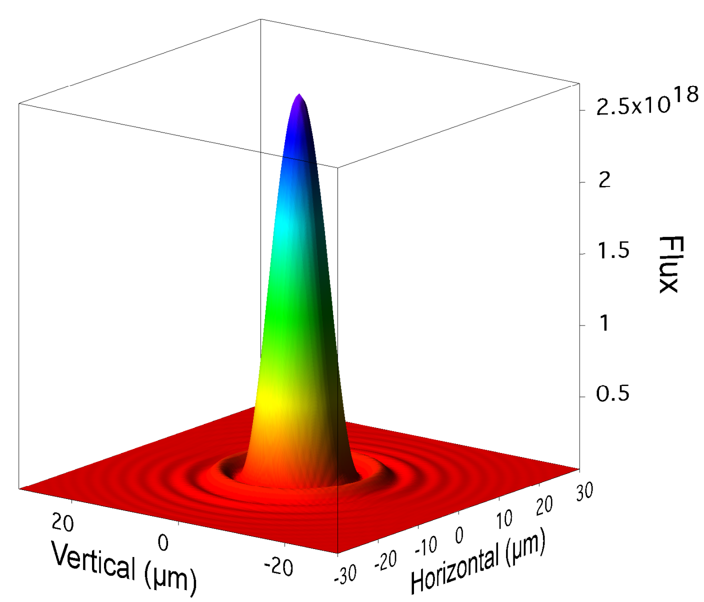
e beam | ID 10 keV | ID 9.9 keV

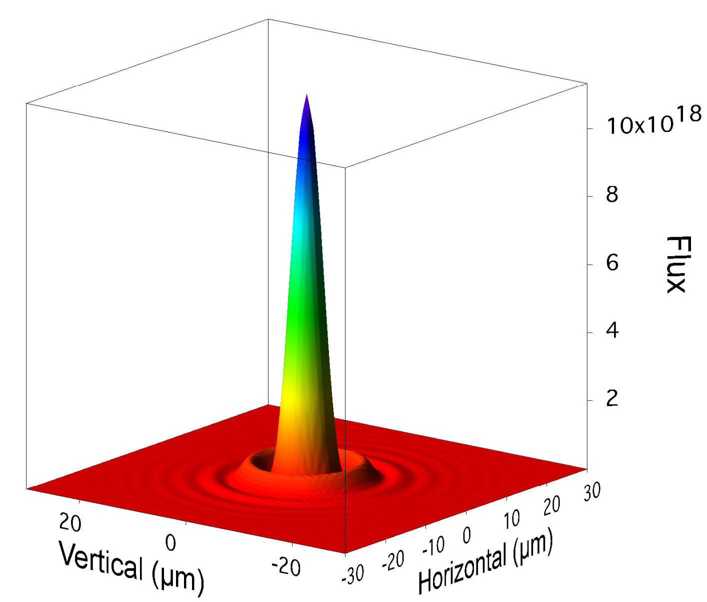












Convolution @ Source .
@ Sample?

$2.5\ 10^{14}$ p/s/0.1%

$4.5\ 10^{14}$ p/s/0.1%

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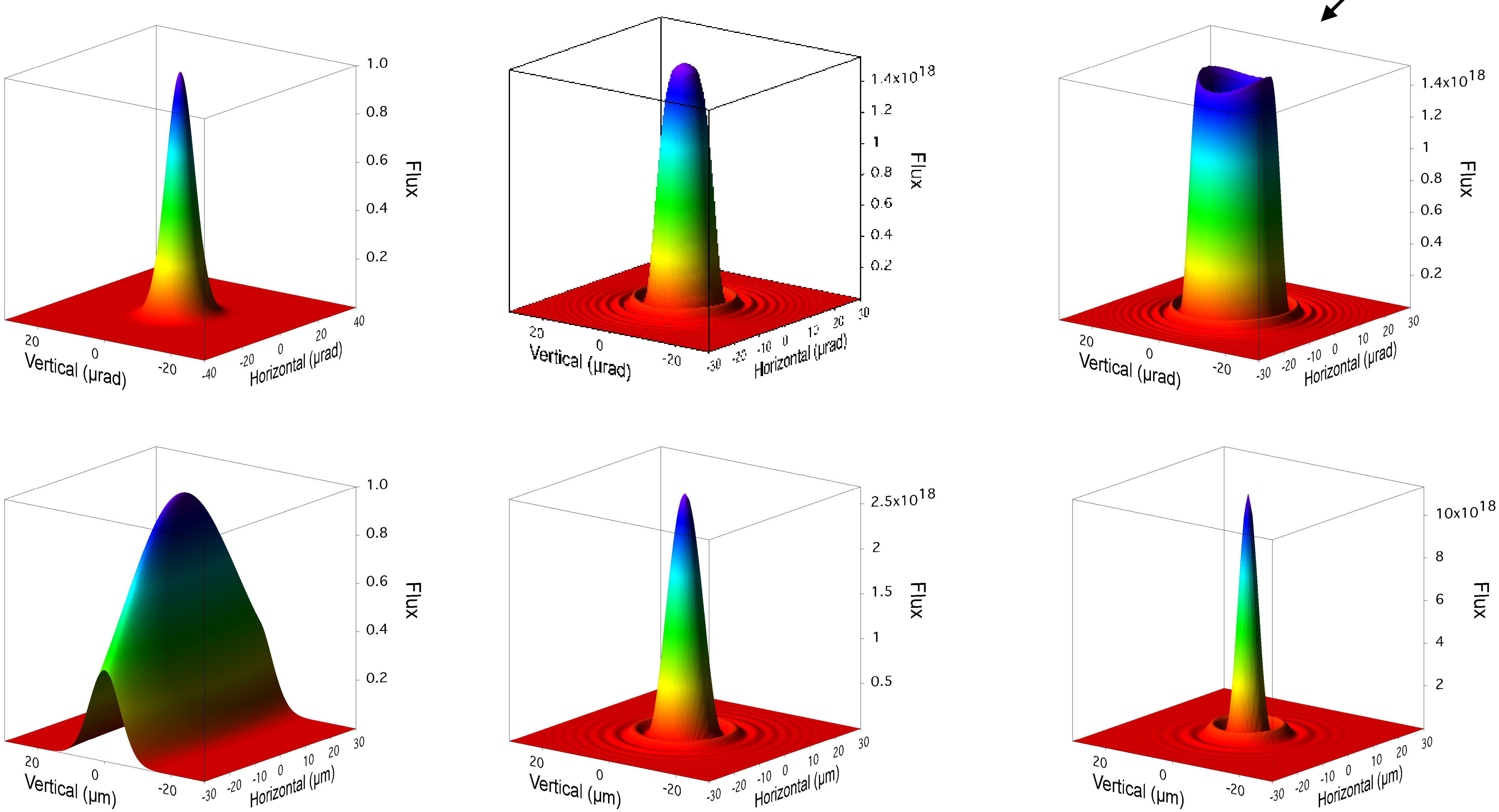
Single e emission

e beam | ID 10 keV | ID 9.9 keV



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Birth of SHADOW

Written in the transition from Tantalus to Aladdin
Beginning of the 80s

Scientific motivation:
Grating monochromator design, TGM, ERG, toridal, spherical mirrors.

Monte Carlo ray tracing program ***designed*** to simulate X-ray optical systems

Requirements

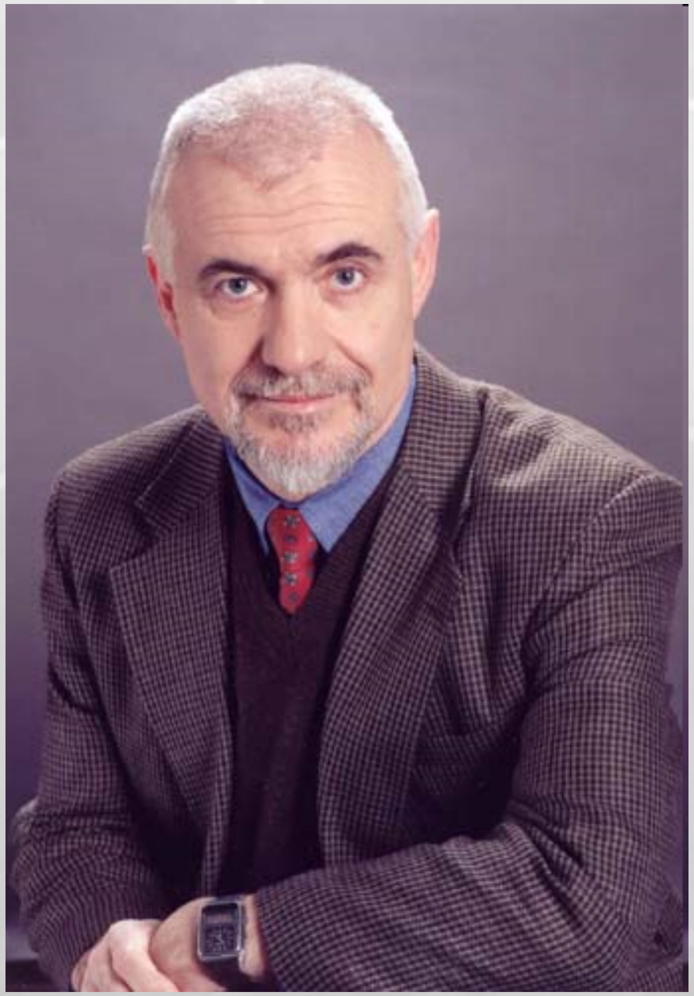
- Accuracy and reliability
- Easy to use
- Flexibility
- Economy of computer resources
- VAX-11 Computers

Efficient MC approach

- Reduced number of rays
- Exact simulation os SR sources
- Vector calculus
- Modular
- User-interface
- Available to users

Two years development

Fortran 77+VAX/VMS extensions



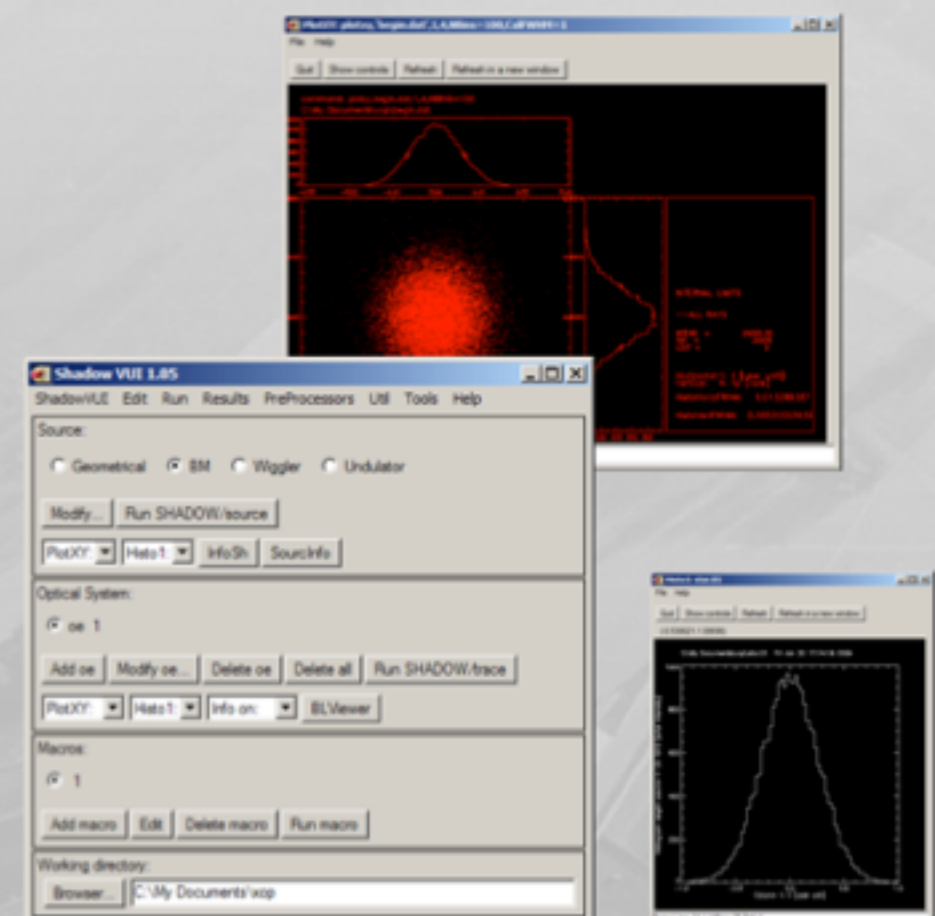
Actively expanded by collaborations
Many with Manuel

XOP+ShadowVui

- XOP
  - quick calculations (synchrotron spectra, reflectivities, rocking curves, attenuation coeffs. etc.)
  - generic data visualization and analysis
  - specific applications ("extensions")

  - Collaboration work ESRF (M Sanchez del Rio)-APS (Roger Dejus)
  - Freely available to users (>10 years)
  - Large user community (>400 users in tens of laboratories)
  - Multiplatform (Windows, Unix, MacOSX)
  - Written in IDL (using Fortran and C modules). Embedded license.

- ShadowVUI: interface that uses the standard SHADOW calculation engine
  - "Easy" to use
  - High performance graphics
  - Macro language
  - Tutorials
  - BLViewer



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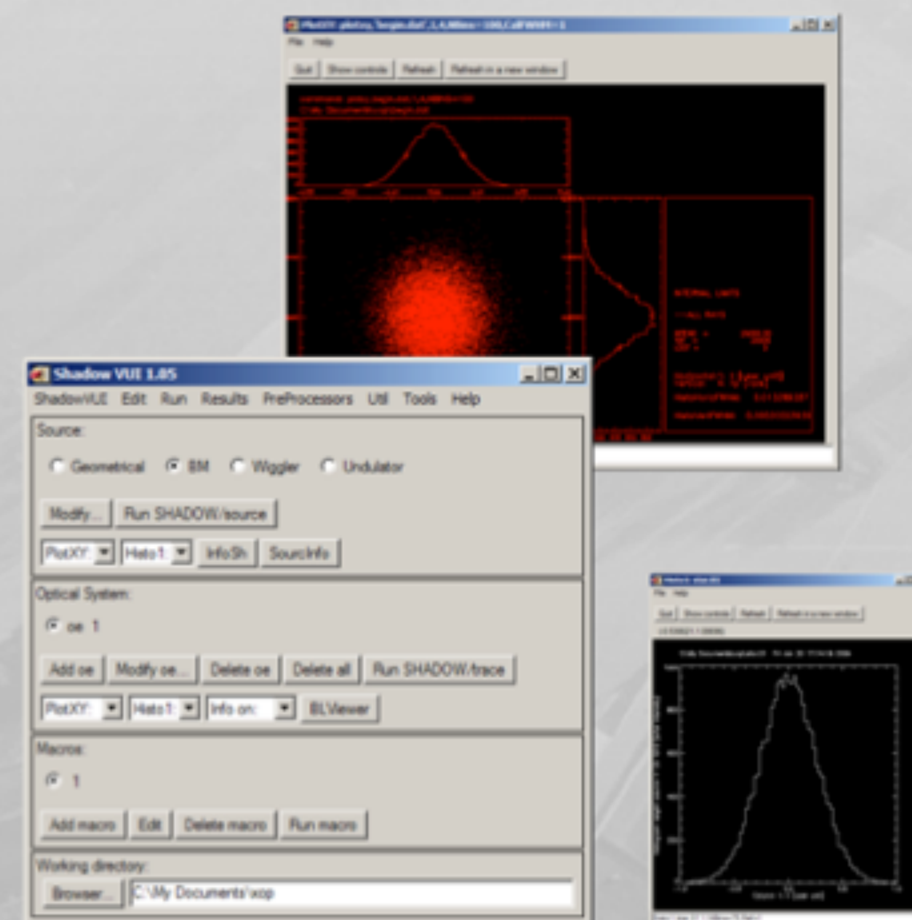
But look awful



What SHADOW can do?

- Beam cross sections (focal spot, PSF, etc)
  - source characteristics (dimensions, depth, emittances)
  - vignetting (apertures, dimension of oe's)
  - effect of mirror shape: aberrations, errors…
  - effect of mirror imperfections (slope errors, roughness?)
- Energy resolution
- Flux and power (number of photons at a given position, absorbed/transmitted power, etc)
- Other aspects? (polarization, coherence effects, etc.)

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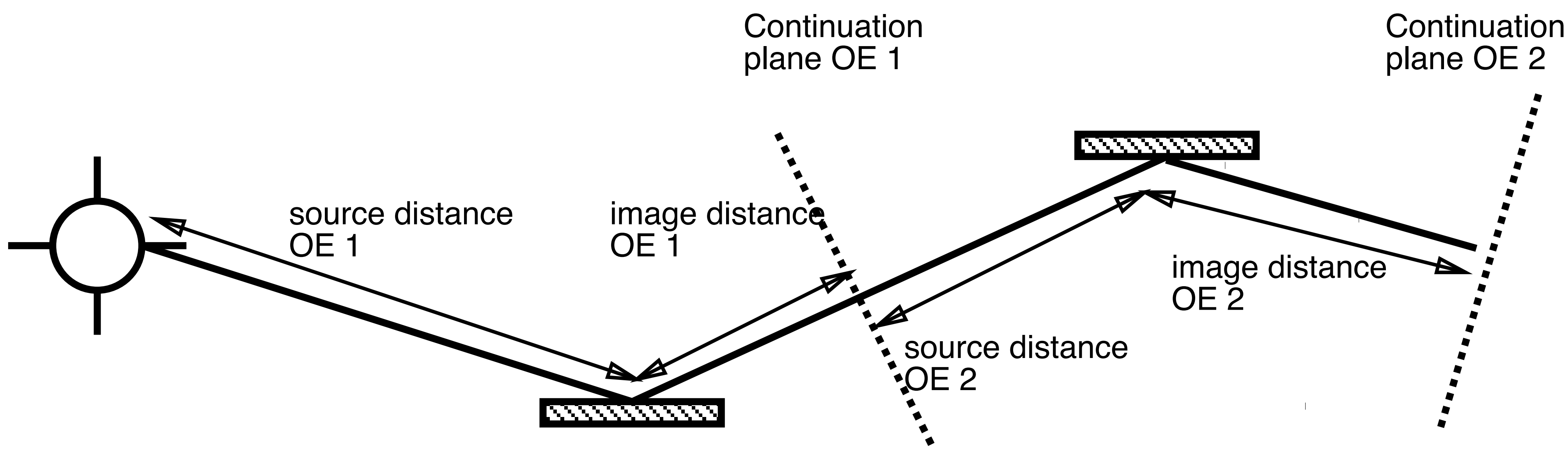
***SHADOW3*: a new version of the synchrotron X-ray optics modelling package**

J. Synchrotron Rad. (2011). **18**, 708–716

Manuel Sanchez del Rio,[a]* Niccolo Canestrari,[b,a] Fan Jiang[c] and Franco Cerrina[c]†

API: Scripts, macros: C, Fortran, Python

SHADOW Optical system

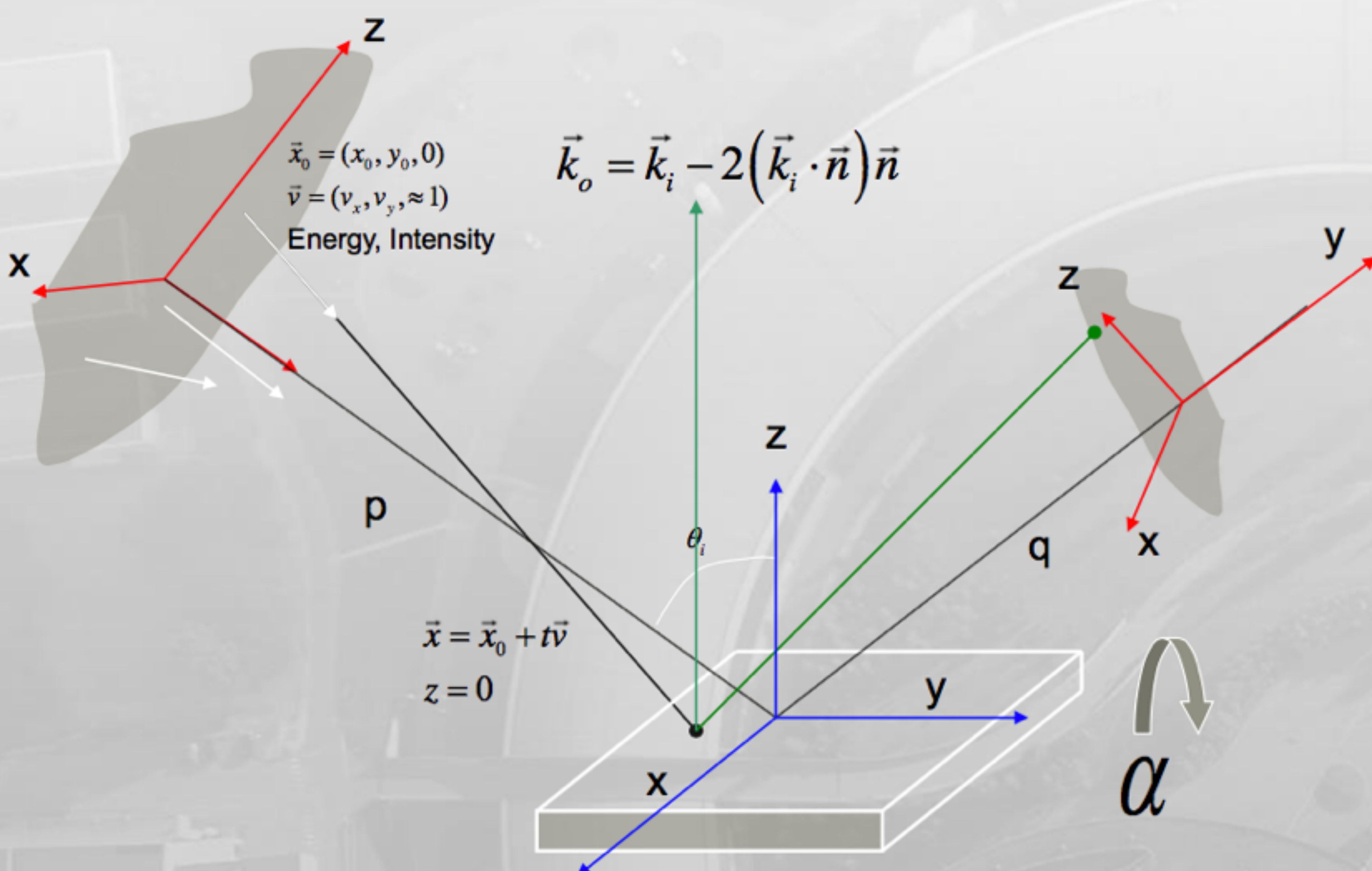


Object:	Source	OE 1		OE 2	
Namelist (starting)	START.00	START.01		START.02	
Namelist (ending)	END.00	END.01		END.02	
data (binary)	BEGIN.DAT	MIRR.01	STAR.01	MIRR.02	STAR.02

Figure 1.1: Sample layout with source and optical system.

Principle of Ray Tracing

Trace (the beamline)

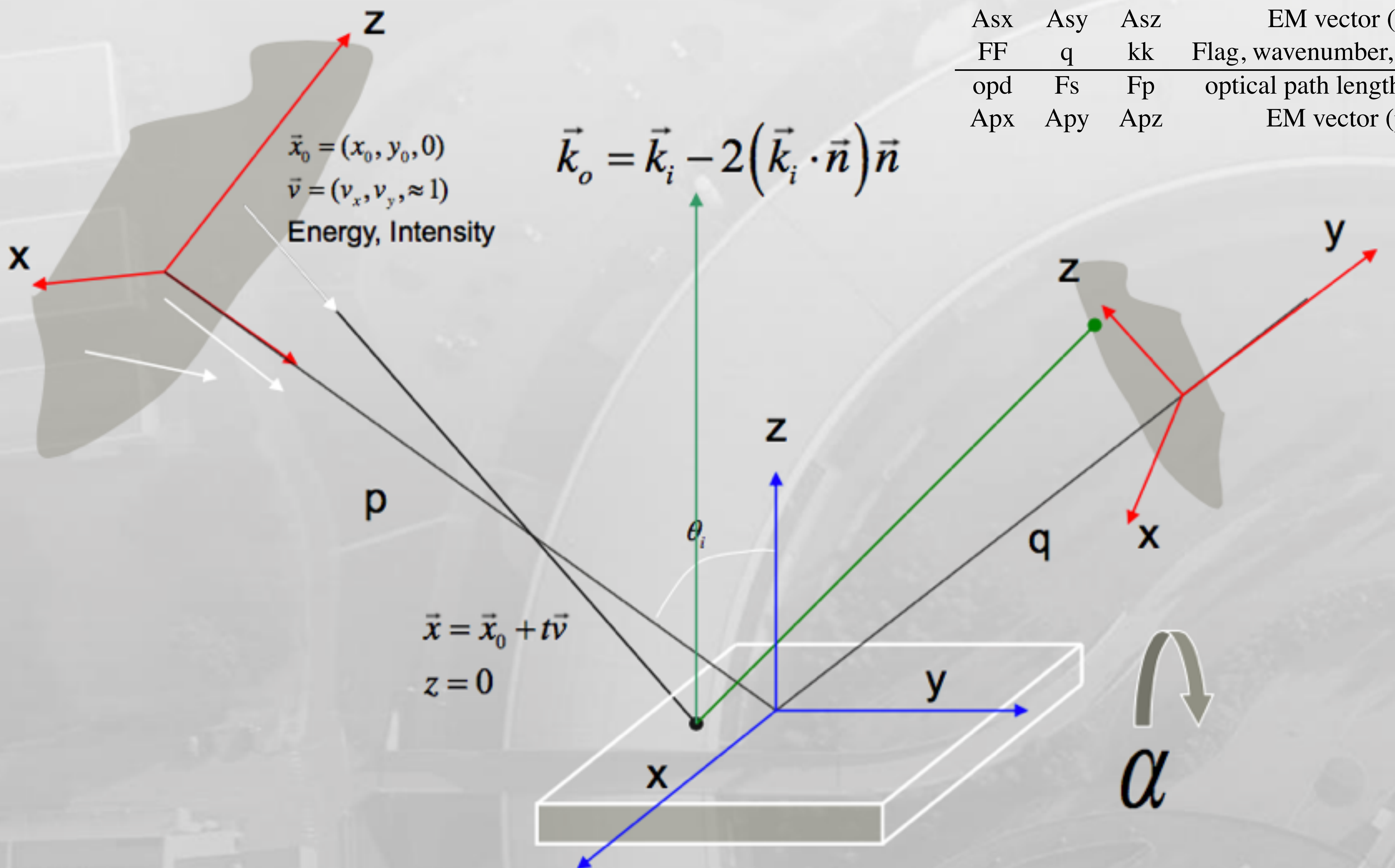


Principle of Ray Tracing

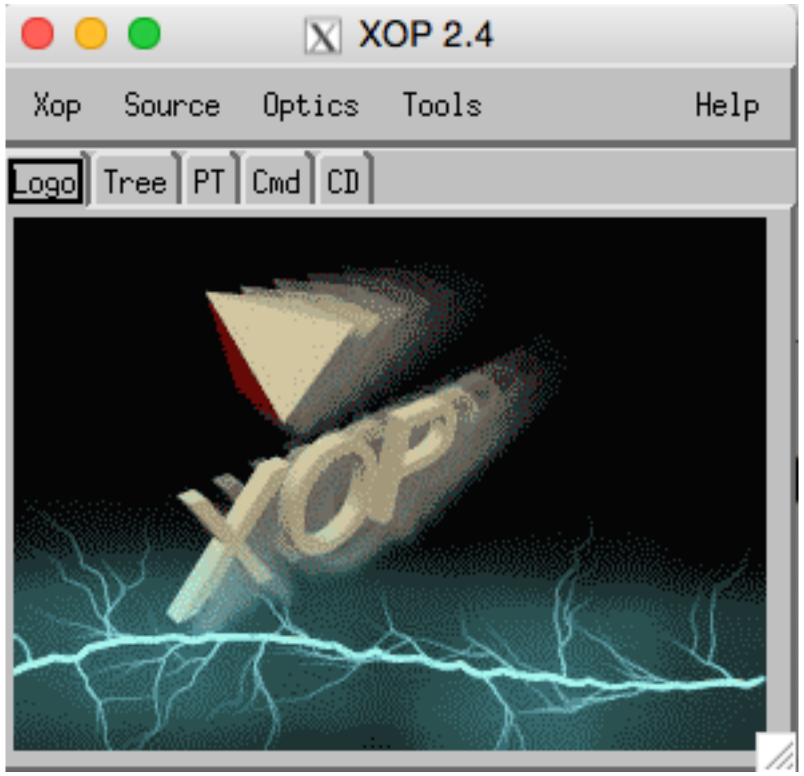
Trace (the beamline)

Ray:

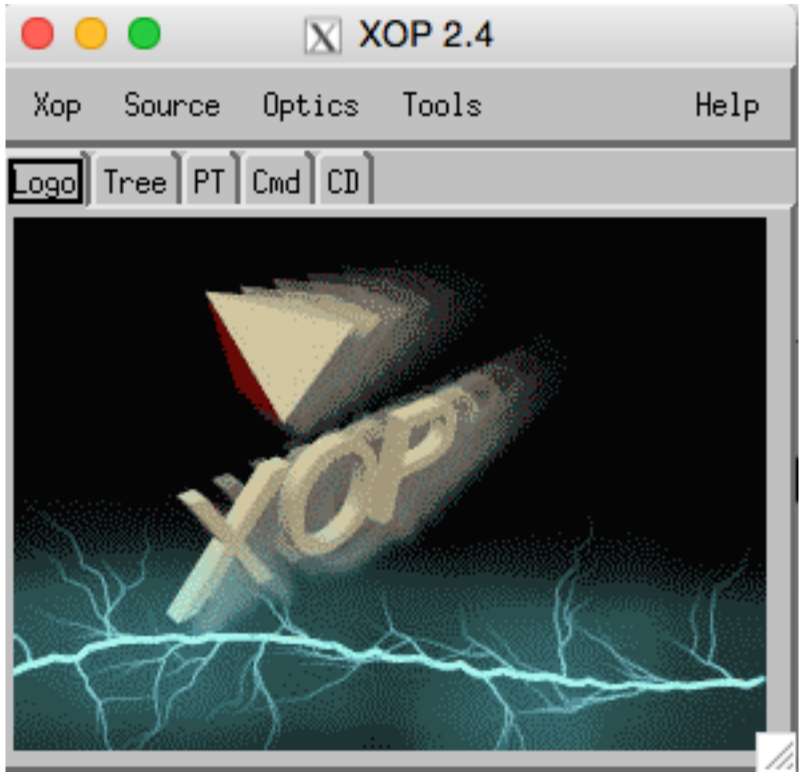
X	Y	Z	Spatial coordinate
X’	Y’	Z’	Direction
Asx	Asy	Asz	EM vector (s-)
FF	q	kk	Flag, wavenumber, ray index
opd	Fs	Fp	optical path length, phases
Apx	Apy	Apz	EM vector (p-)

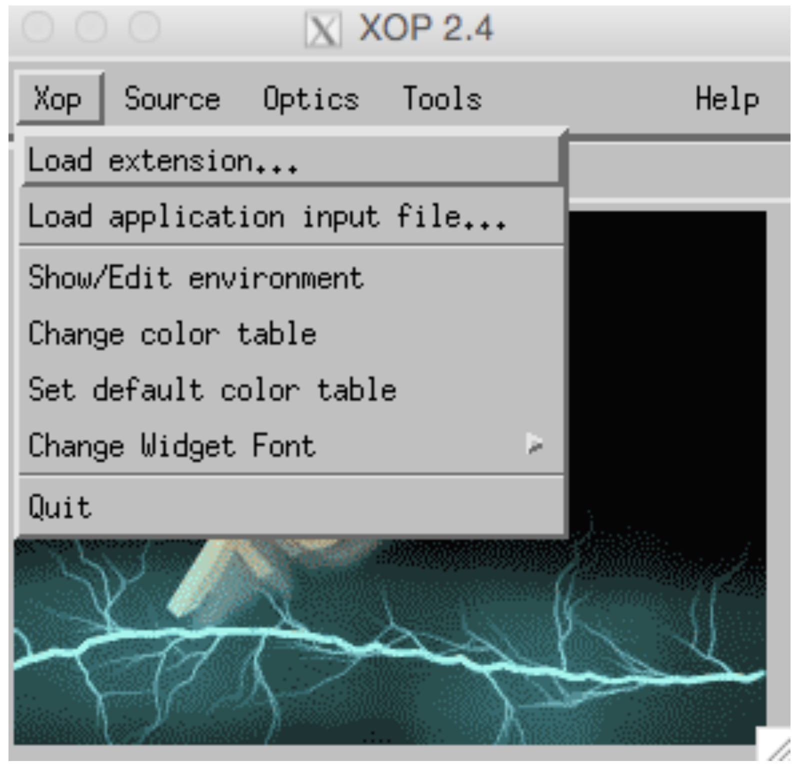


Start SHADOW



Start SHADOW





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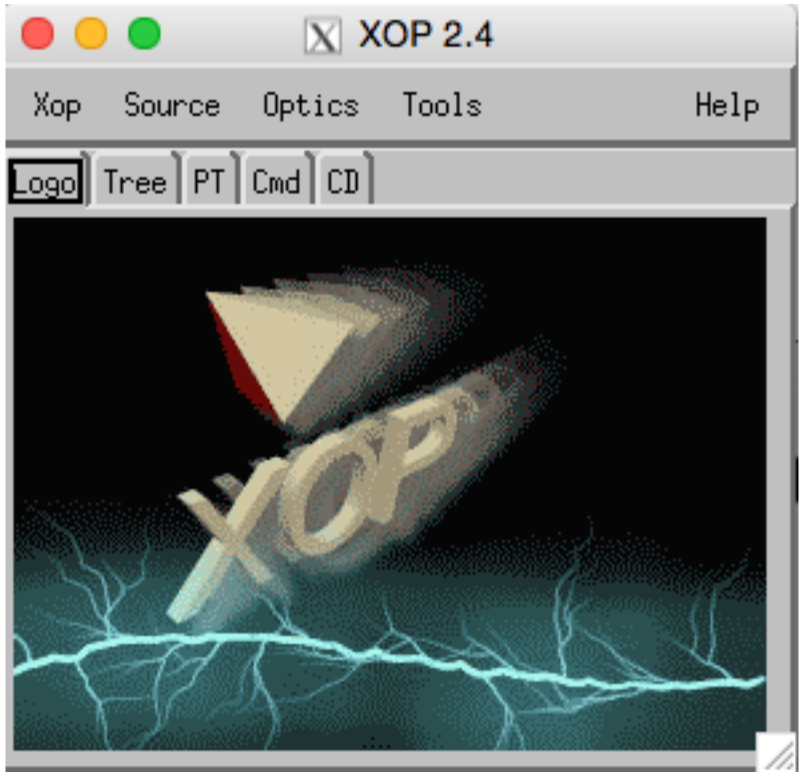
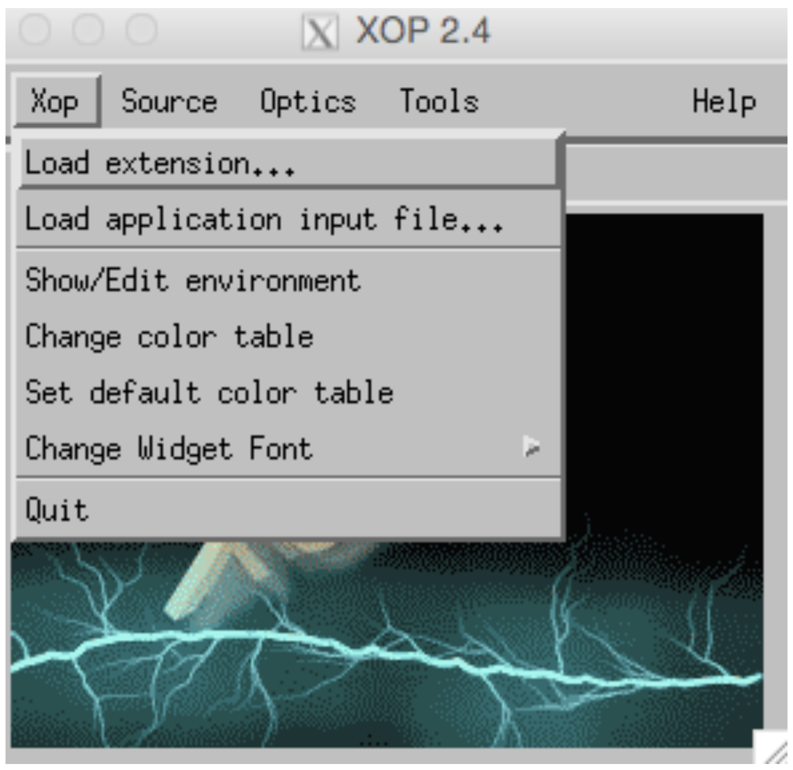
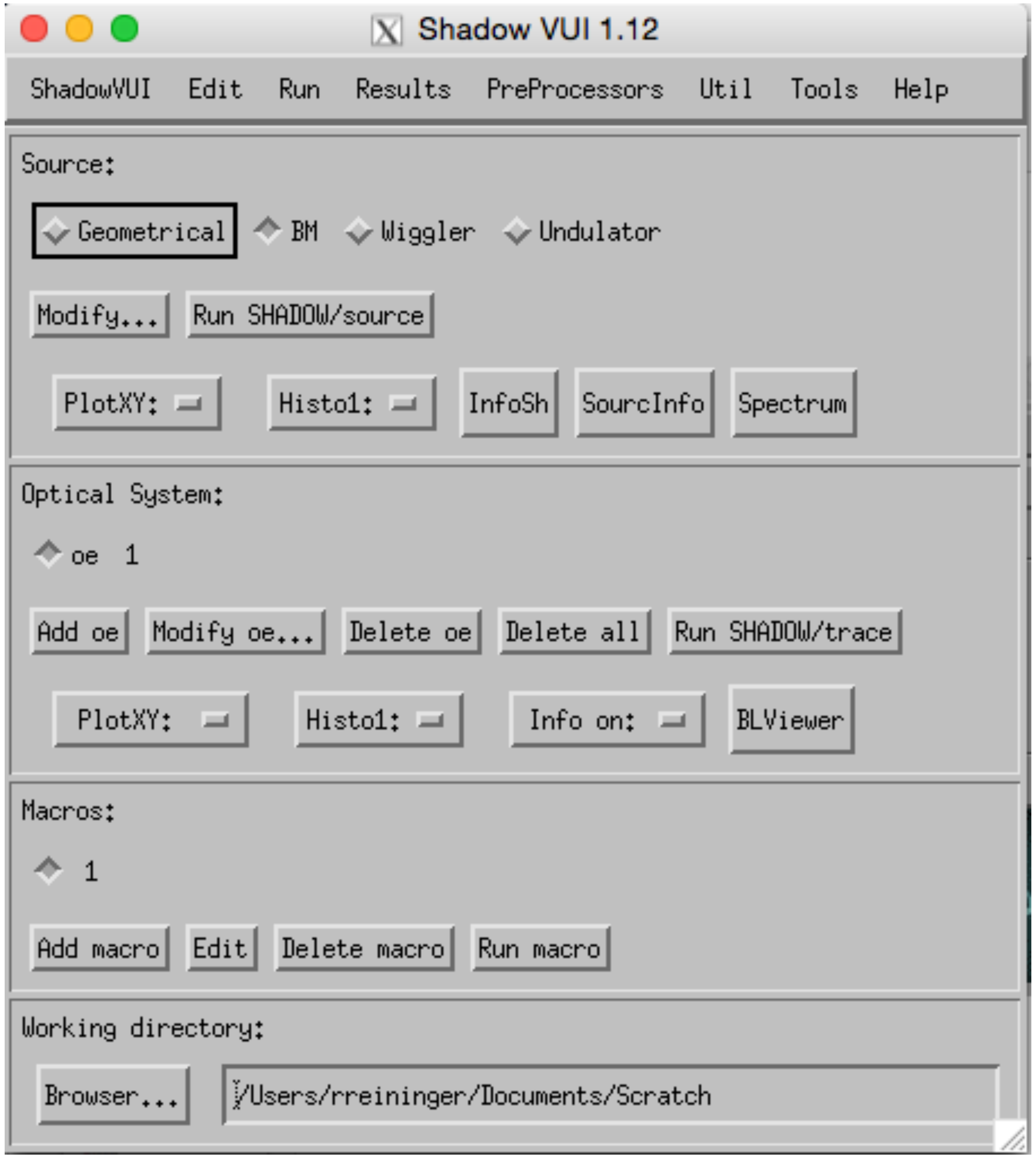
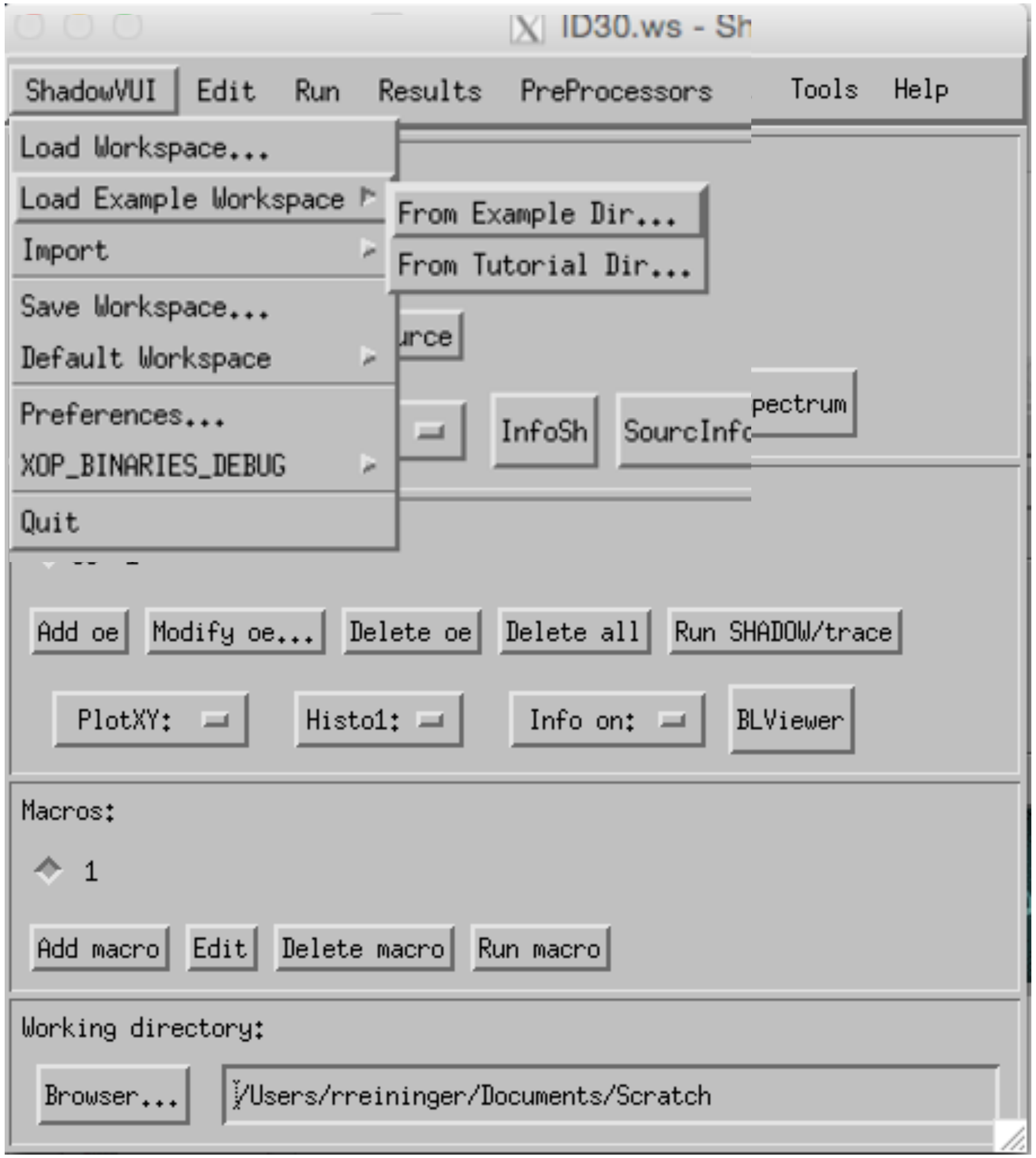




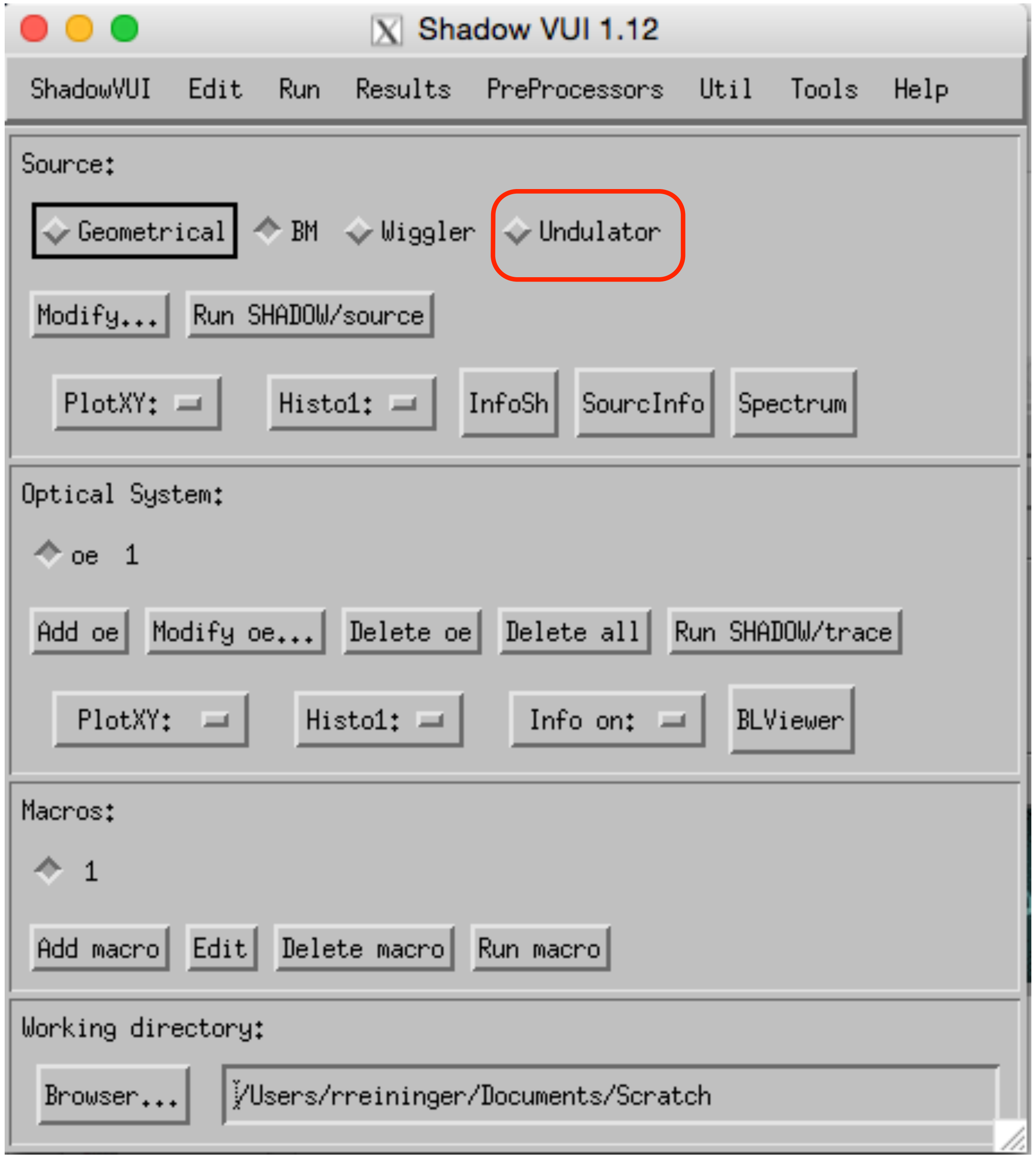
SHADOW VUI Screen



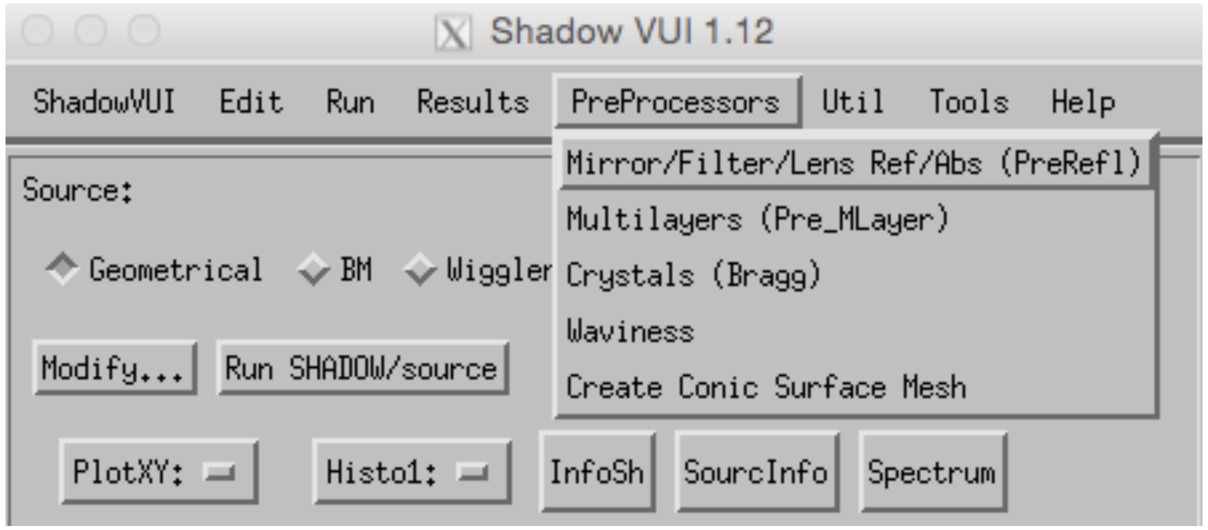
SHADOW VUI Screen

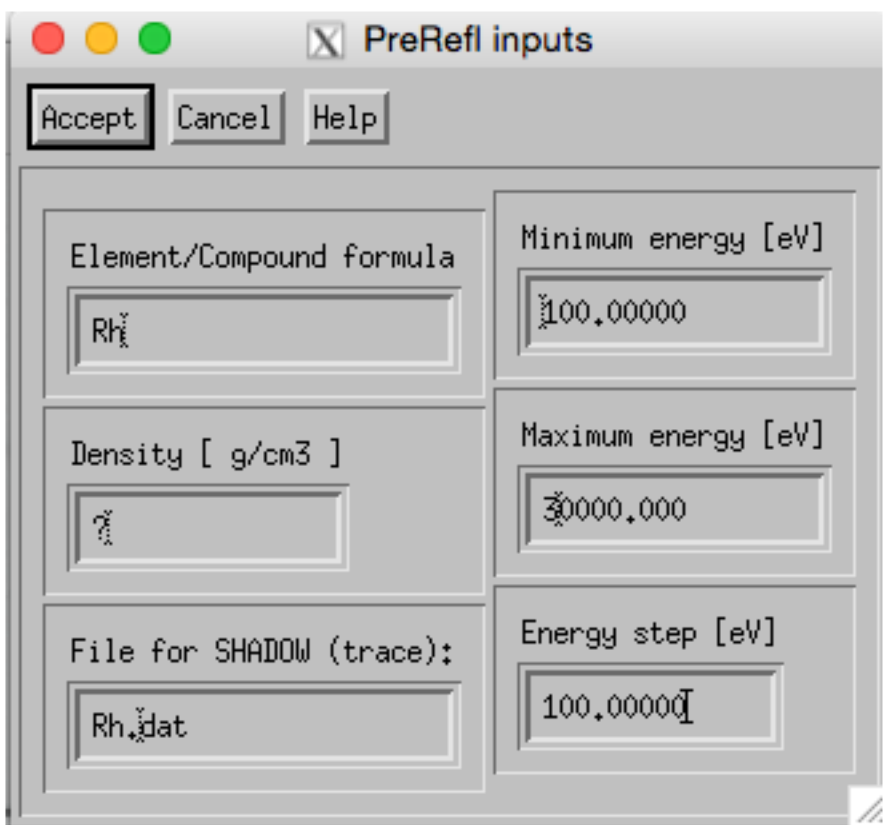


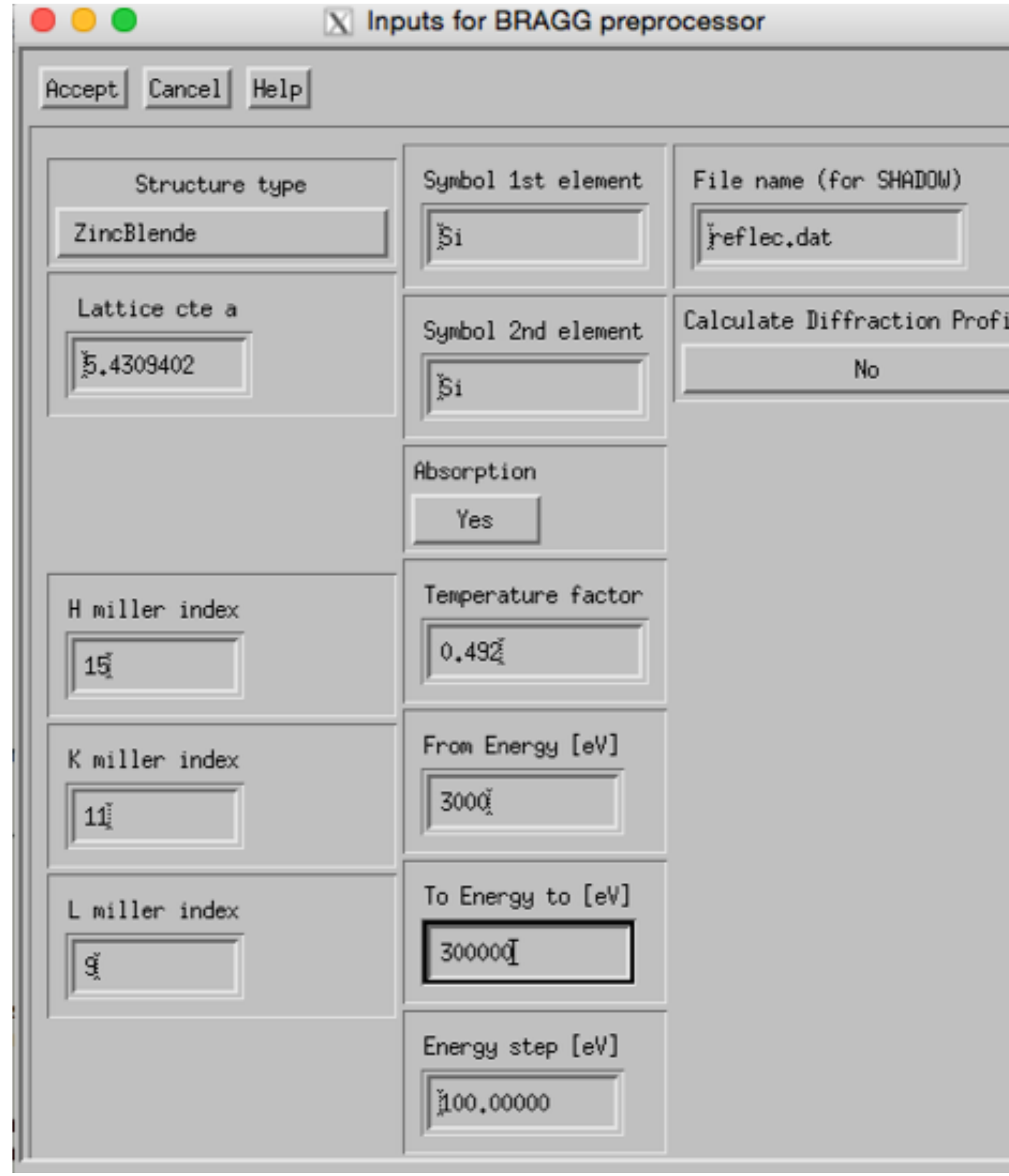
SHADOW VUI Screen



How to include Optical Constants







Run two times in Mac

Single Optic Focusing

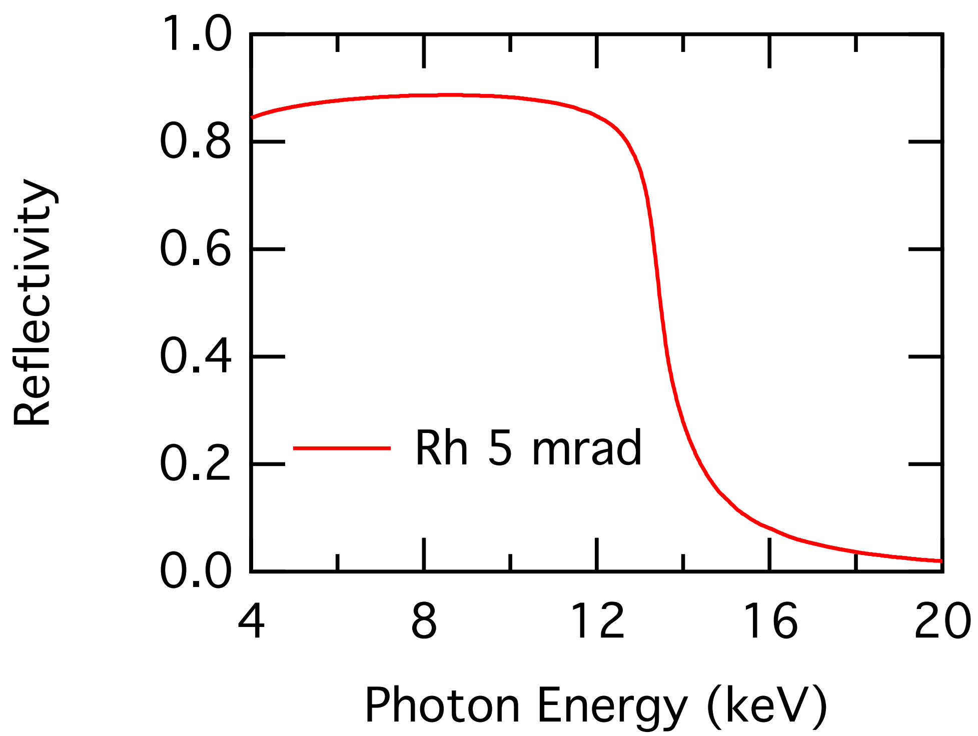
2.4 m long ID

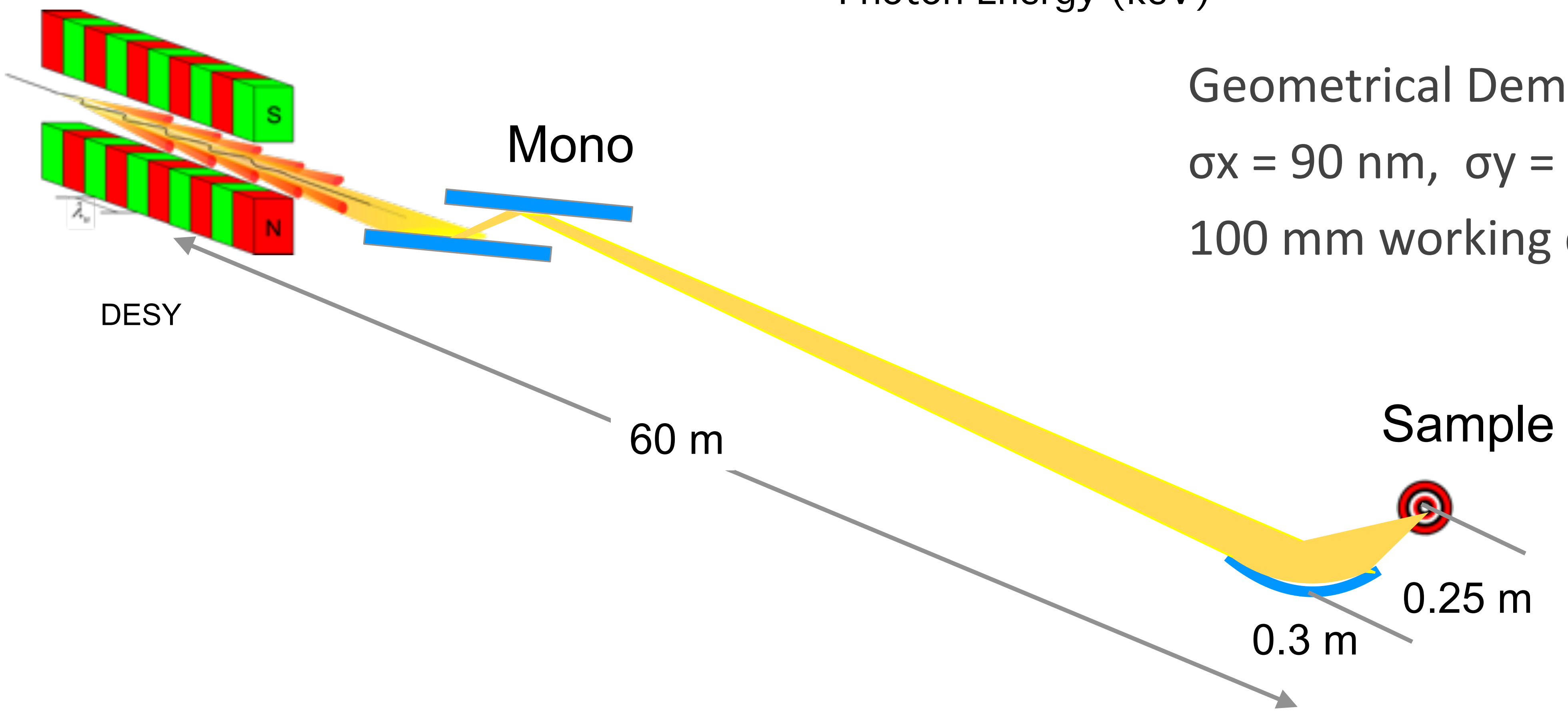
E = 12 keV

Σx = 21.5 µm, Σy = 4.6 µm

Σ’x = 4.5 µrad, Σ’y = 3.7 µrad

s polarized



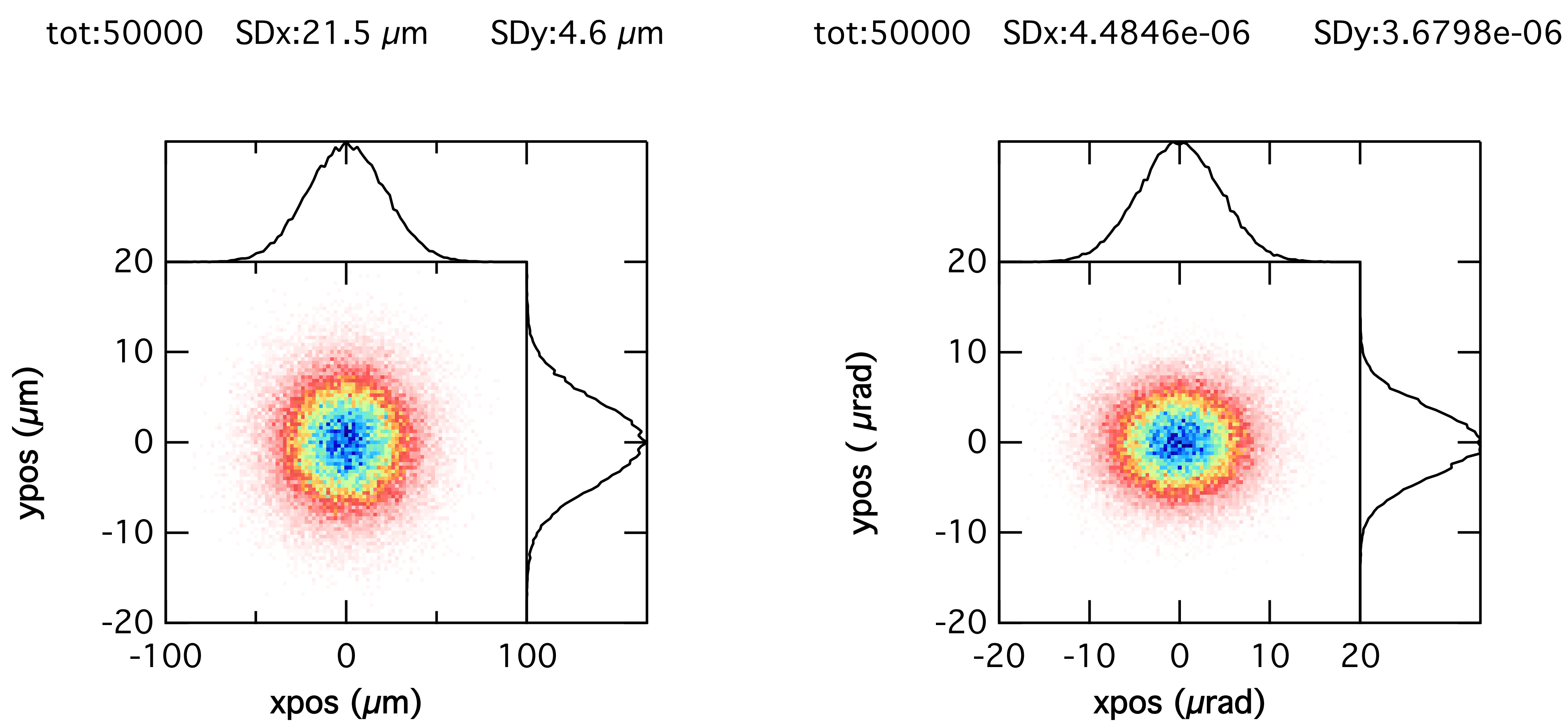


Geometrical Demag: 240

σx = 90 nm, σy = 20 nm

100 mm working distance

Source

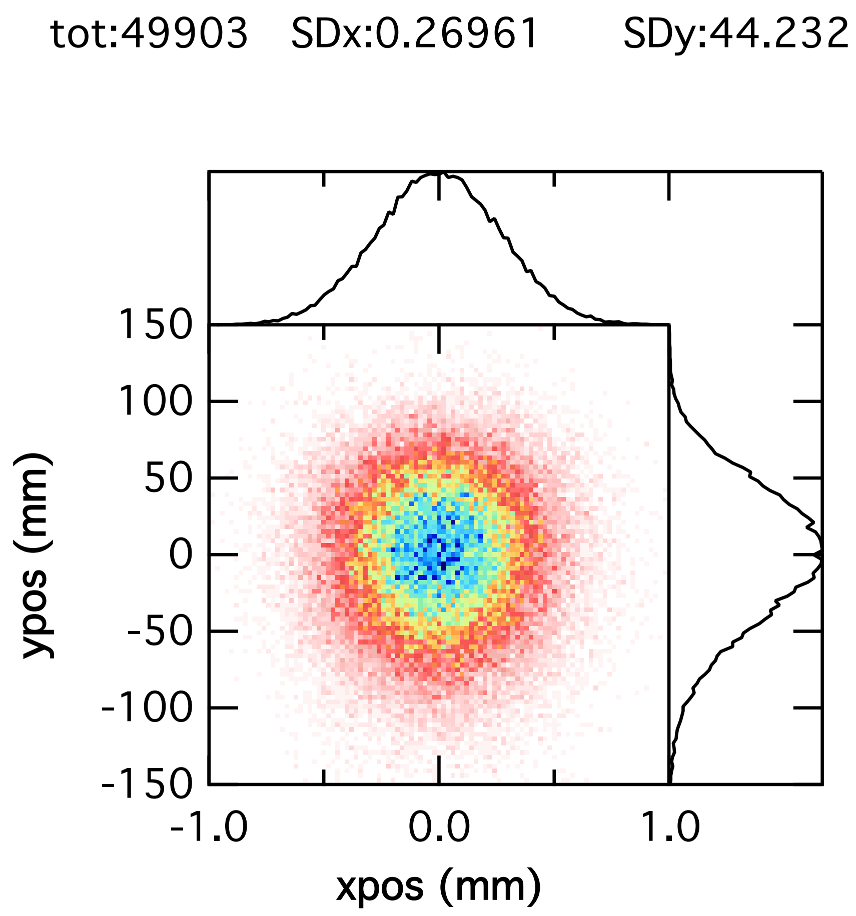


Shadow plots using SRCalc (uses Igor), available

Mirror Illumination

Intensity not included

Only Rays

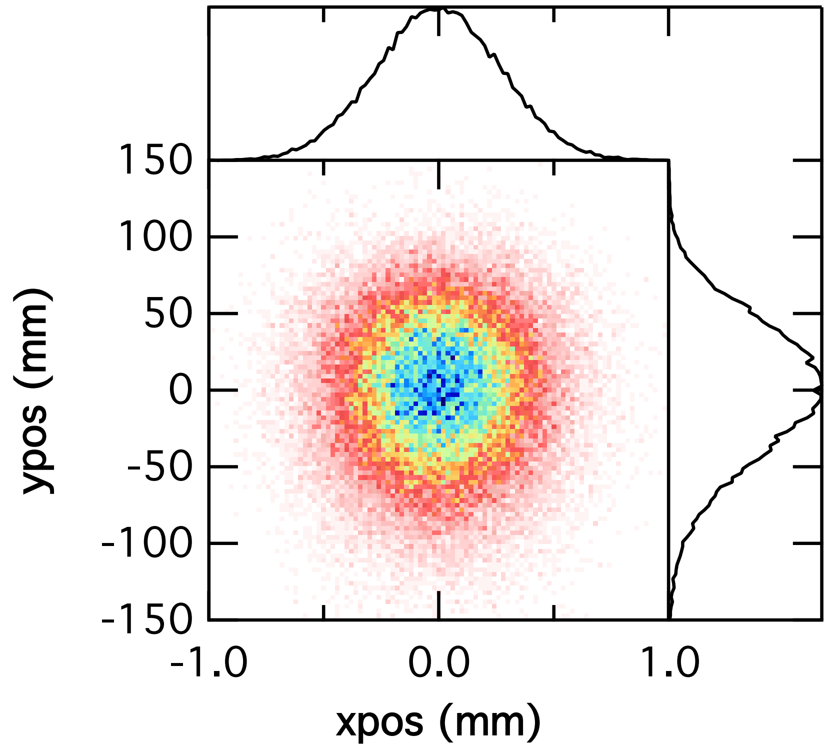


Mirror Illumination

Intensity not included

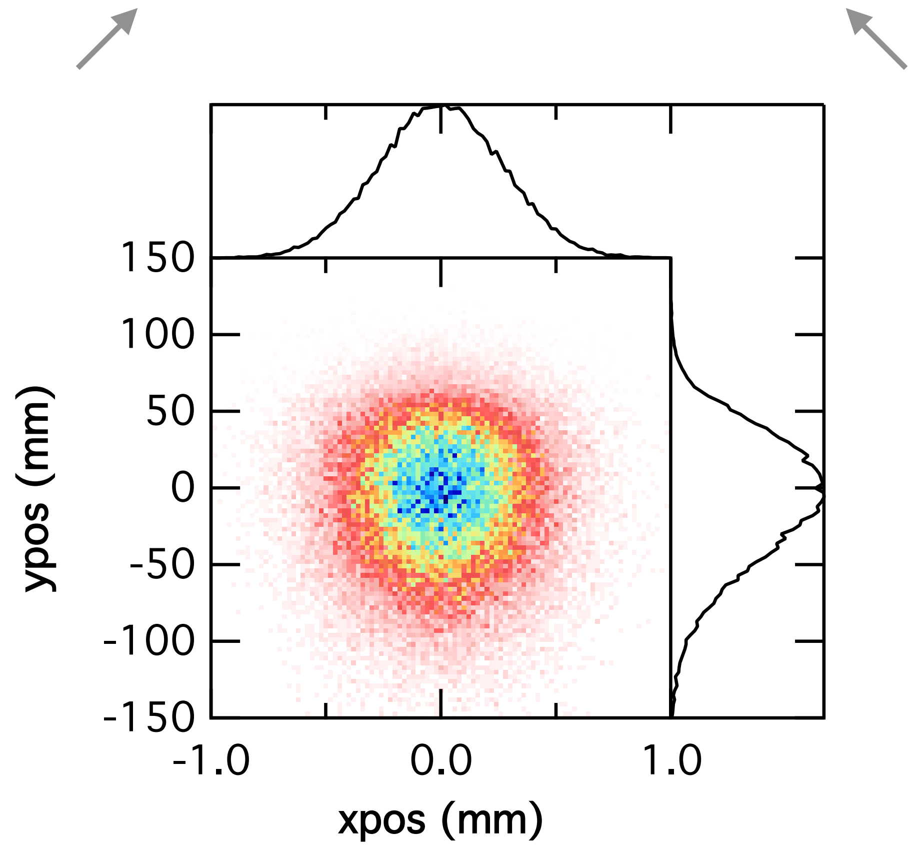
Only Rays

tot:49903 SDx:0.26961 SDy:44.232



Intensity included

tot:39518 SDx:0.26955 SDy:41.358



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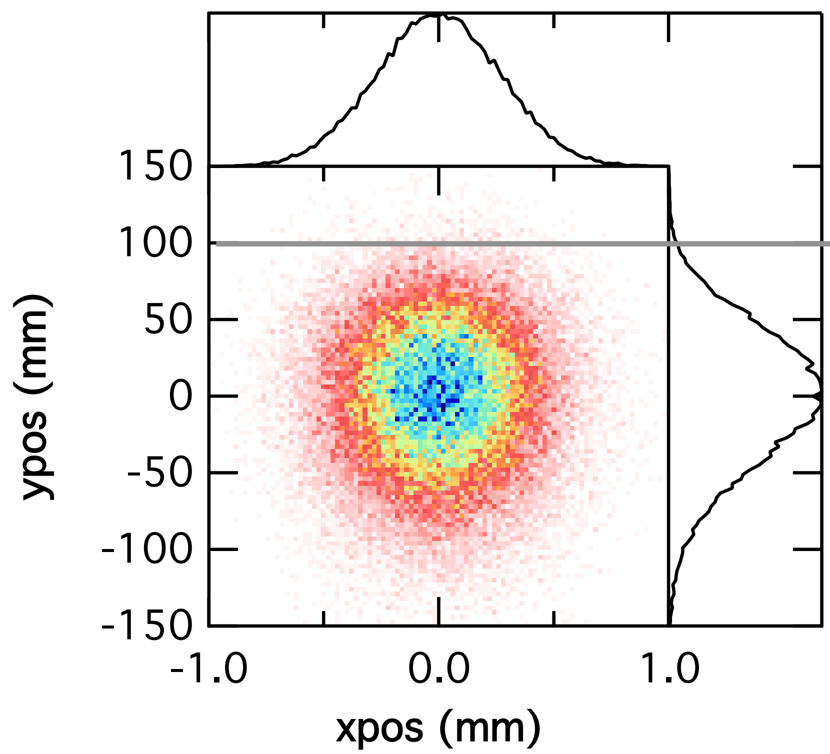

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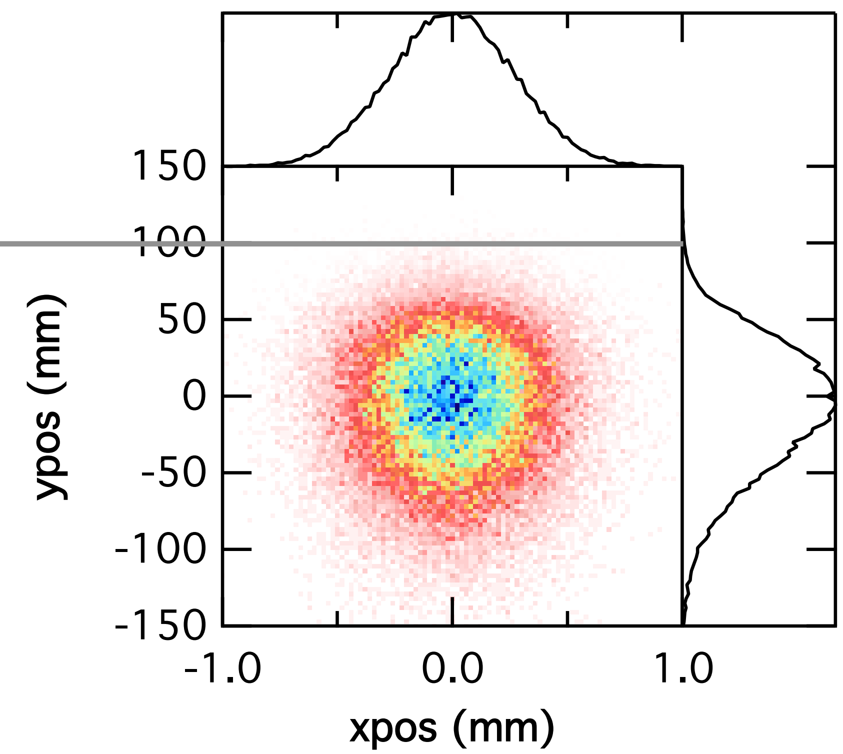
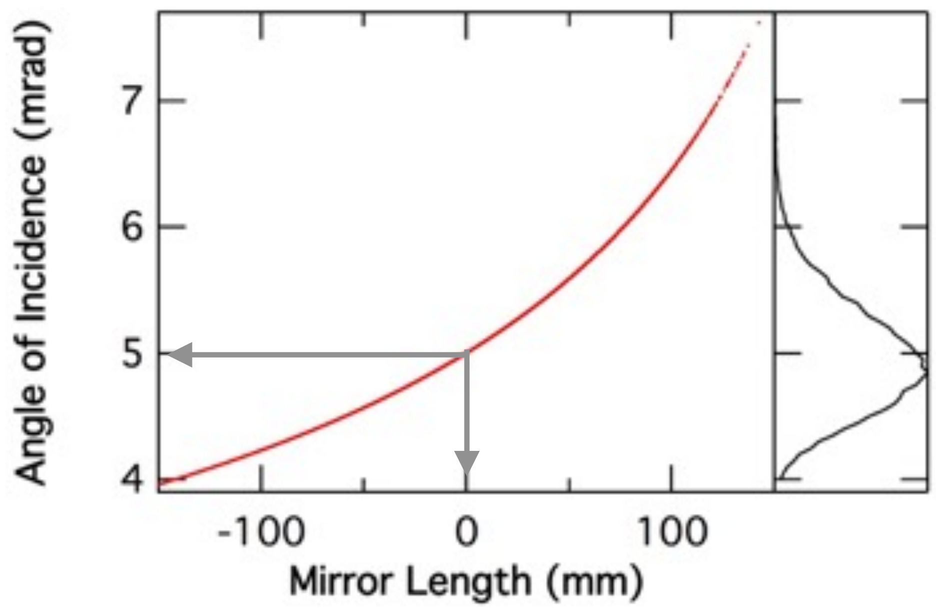
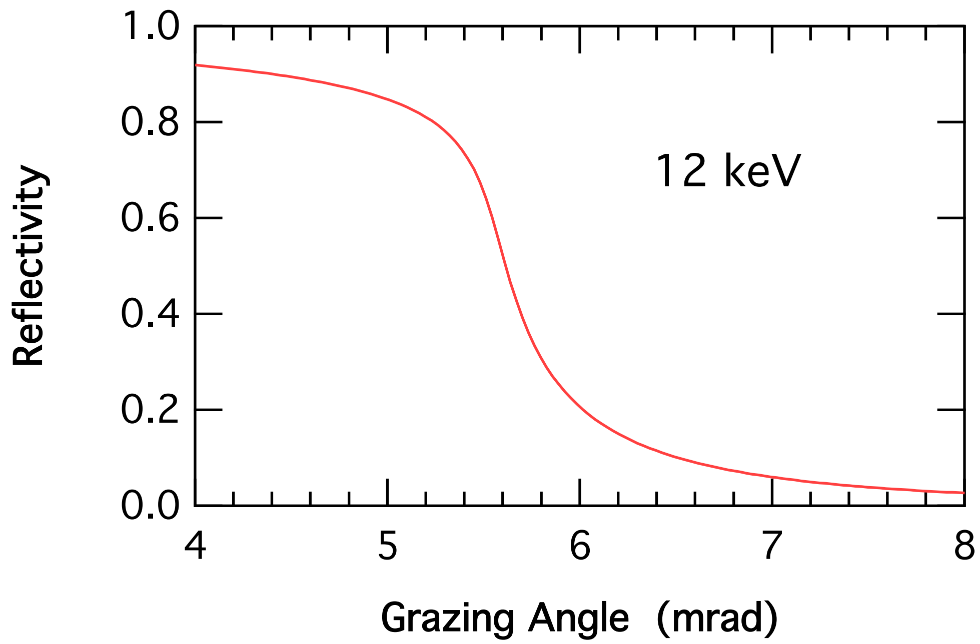


Mirror Illumination Reflectivity





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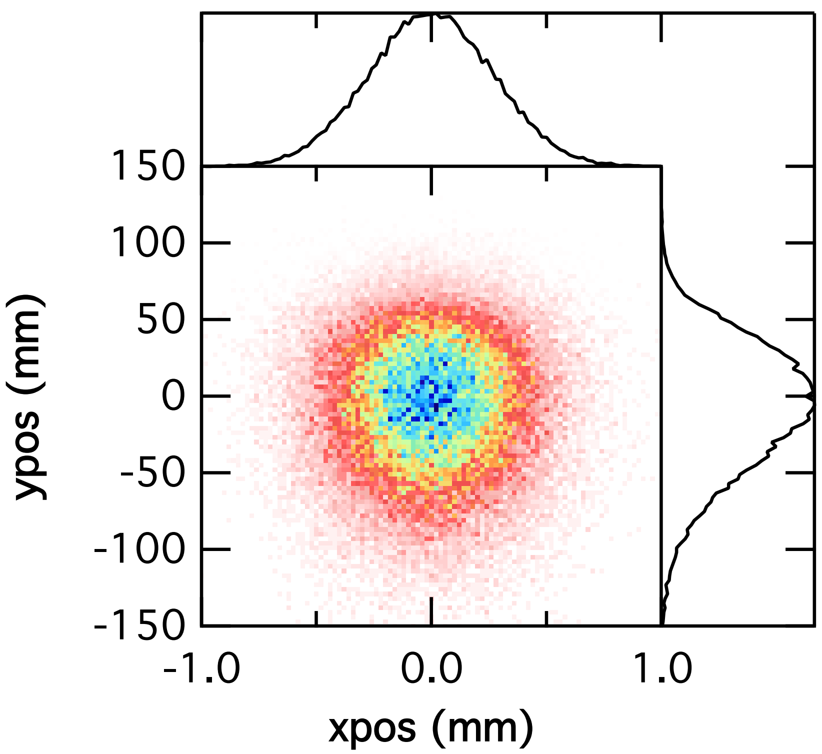


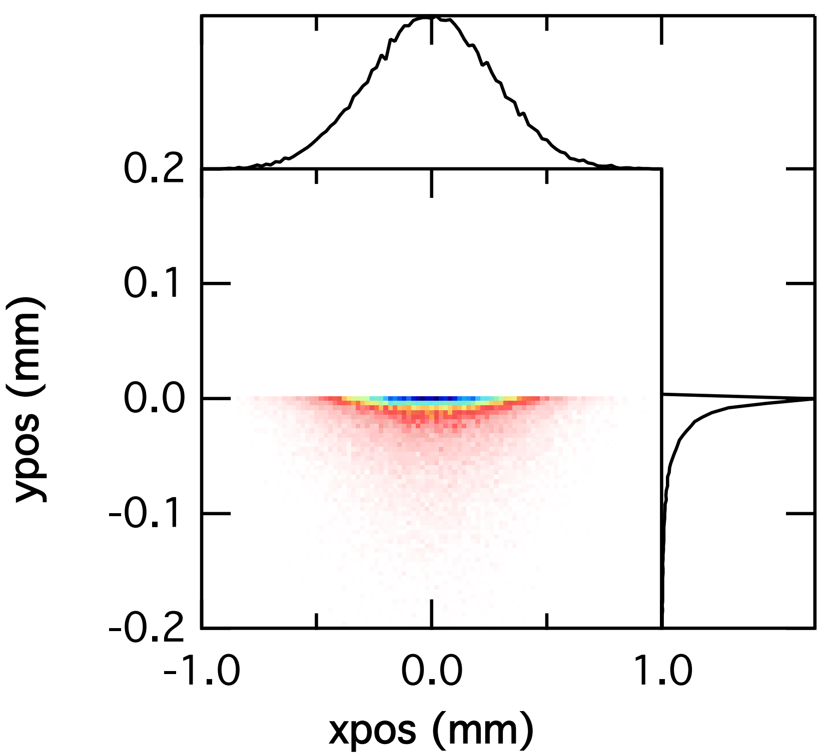
Different mirrors

From geometry

$\sigma x = 90$ nm, $\sigma y = 20$ nm

Spherical

tot:39138 SDx:270 μm SDy:33 μm

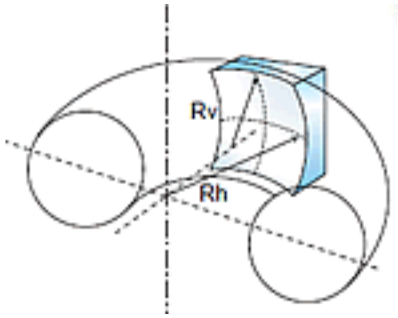


x: Practically no focus
y: Coma

Different mirrors

From geometry

σx = 90 nm, σy = 20 nm



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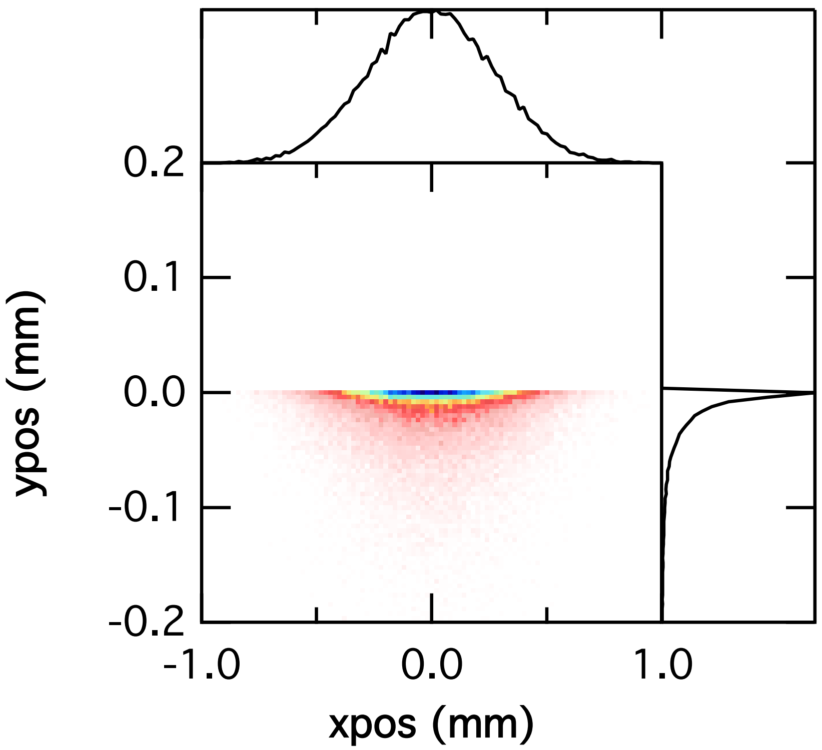
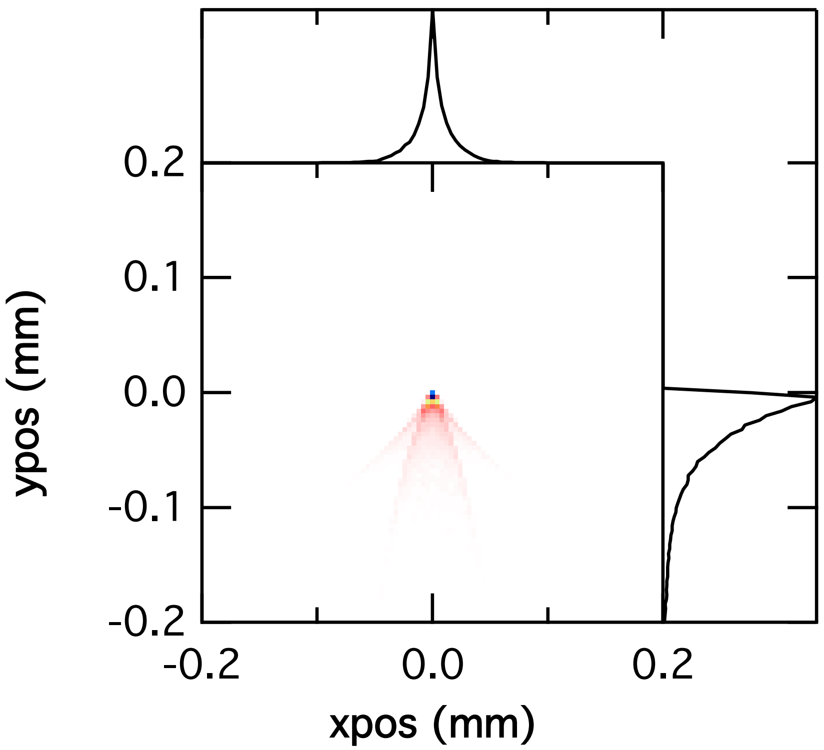
tot:39138   SDx:270 μm   SDy:33 μm



Toroidal
tot:39491   SDx:19 μm   SDy:38 μm



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From geometry

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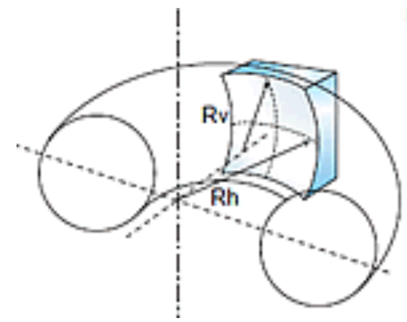
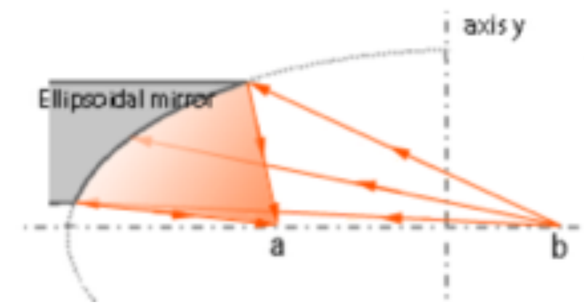
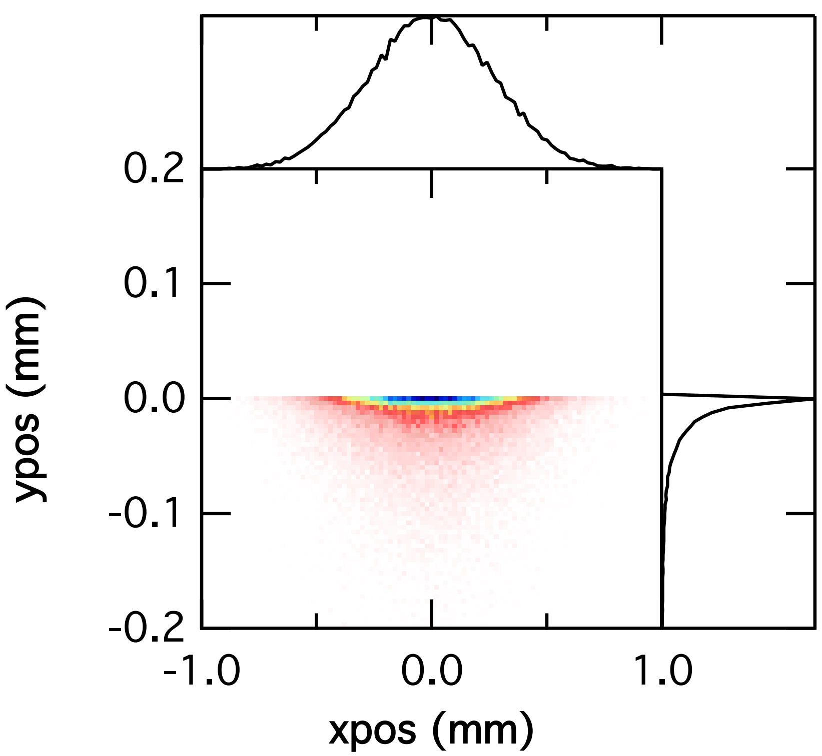
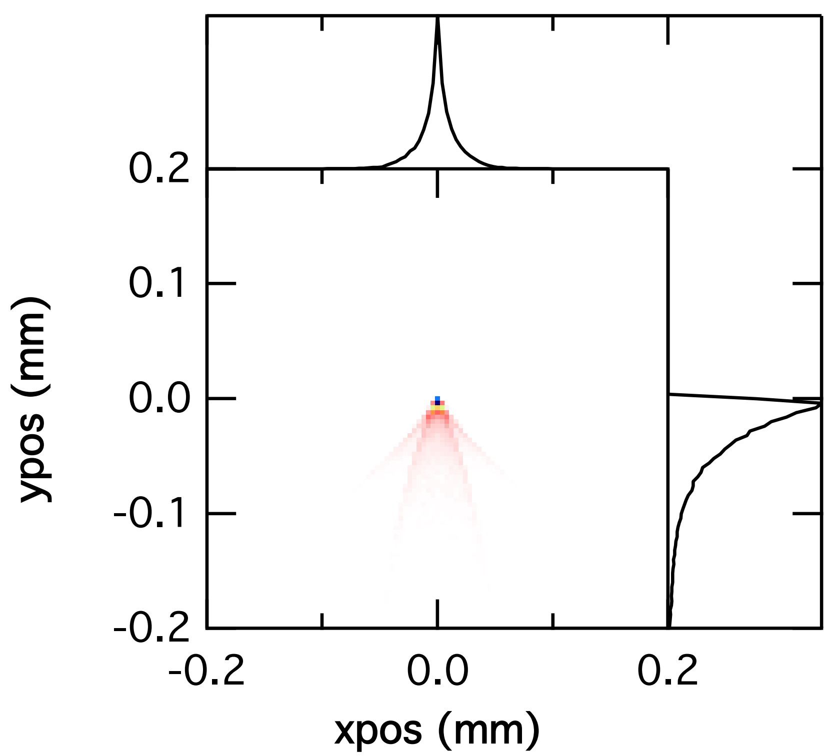




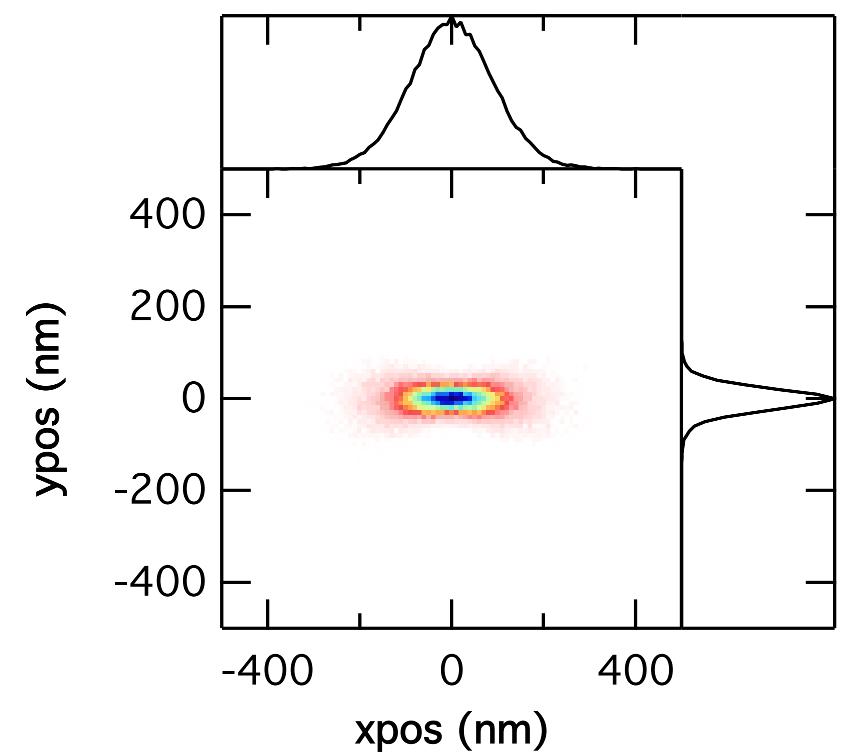
Spherical
tot:39138   SDx:270 μm   SDy:33 μm



Toroidal
tot:39491   SDx:19 μm   SDy:38 μm



Ellipsoidal
tot:38876   SDx:93 nm   SDy:28 nm

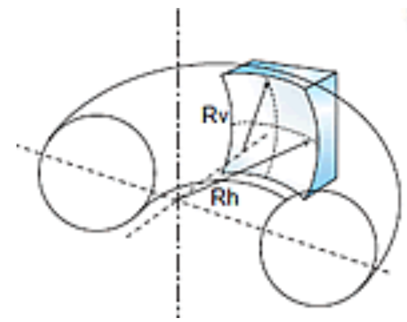


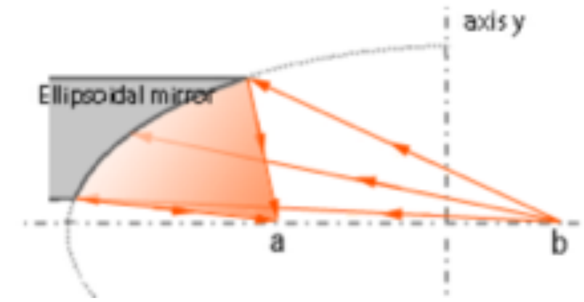
x: Practically no focus
y: Coma

Different mirrors

From geometry

σx = 90 nm, σy = 20 nm





Spherical
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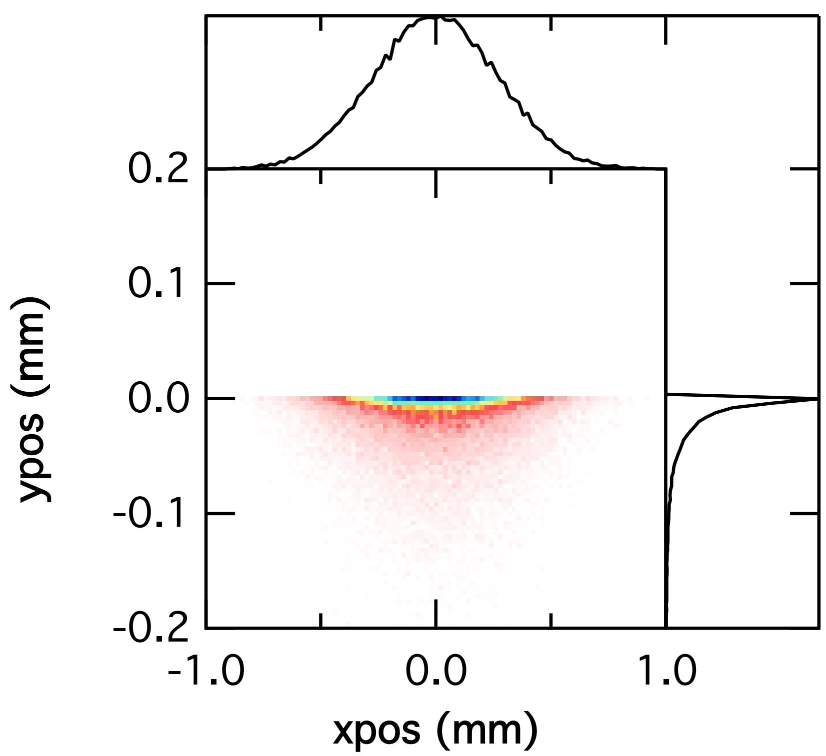
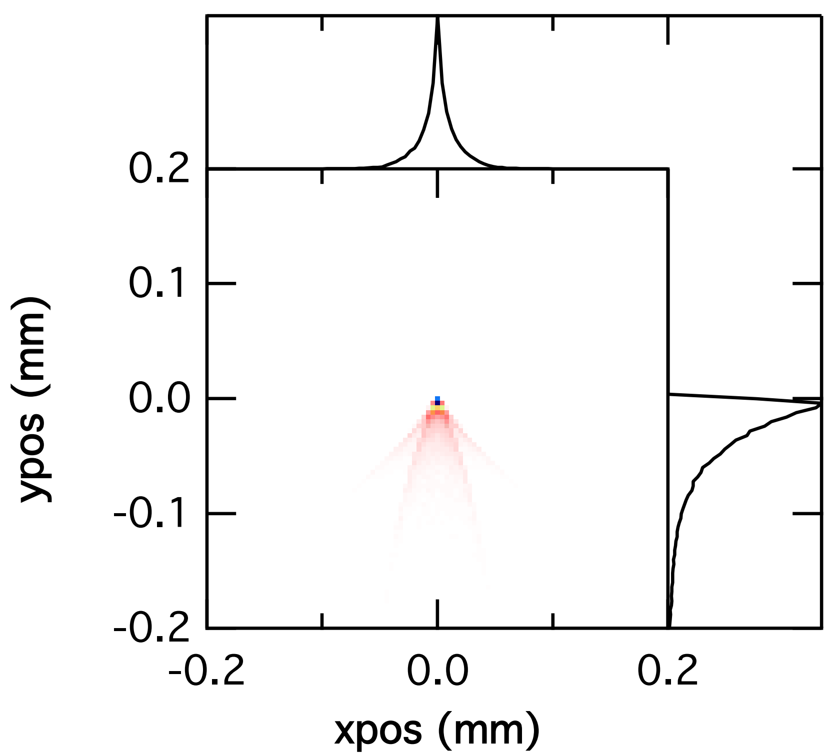
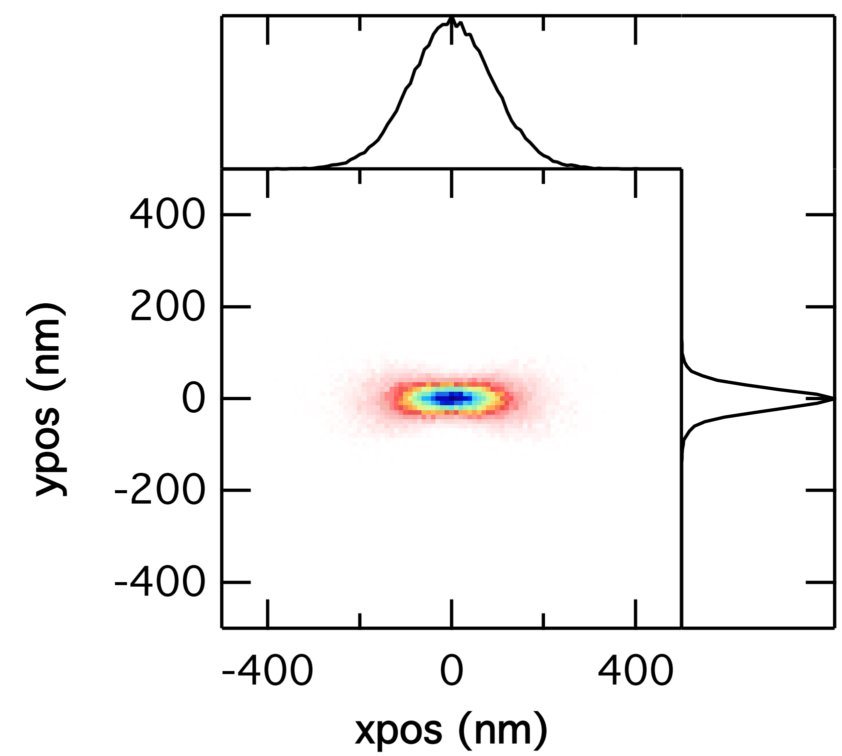


Toroidal
tot:39491 SDx:19 μm SDy:38 μm



Ellipsoidal
tot:38876 SDx:93 nm SDy:28 nm



x: Practically no focus
y: Coma

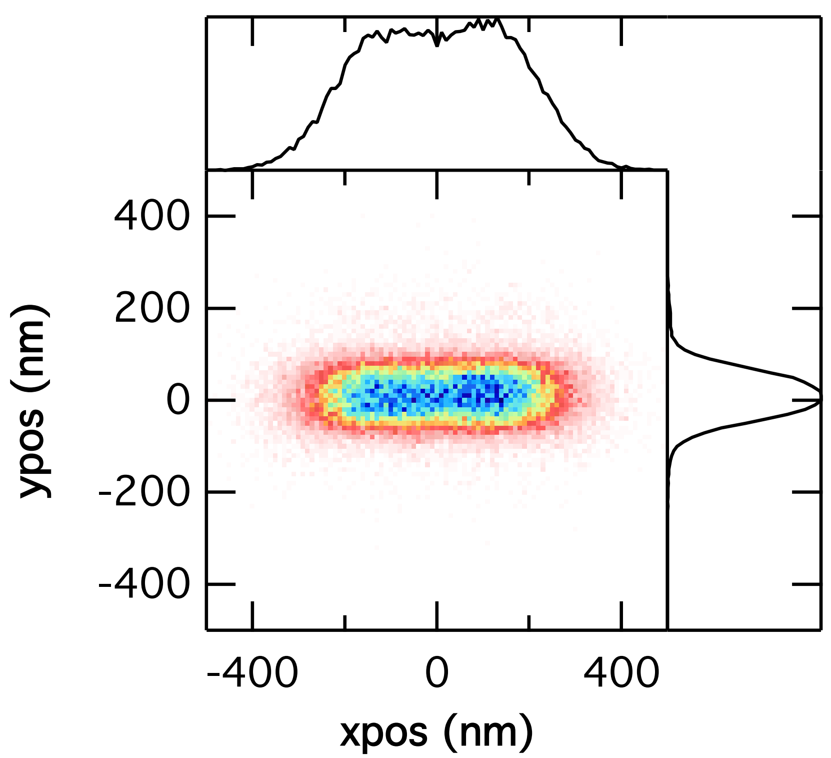
Not quite!

Figure errors and/or Diffraction

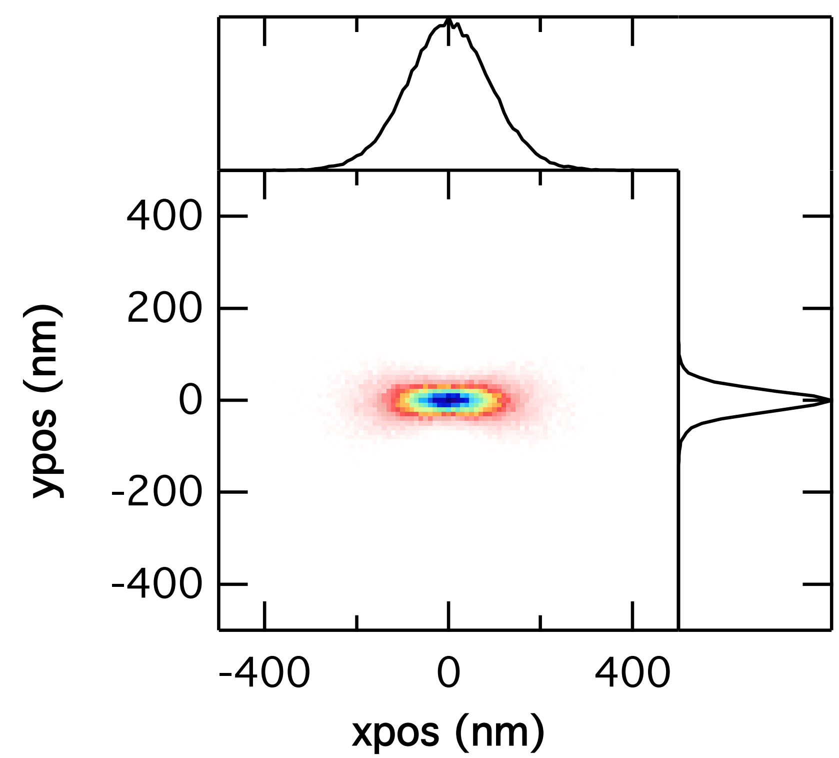
From geometry

σx = 90 nm, σy = 20 nm

Ellipsoidal state of the art FE ~ 2 nm RMS
tot:38790   SDx160 nm   SDy:52 nm

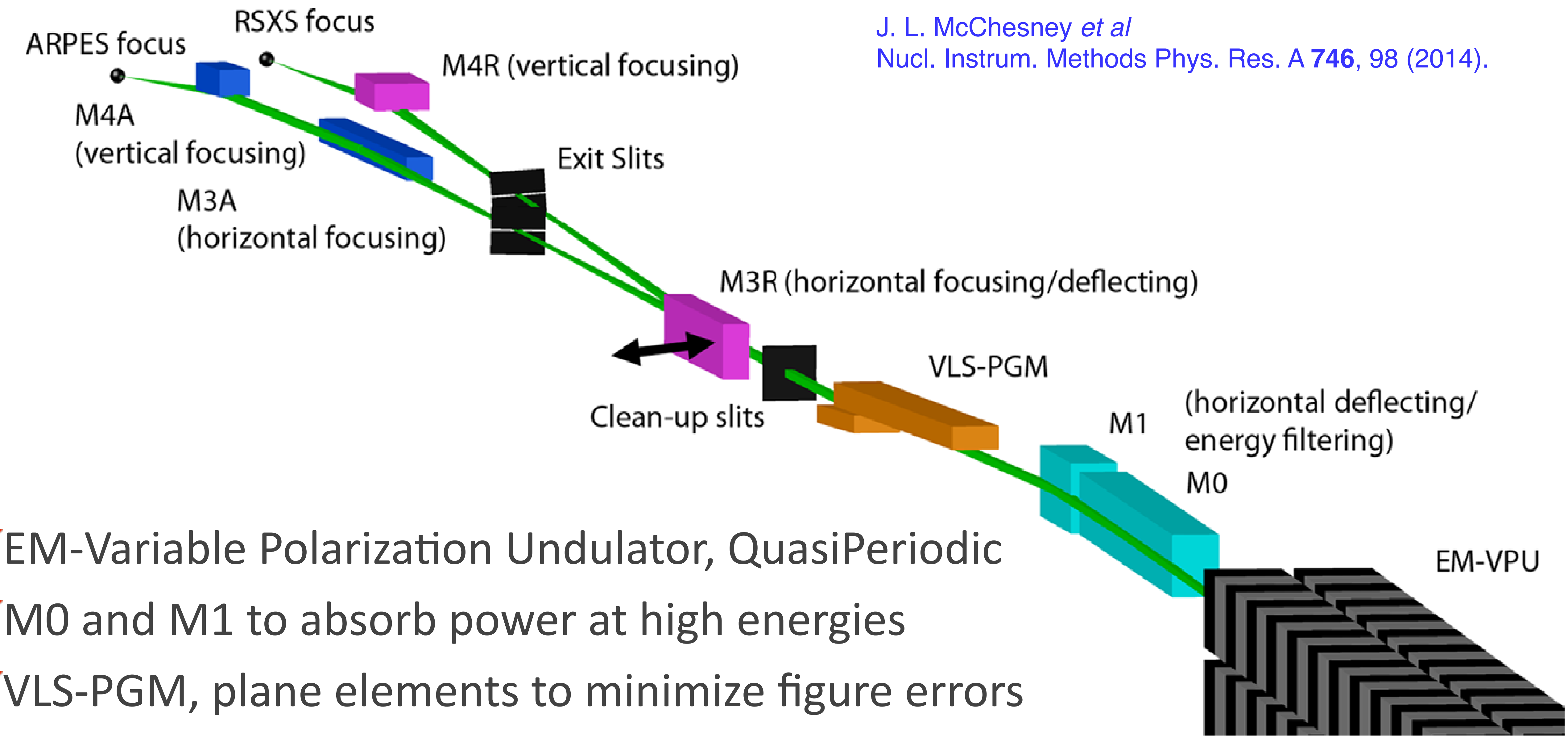


Ellipsoidal
tot:38876   SDx:93 nm   SDy:28 nm



State of the Art XUV beamline: IEX @ APS

J. L. McChesney *et al*
Nucl. Instrum. Methods Phys. Res. A **746**, 98 (2014).

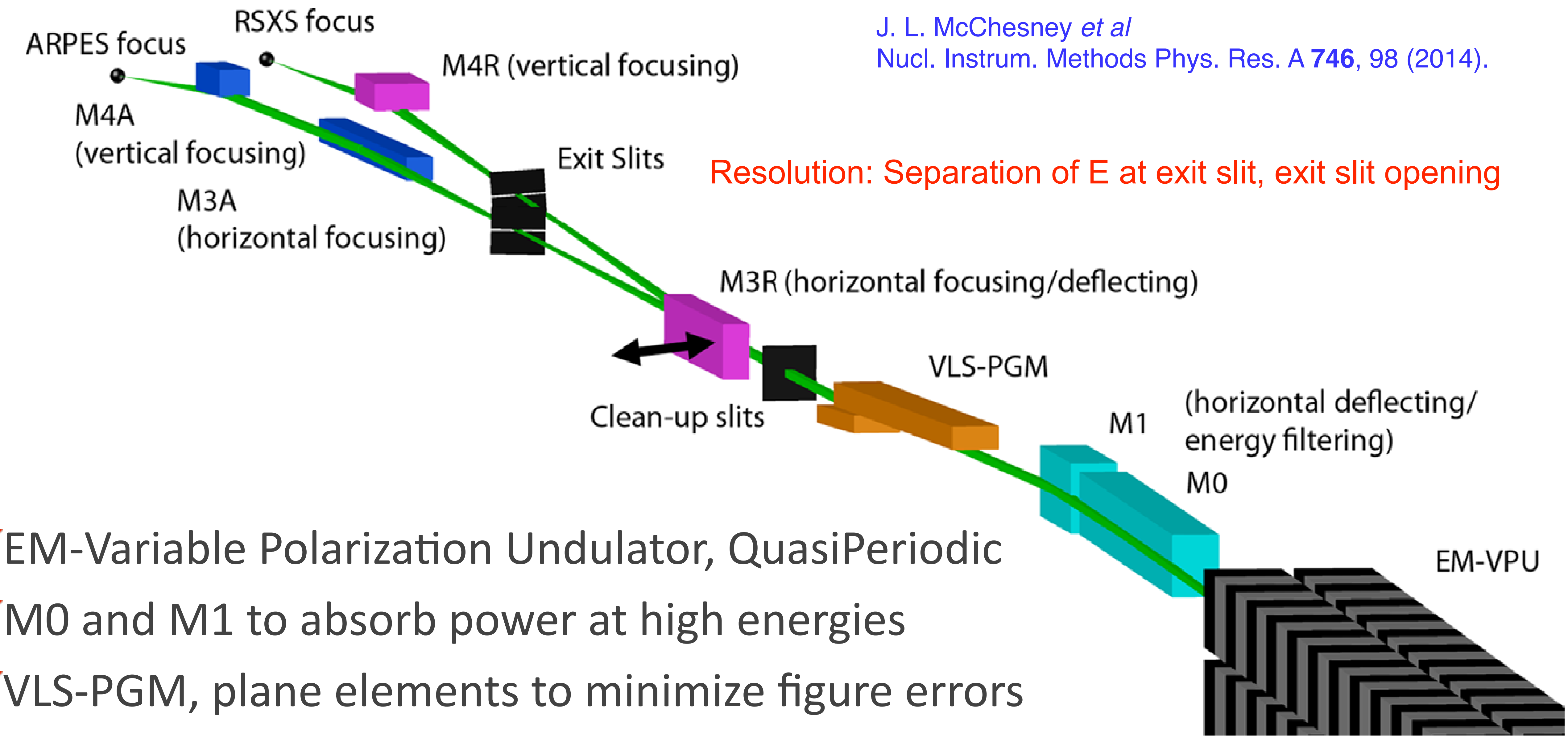


- ☑ EM-Variable Polarization Undulator, QuasiPeriodic
- ☑ M0 and M1 to absorb power at high energies
- ☑ VLS-PGM, plane elements to minimize figure errors
- ☑ Two branches
  - ☑ ARPES: High resolution, small spot
  - ☑ RSXS: High flux, low divergence
- ☑ 250 - 2200 eV

State of the Art XUV beamline: IEX @ APS

J. L. McChesney *et al*
Nucl. Instrum. Methods Phys. Res. A **746**, 98 (2014).

Resolution: Separation of E at exit slit, exit slit opening



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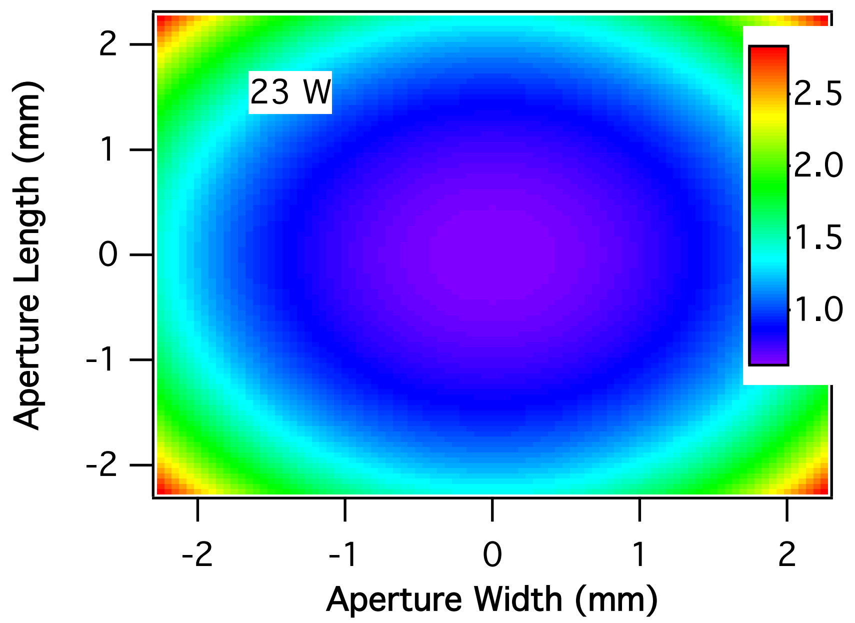
- ☑ Two branches
  - ☑ ARPES: High resolution, small spot
  - ☑ RSXS: High flux, low divergence
- ☑ 250 - 2200 eV

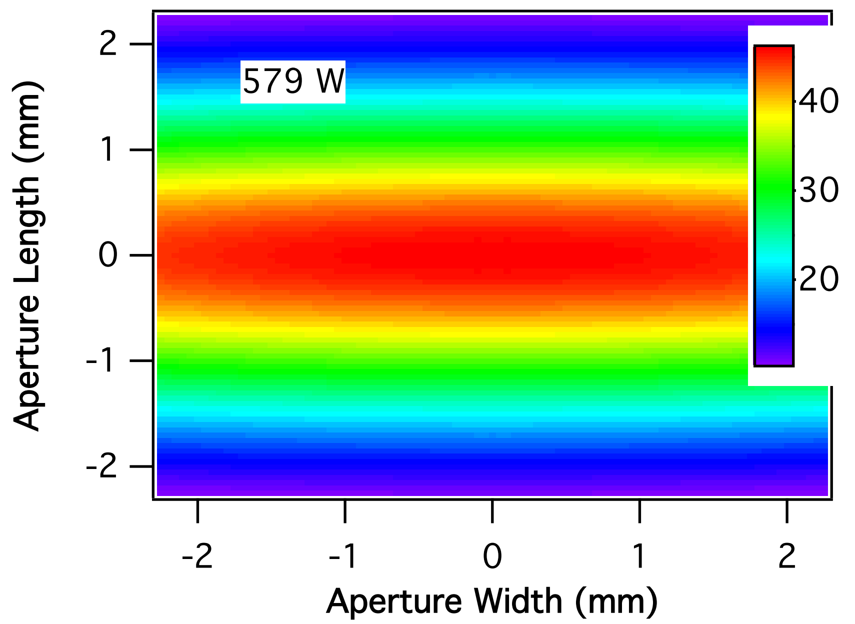
Power Density: SRCalc (Urgent)

Circular:
k_x=2.8
k_y=2.8



Source:
7 GeV
0.1 A
ID: EM, QP
38 periods
0.125 m
410 eV

Linear:
k_x=0
k_y=4.0



$$\epsilon\ (\mathrm{keV}) = 0.95\ \frac{E^2\ (\mathrm{GeV})}{1 + \left(k_x^2 + k_y^2\right) / 2}\ \frac{1}{\lambda_u\ (\mathrm{cm})}$$

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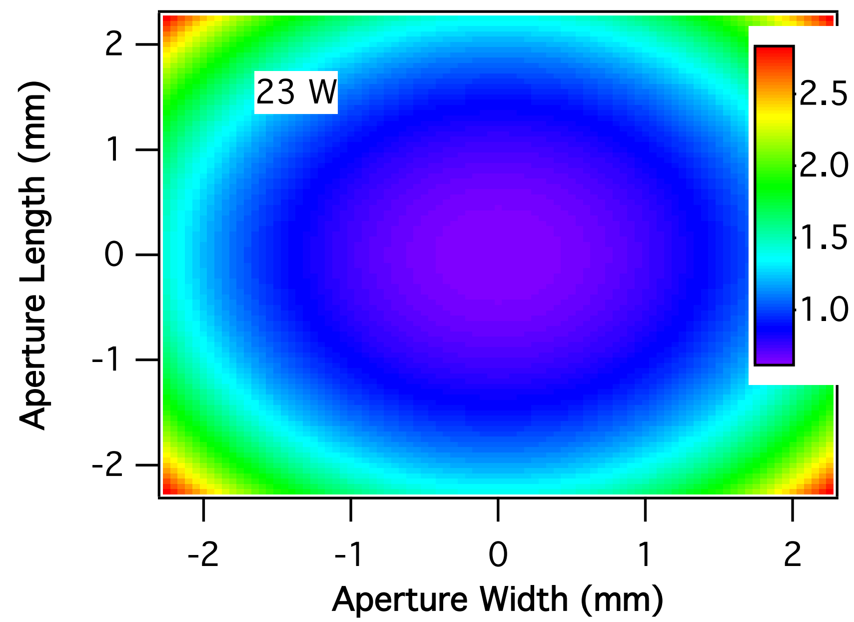
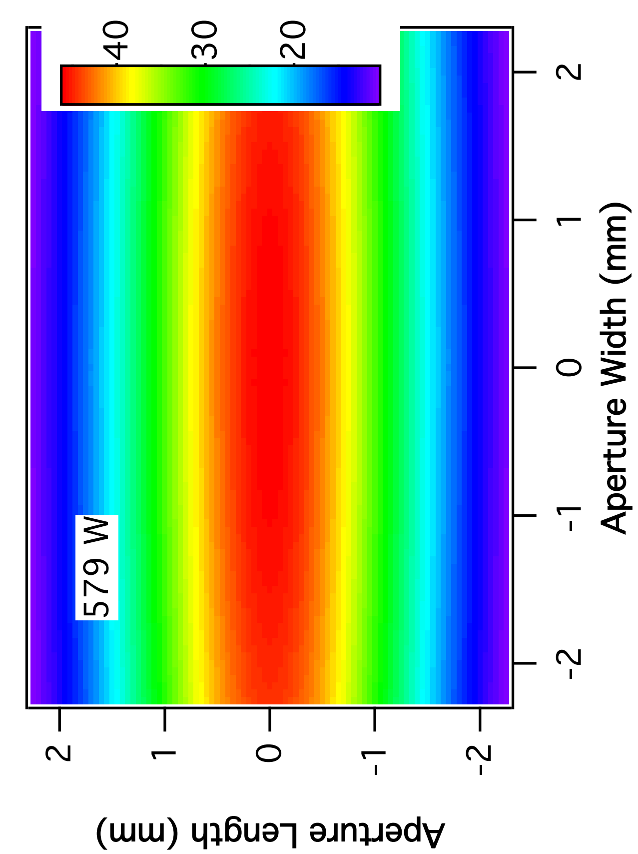


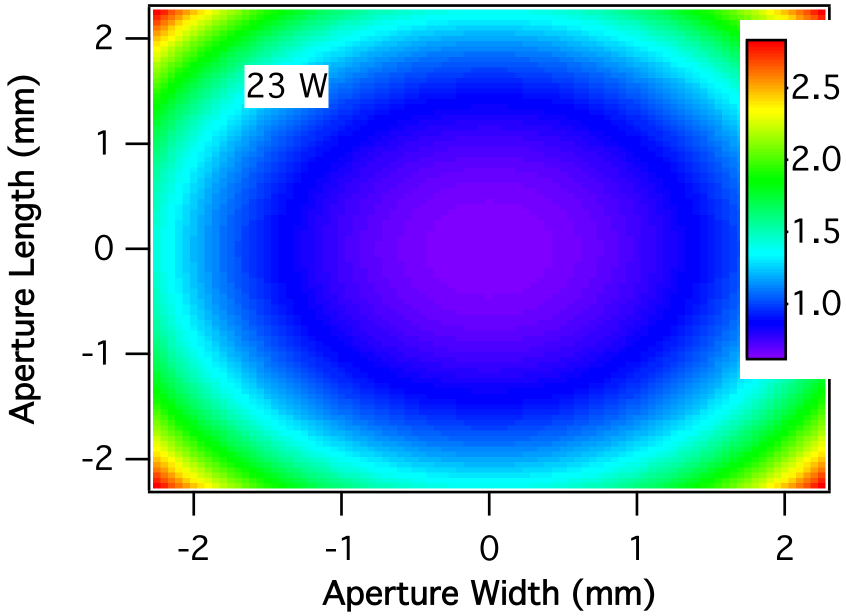
Linear:
k_x=4.0
k_y=0

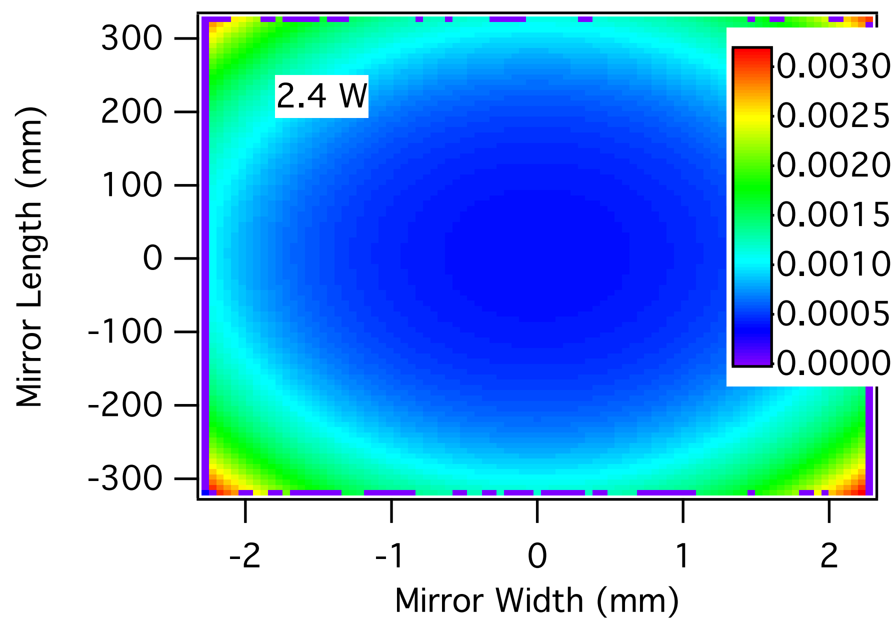


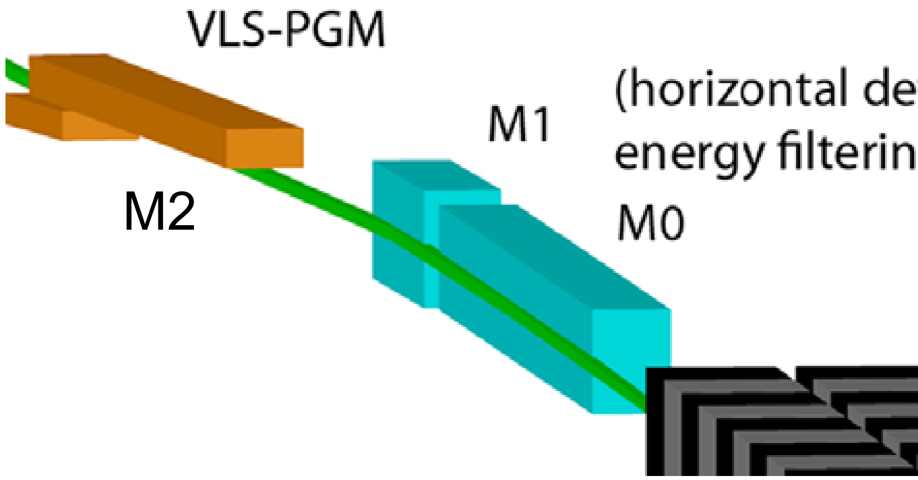
$$\epsilon\ (\mathrm{keV}) = 0.95\ \frac{E^2\ (\mathrm{GeV})}{1 + \left(k_x^2 + k_y^2\right) / 2}\ \frac{1}{\lambda_u\ (\mathrm{cm})}$$

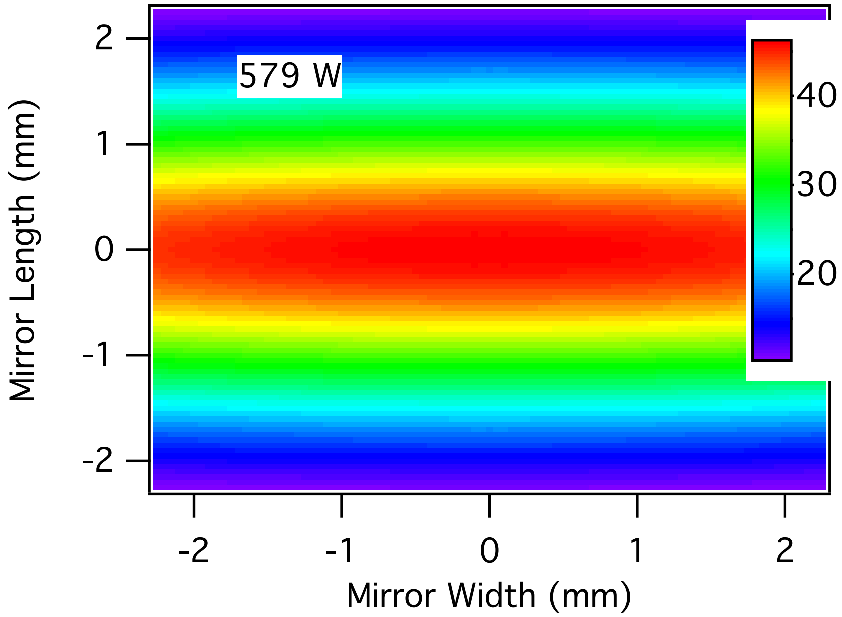
Power Density: SRCalc (Urgent)

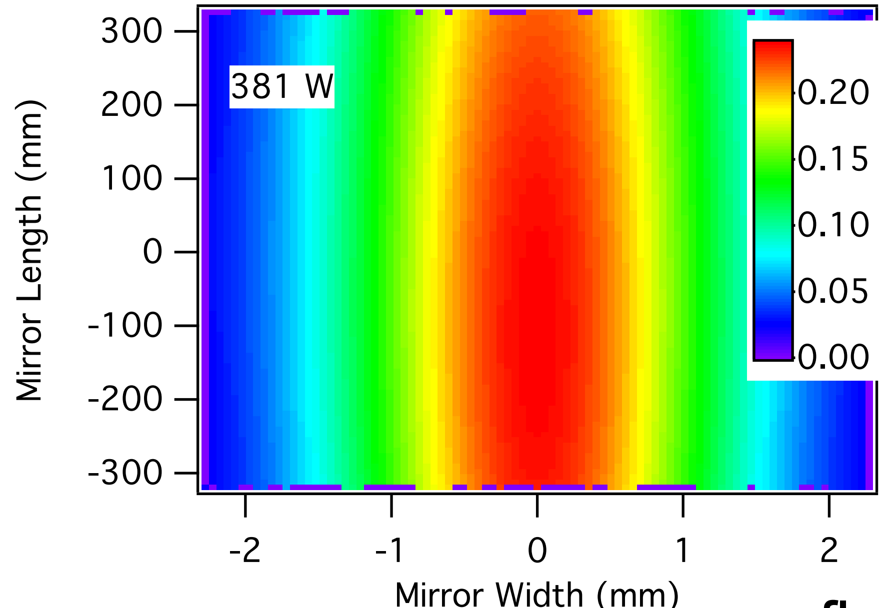
M0: Au Coating







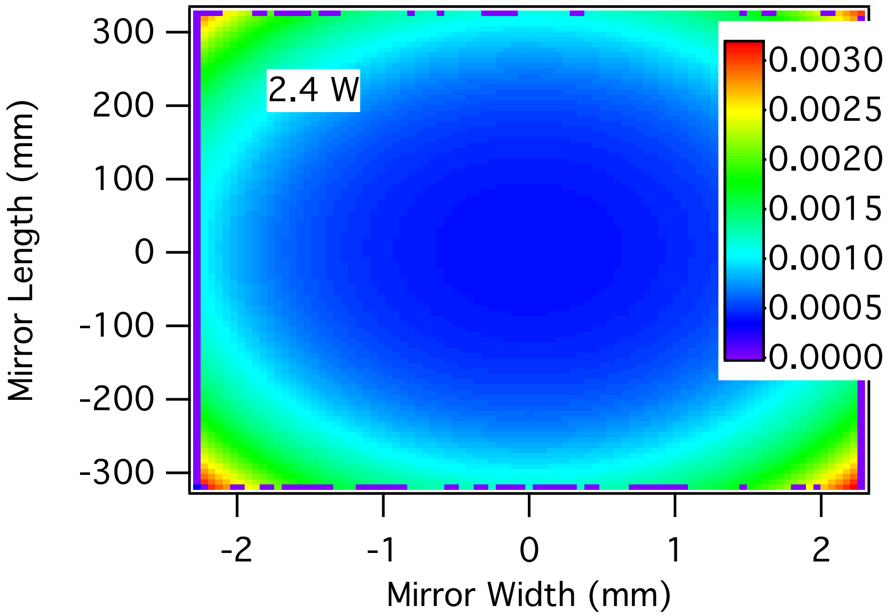


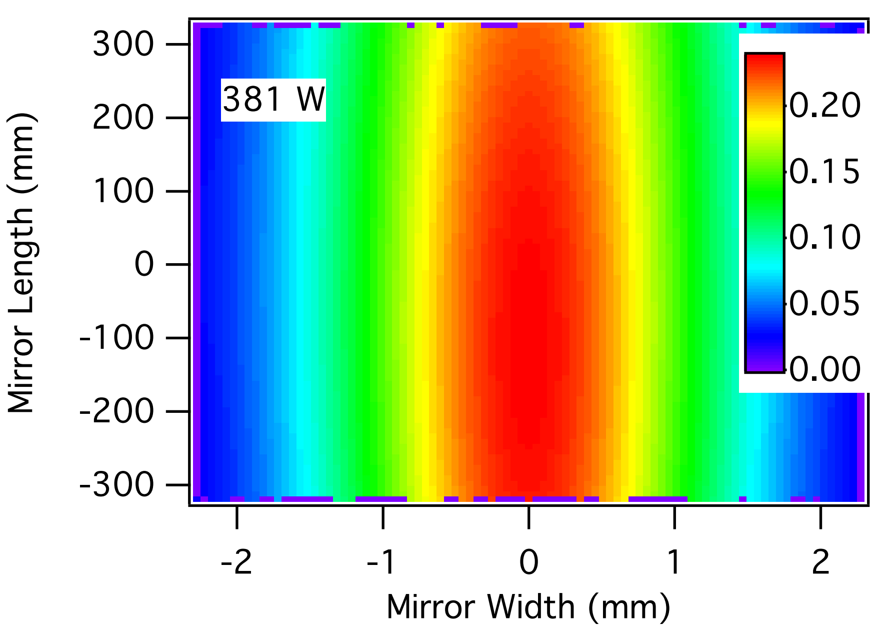


p reflec

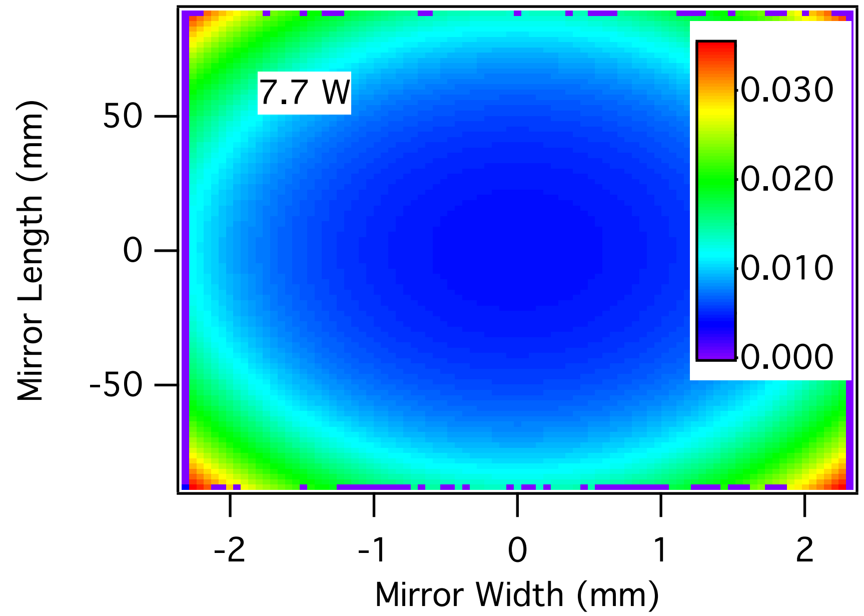
Power Density: SRCalc (Urgent)

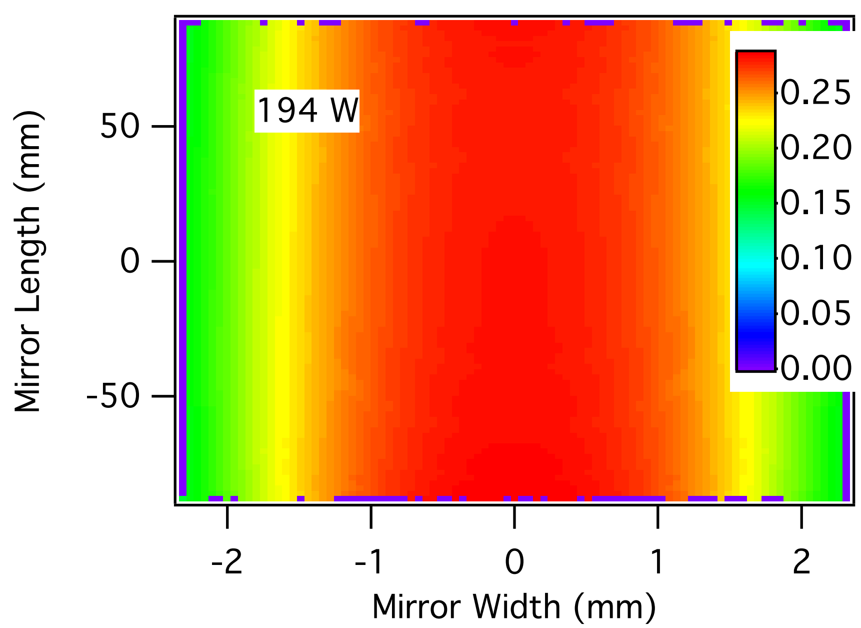
M0: Au Coating



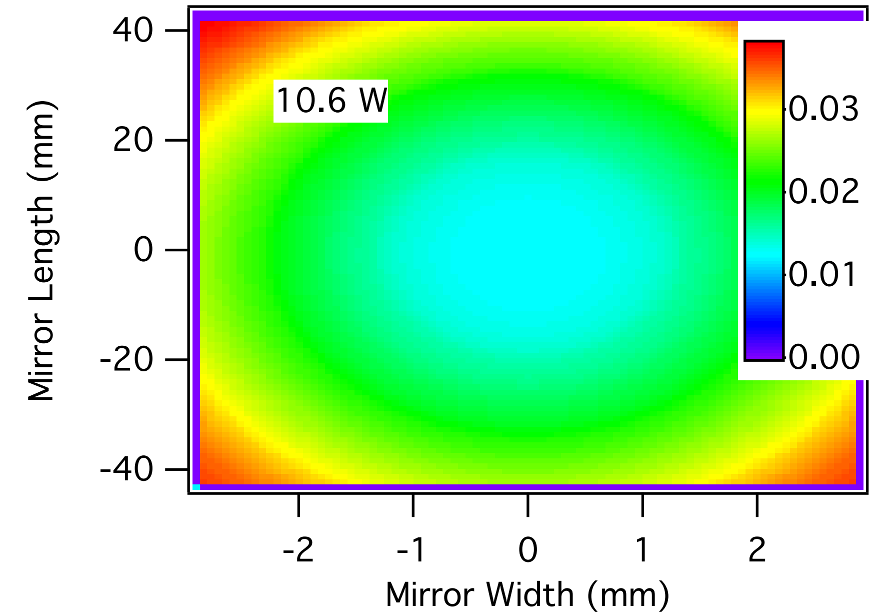


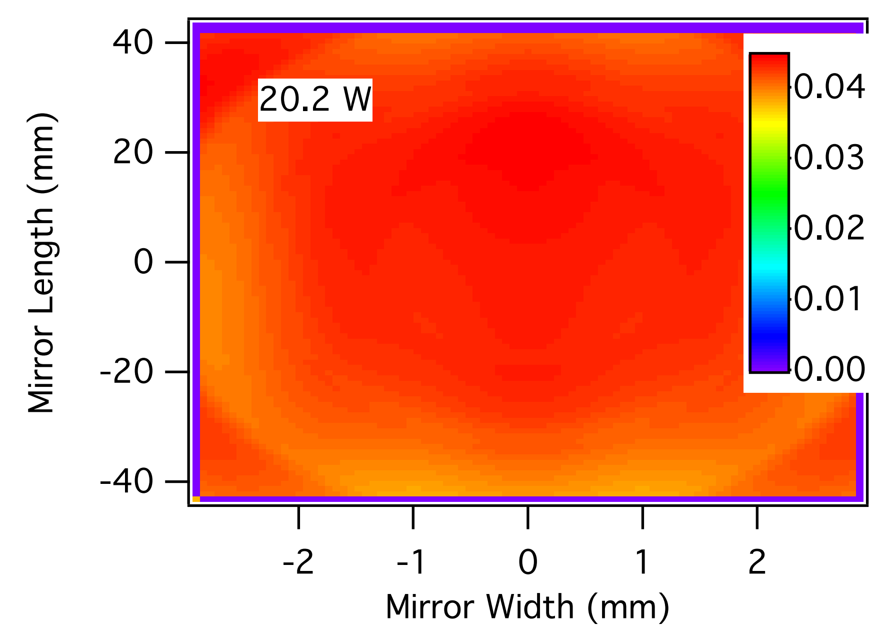
M1: Au Coating





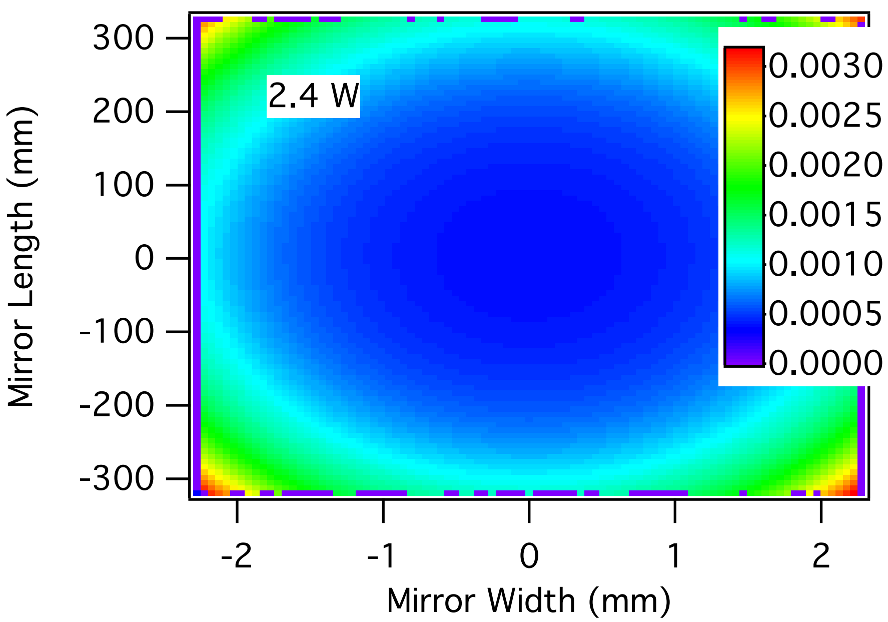
M2: Au Coating

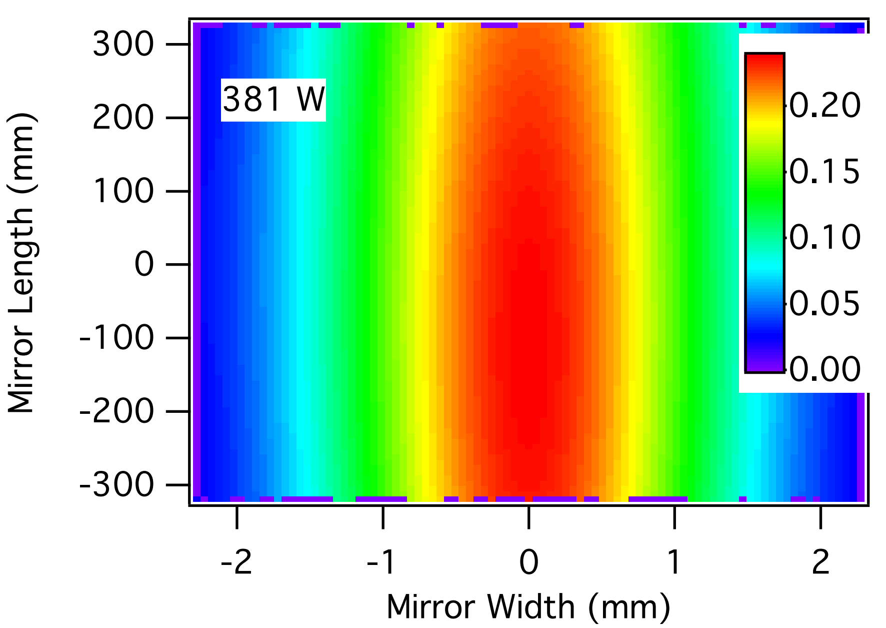




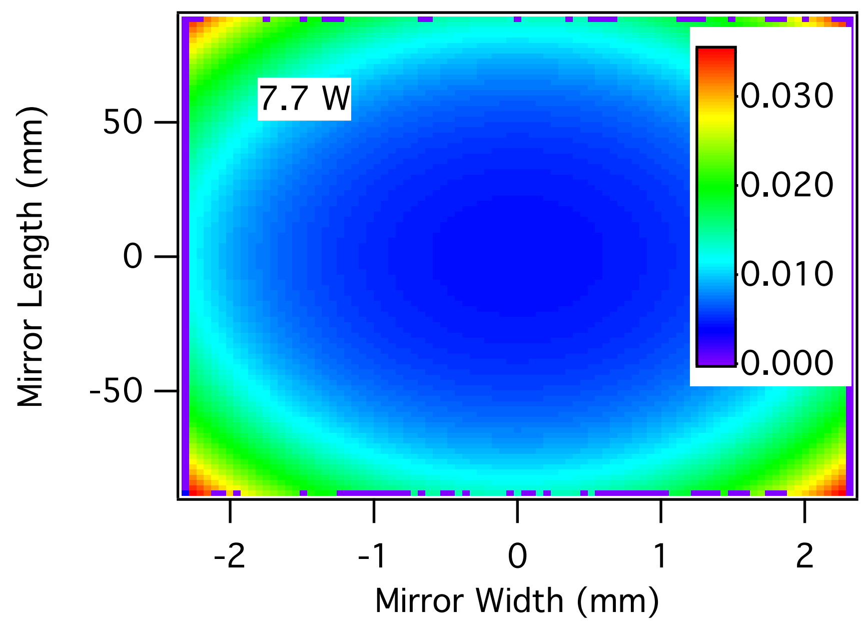
Power Density: SRCalc (Urgent)

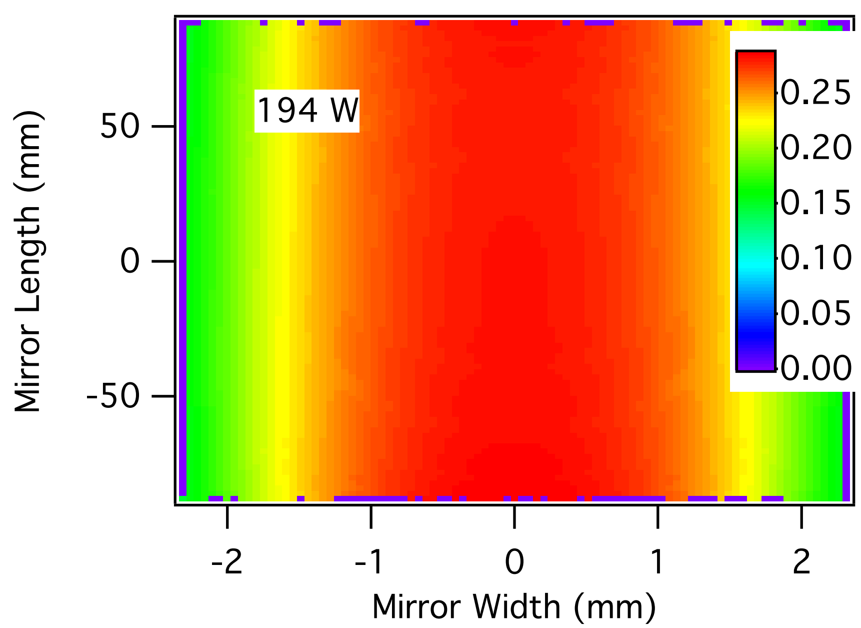
M0: Au Coating



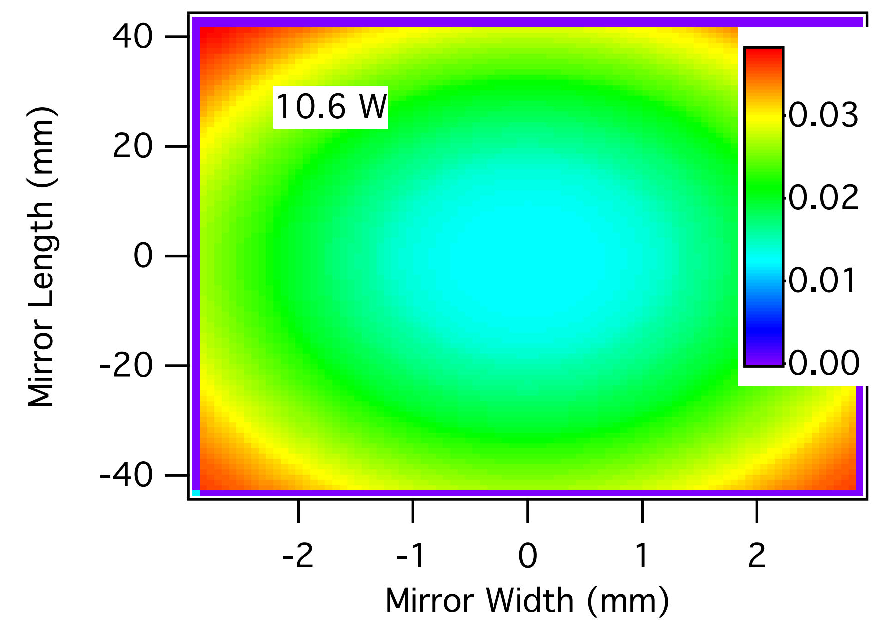


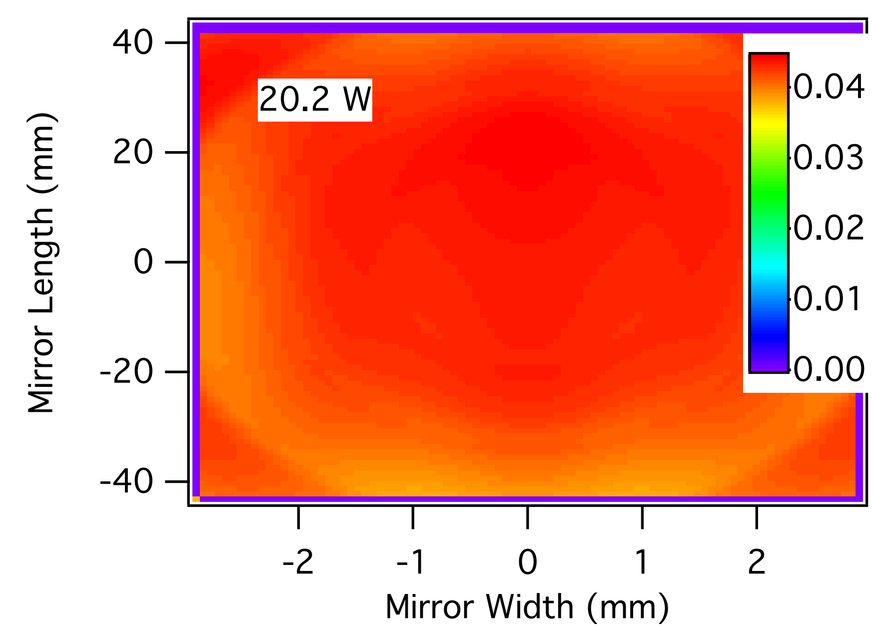
M1: Au Coating



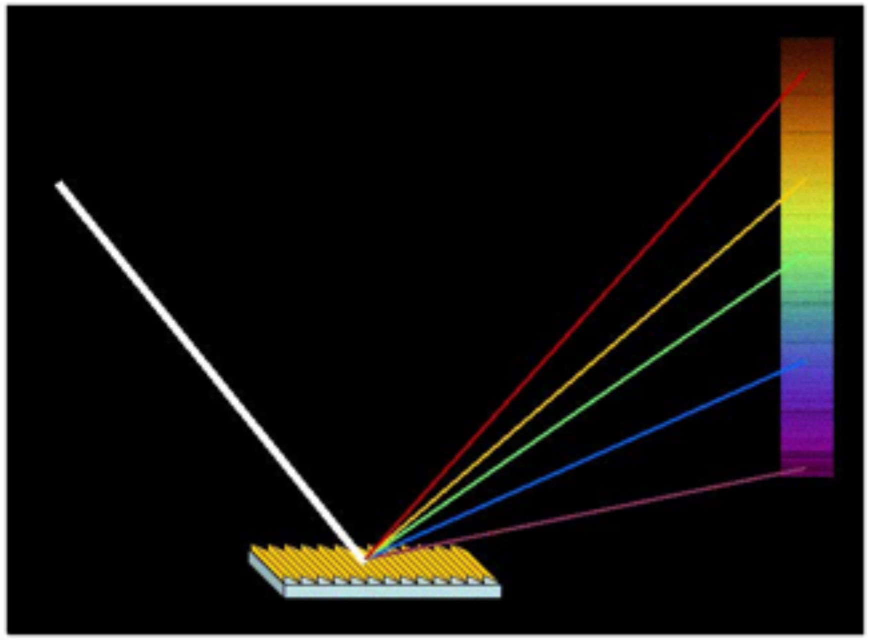


M2: Au Coating
M2: Resolution

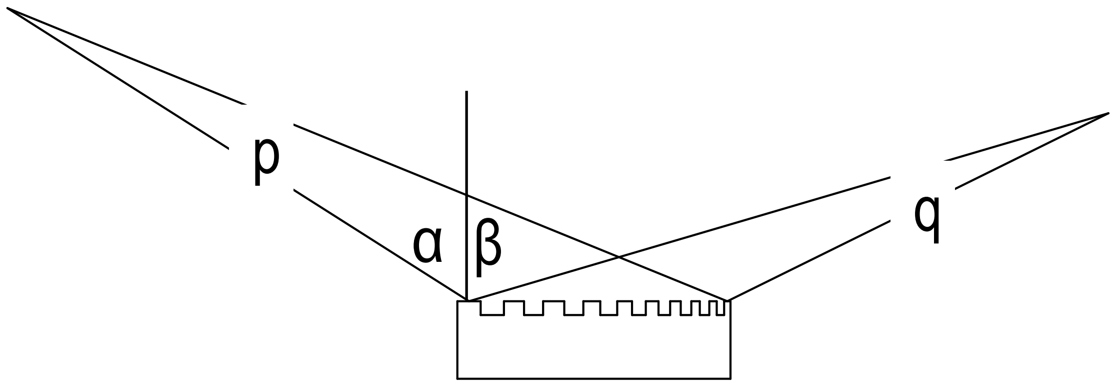




VLS Grating



$$n\,k\,\lambda = \mathrm{Sin}[\alpha] + \mathrm{Sin}[\beta]$$

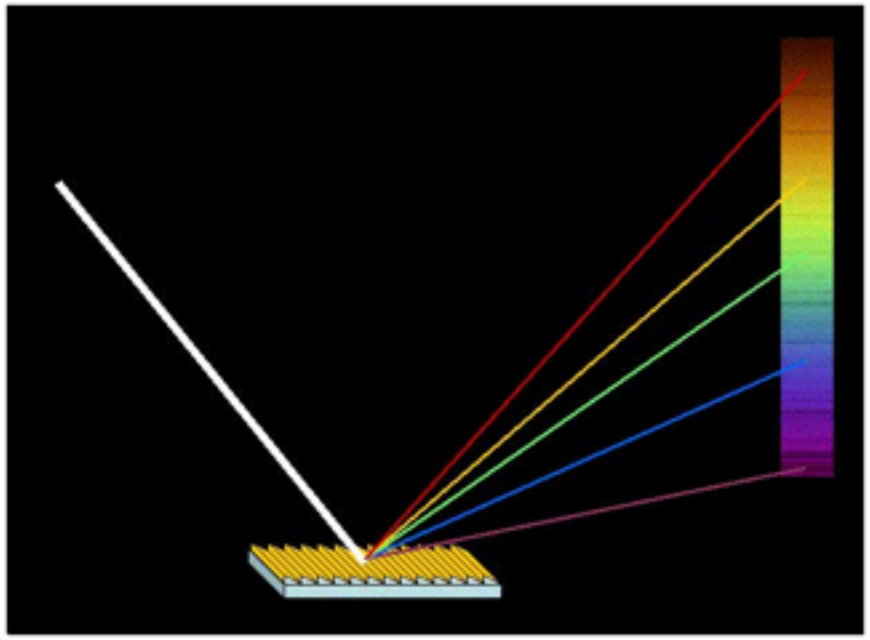


$$k = k0\left(1 + 2\,b2\,w + 3\,b3\,w^2 + \ldots\right)$$

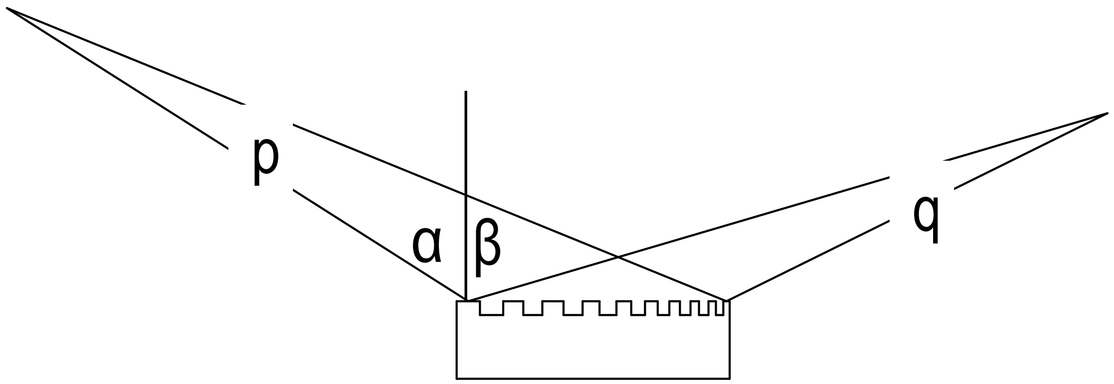
$$f20 = \frac{\mathrm{Cos}[\alpha]^2}{p} + \frac{\mathrm{Cos}[\beta]^2}{q} + 2\,b2\,m\,k0\,\lambda;$$

$$f30 = \mathrm{Sin}[\alpha]\frac{\mathrm{Cos}[\alpha]^2}{p^2} + \mathrm{Sin}[\beta]\frac{\mathrm{Cos}[\beta]^2}{q^2} + 2\,b3\,m\,k0\,\lambda$$

VLS Grating



$$n\,k\,\lambda = \mathrm{Sin}[\alpha] + \mathrm{Sin}[\beta]$$



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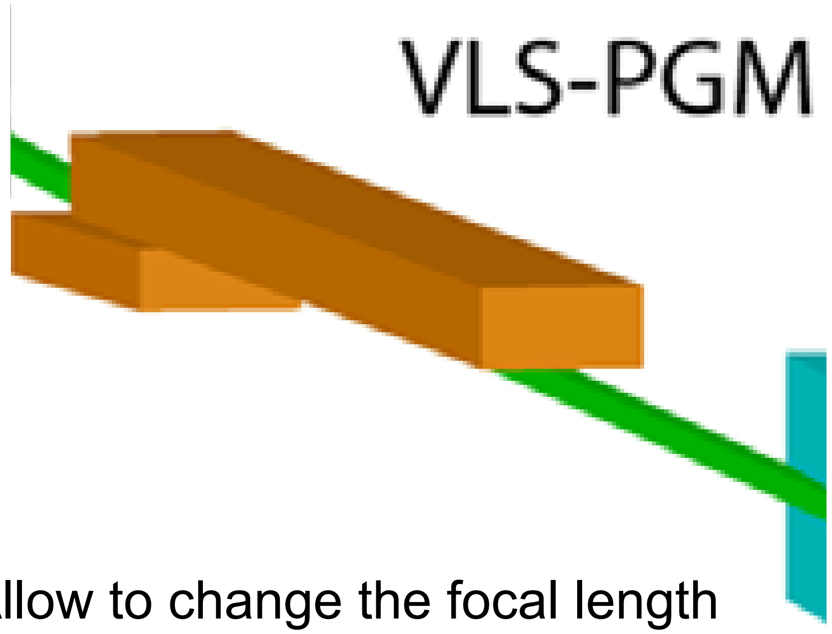
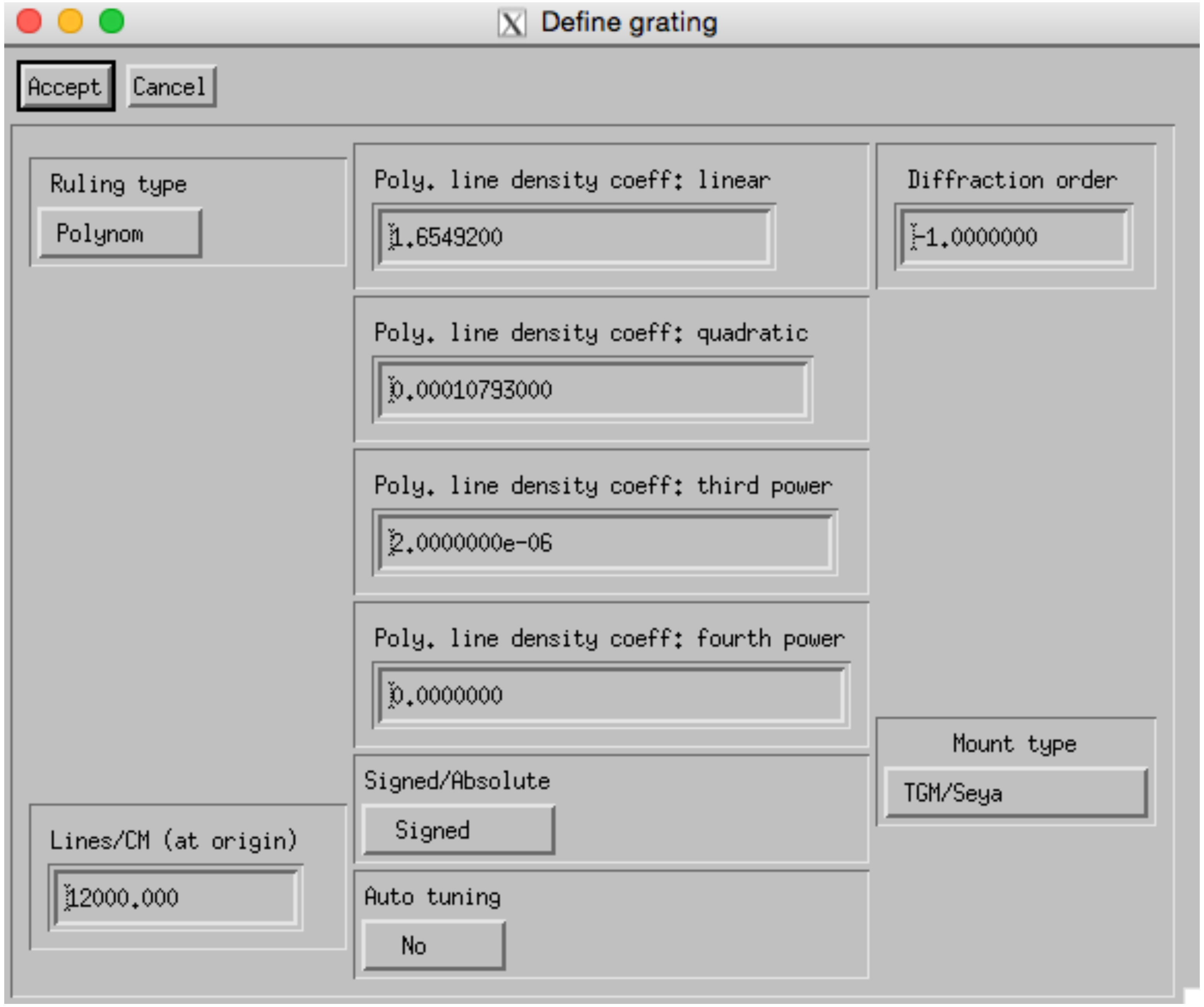
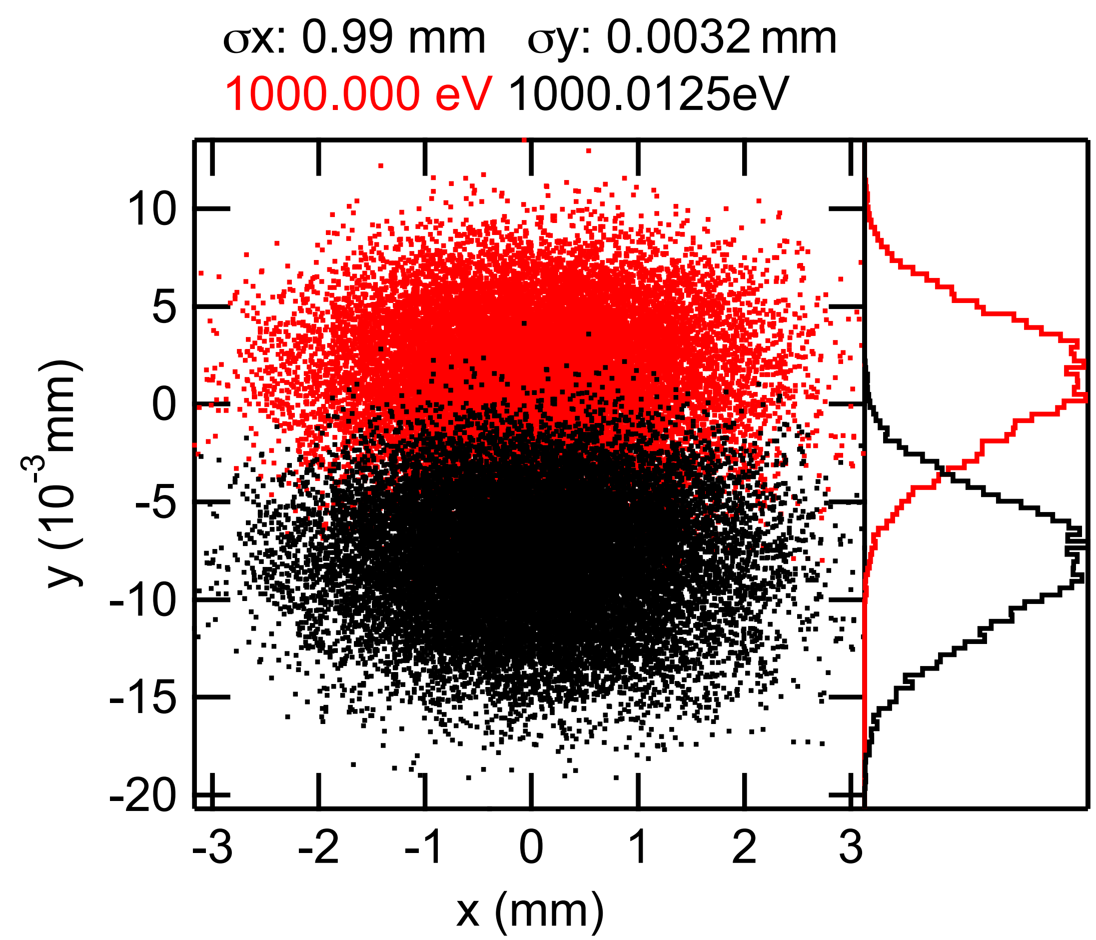


Allow to change the focal length

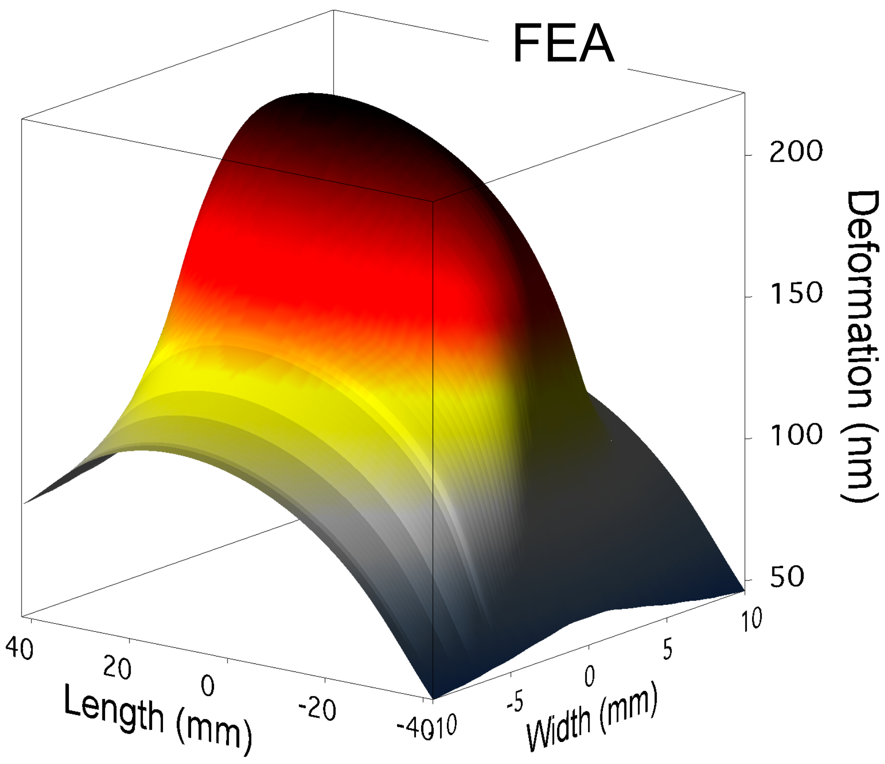
Grating in Shadow



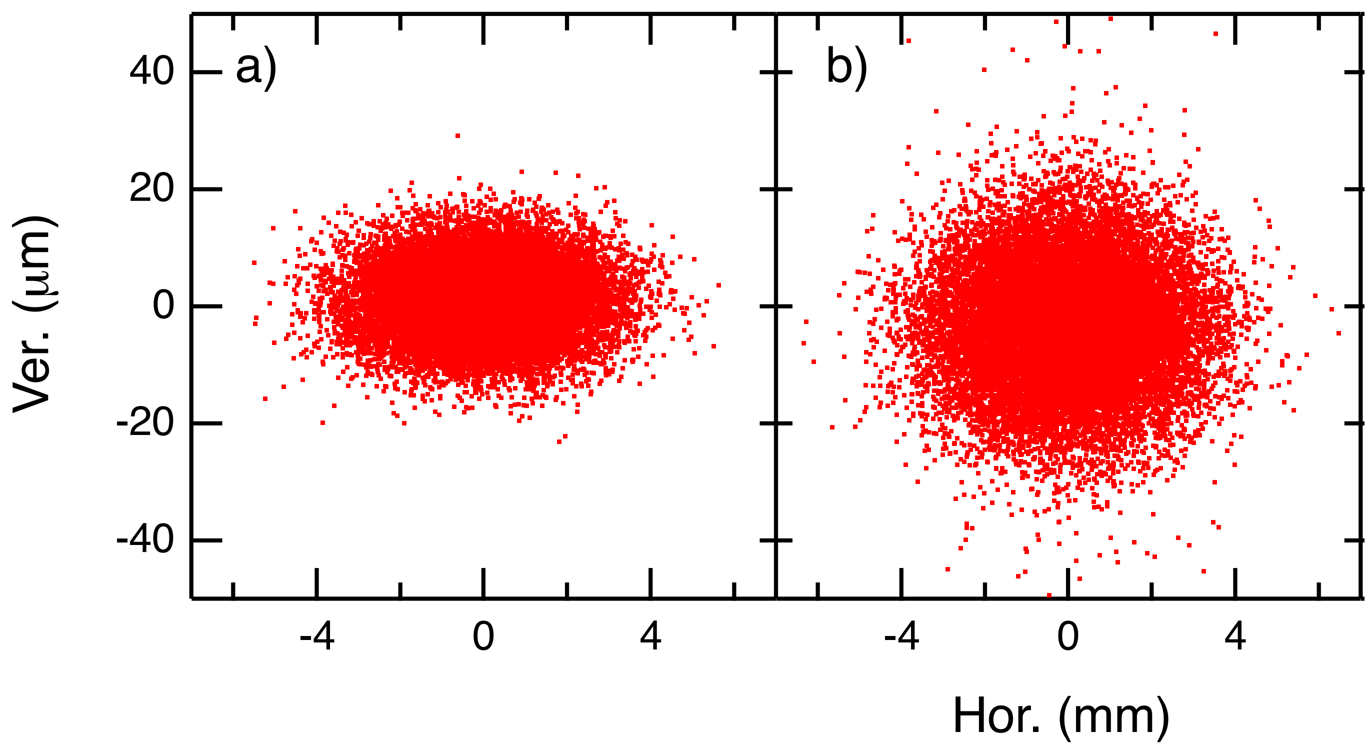
Exit Slit plane
RP 80,000



Correction of Heat Load Deformation M2

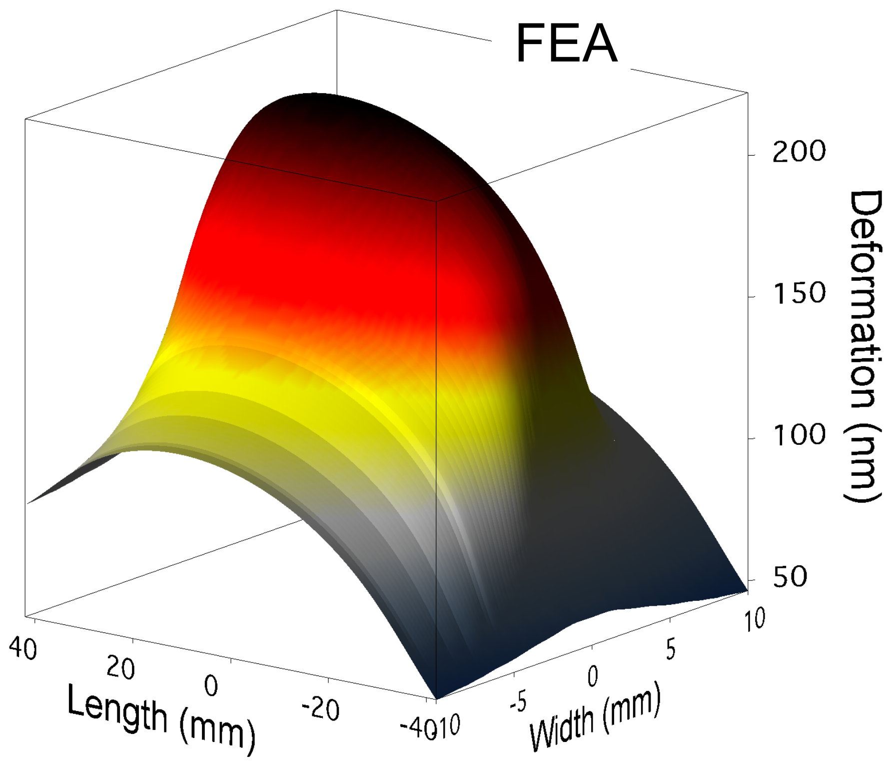


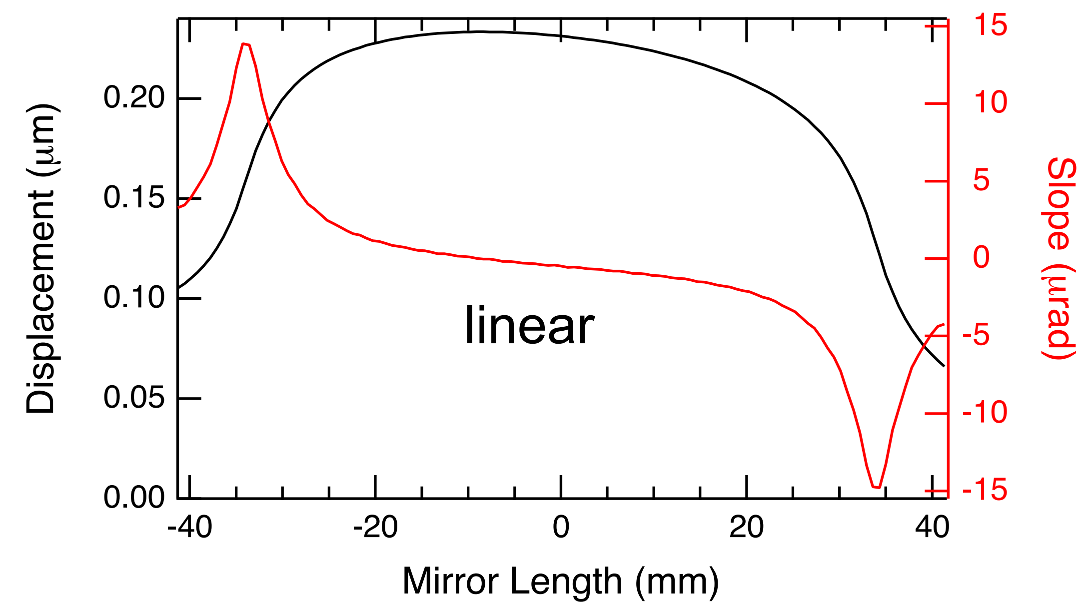
Resolution degradation!



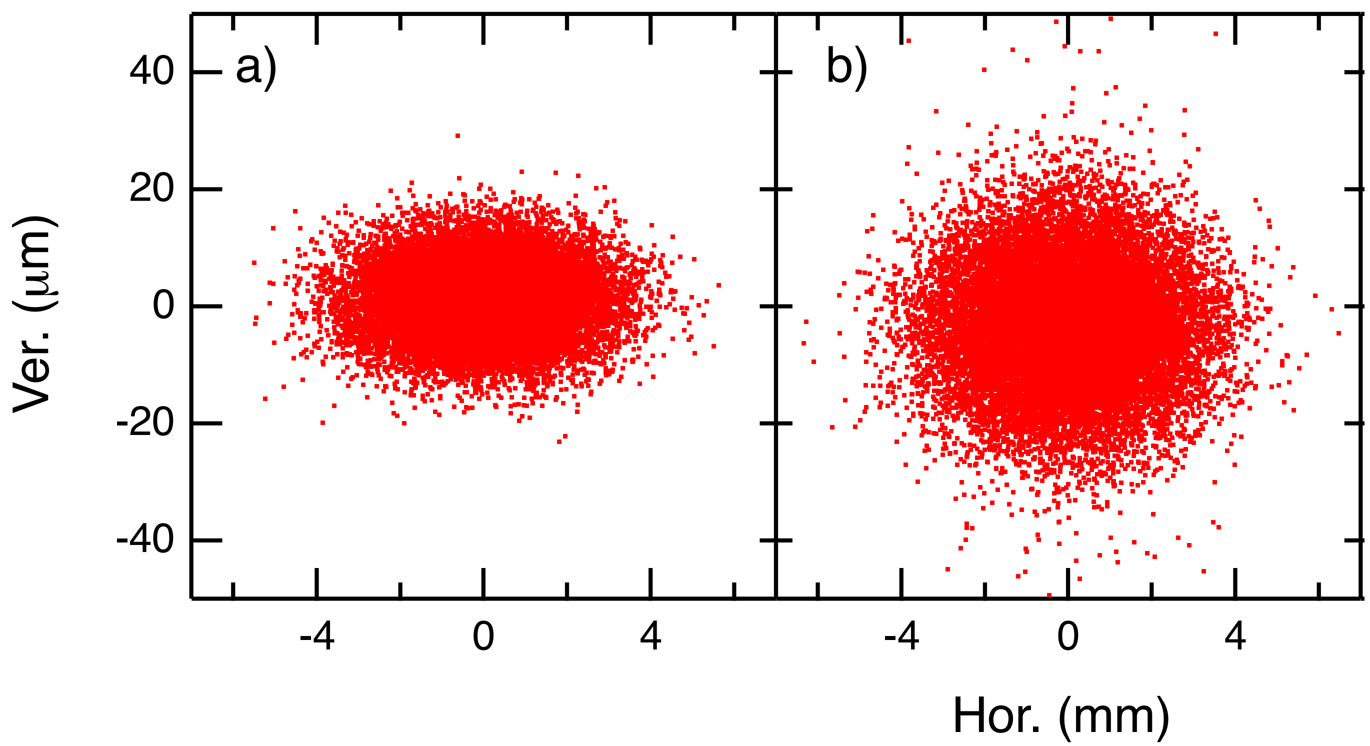
R. Reininger, Nucl. Instrum. Methods Phys. Res. A 649, 139 (2011).

Correction of Heat Load Deformation M2





Resolution degradation!



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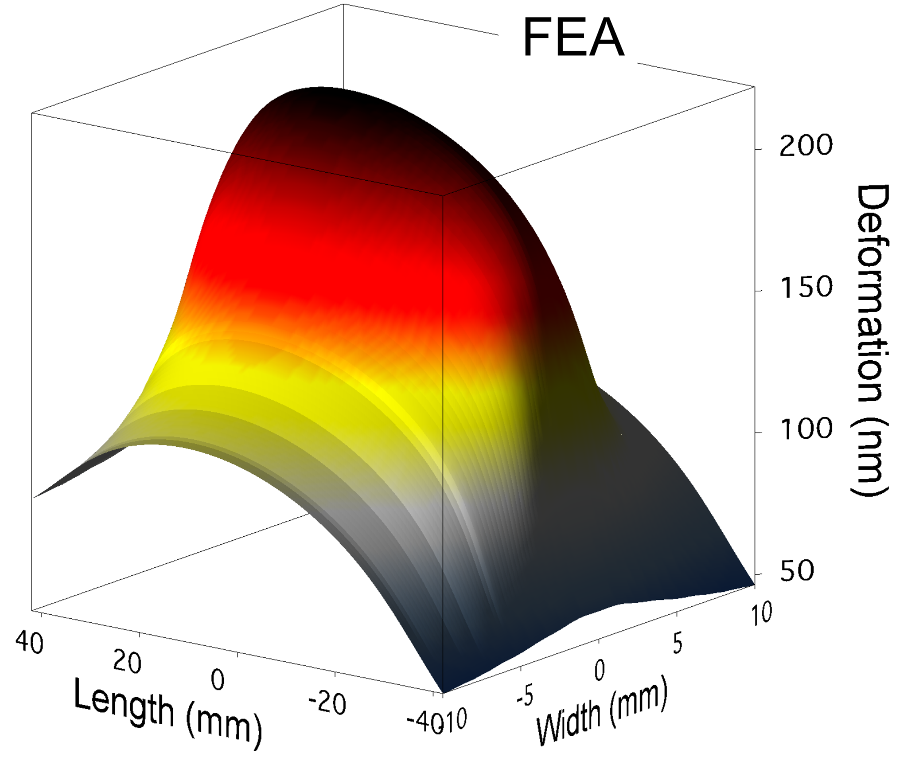
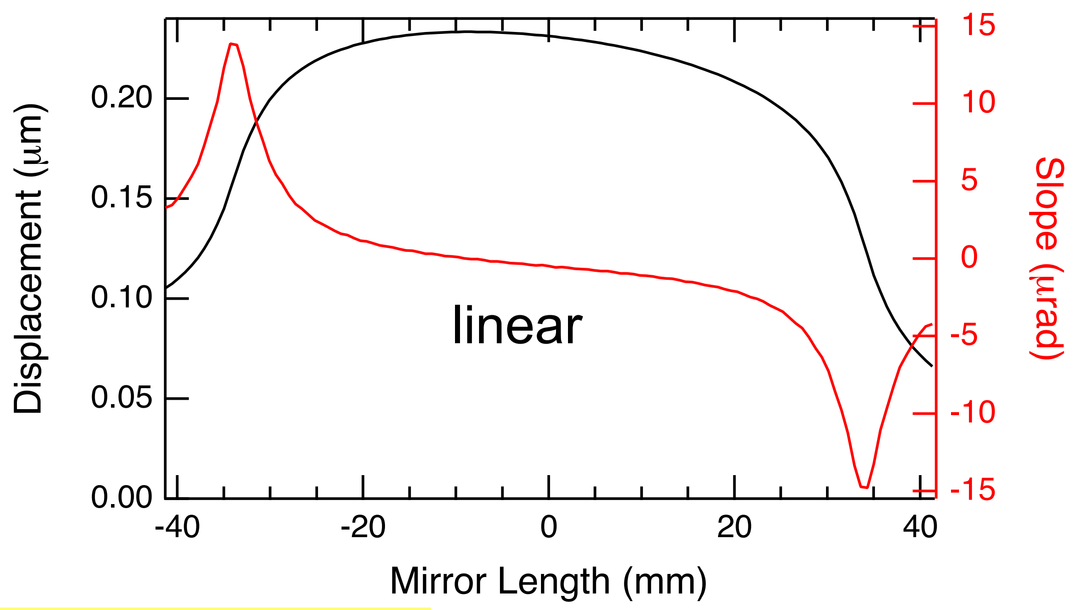
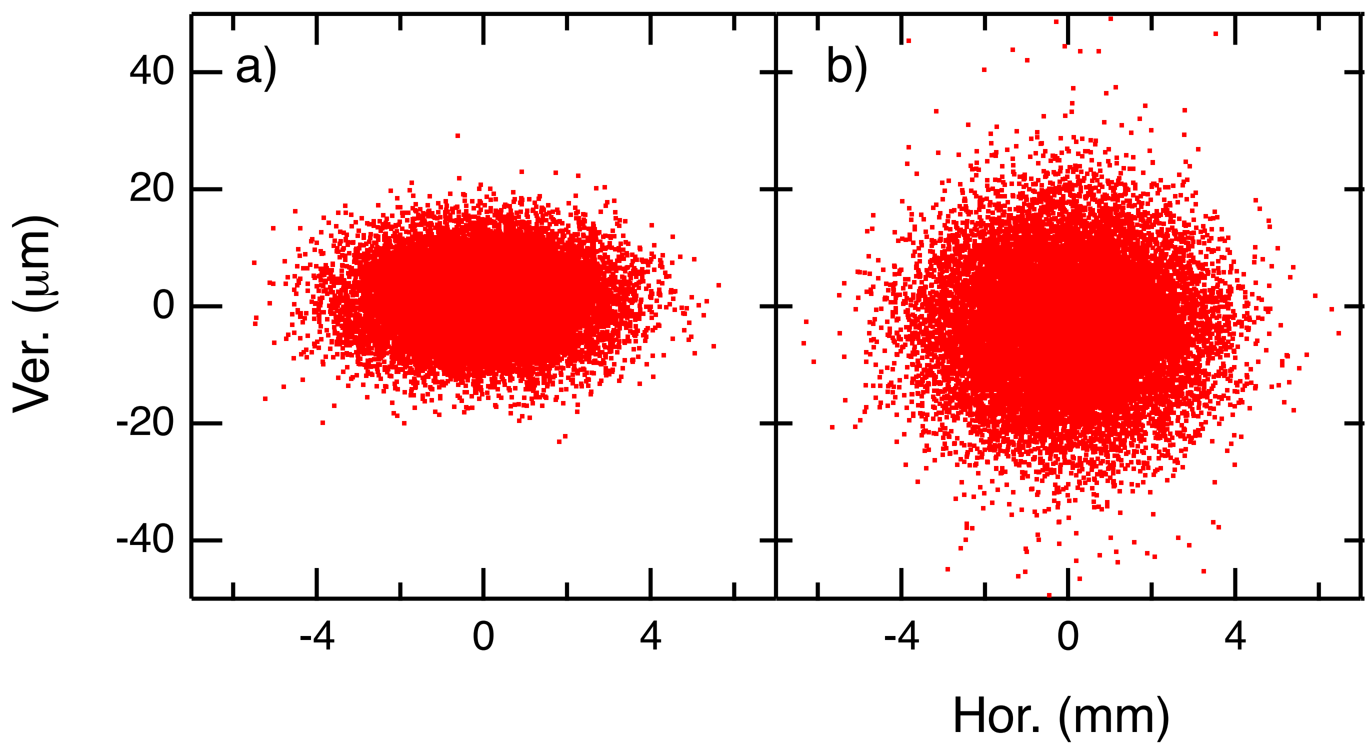
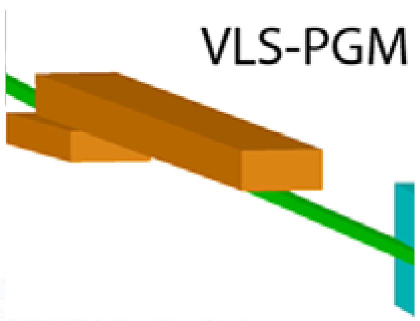




Resolution degradation!





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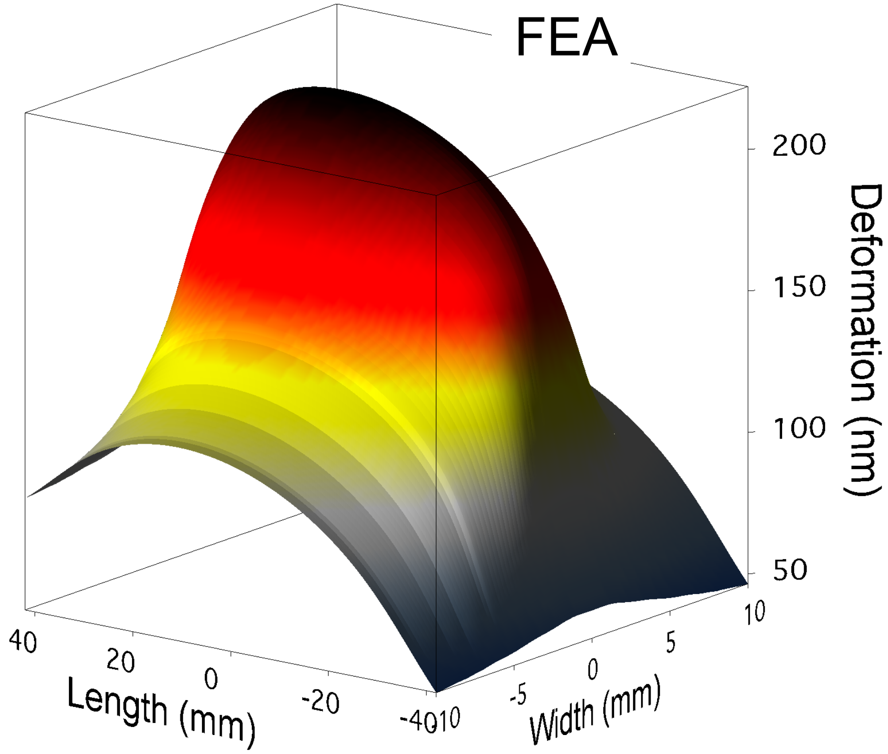
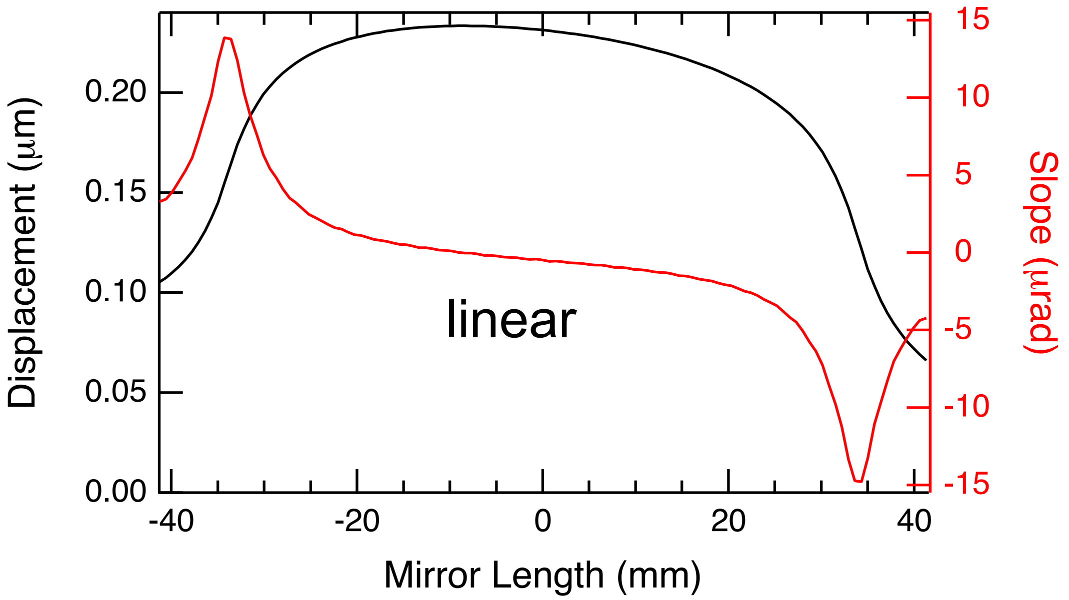
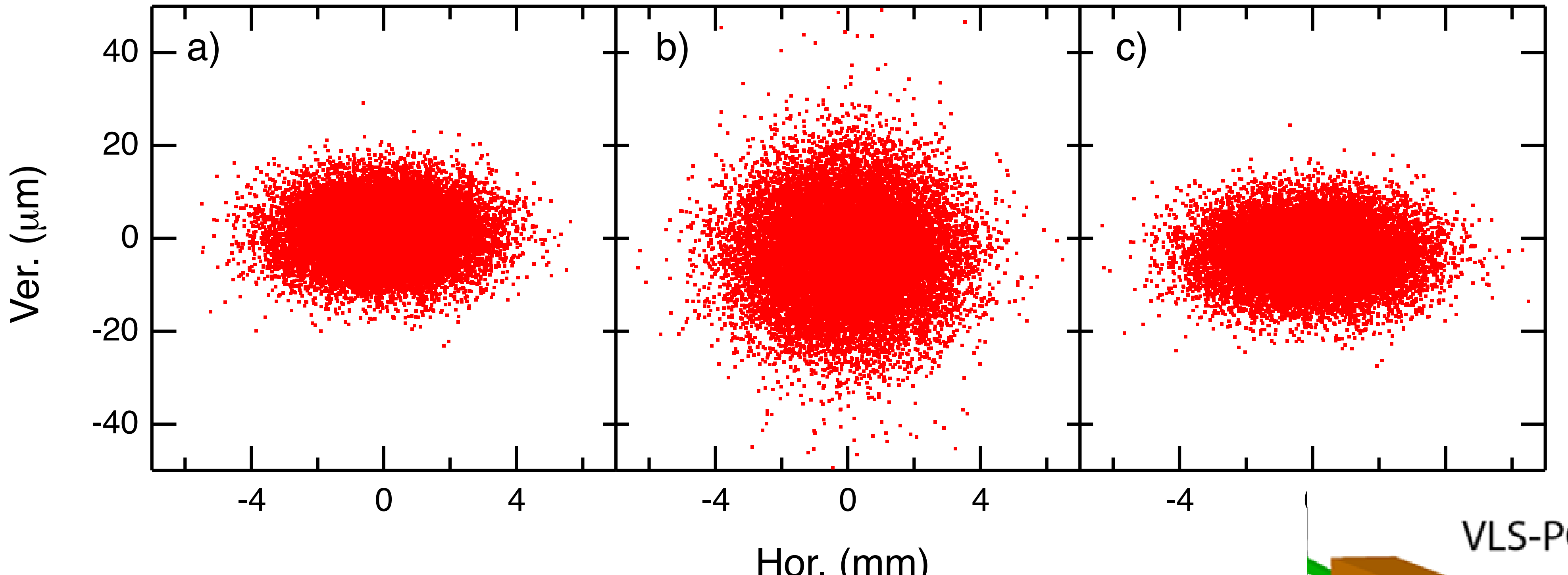
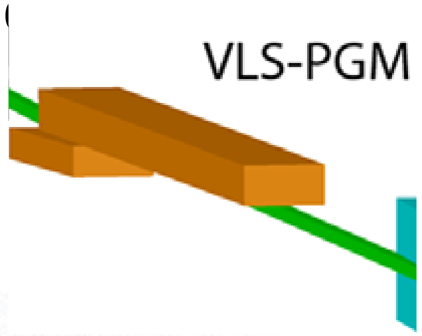




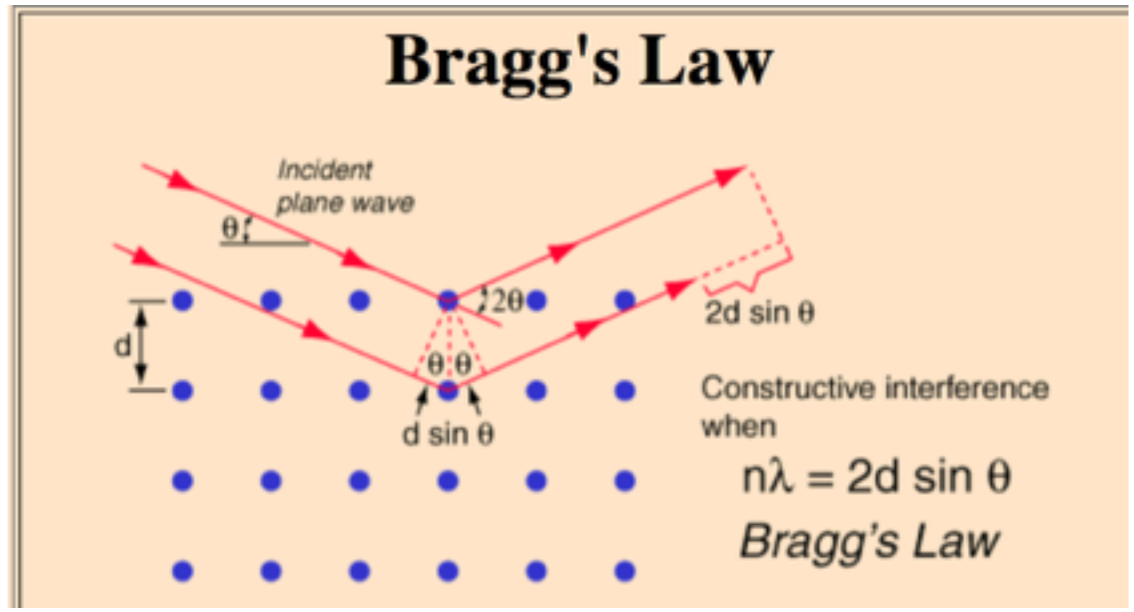
Resolution degradation!





R. Reininger, Nucl. Instrum. Methods Phys. Res. A 649, 139 (2011).

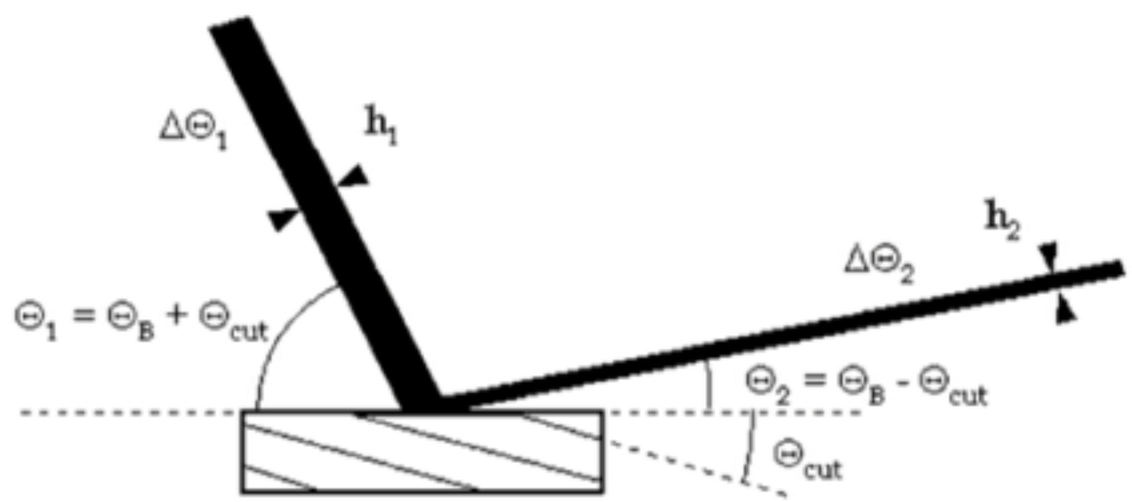
Crystal Diffraction



The asymmetry parameter

$b = -(\sin Q_1) / (\sin Q_2)$

$Q_1 = Q_B + Q_{cut}$	is the angle between the crystal surface and	the incoming beam
$Q_2 = Q_B - Q_{cut}$		the outgoing beam

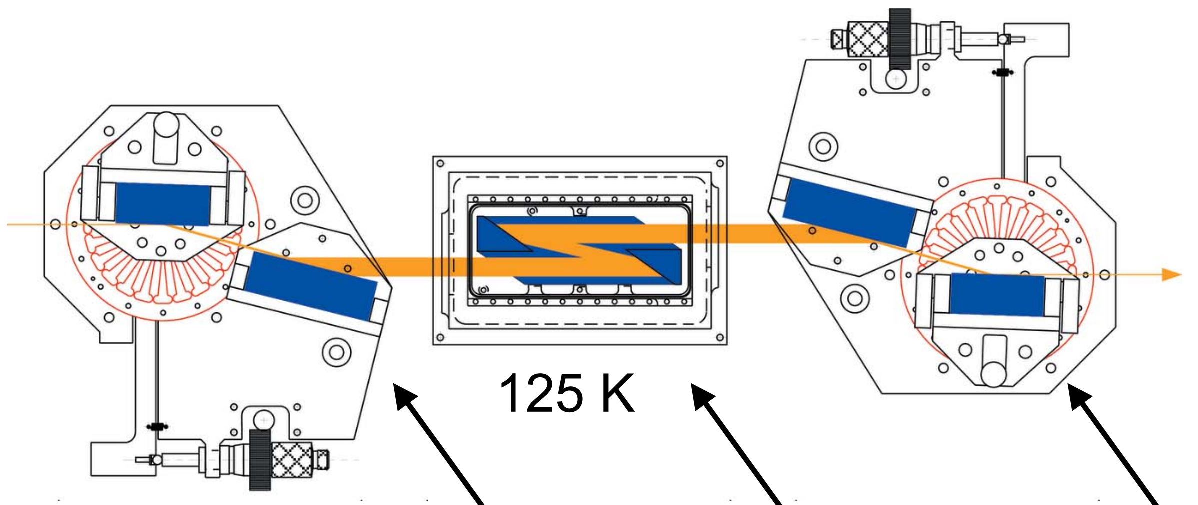


Crystal Monochromator

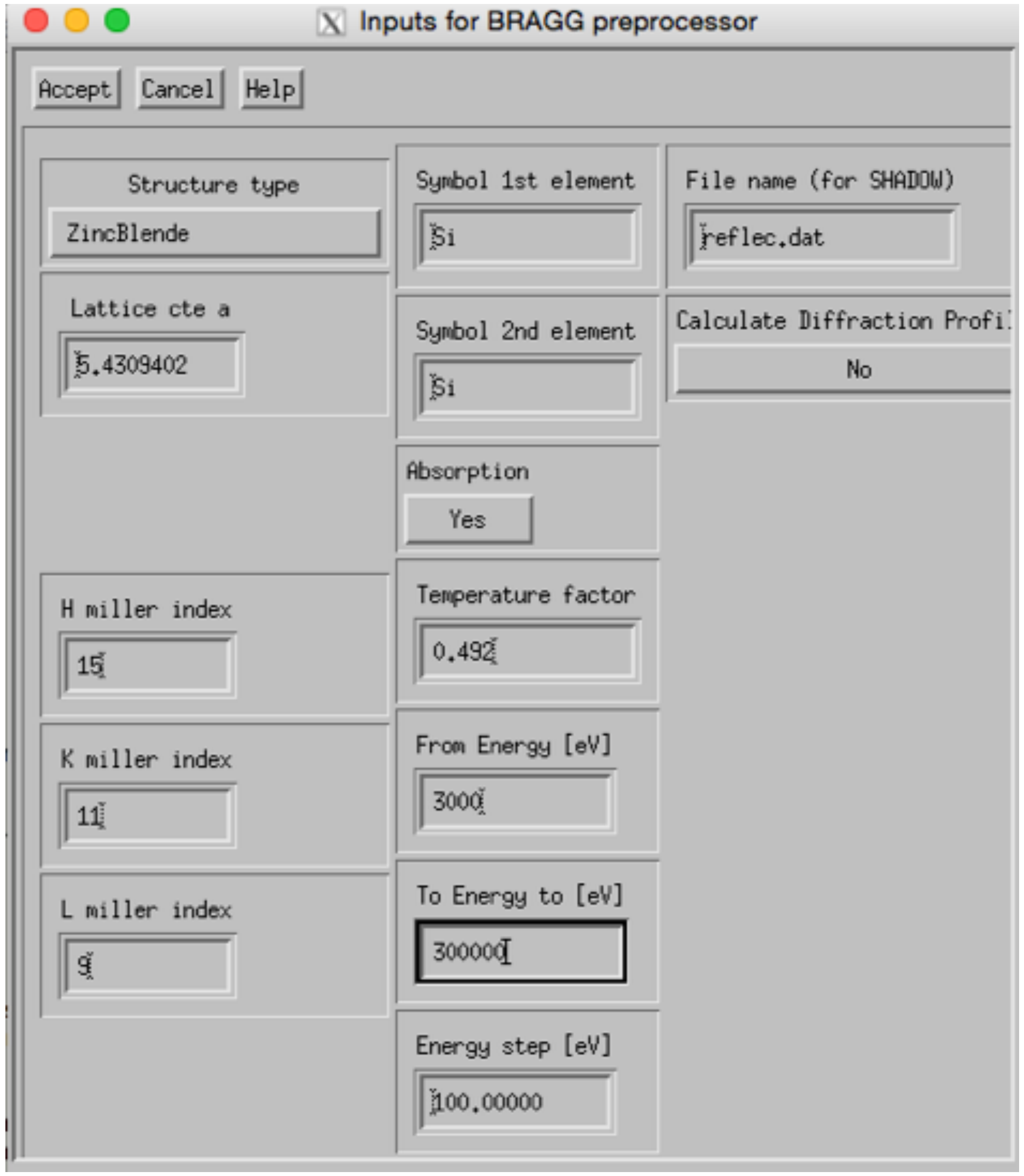
Six-reflection meV-monochromator for synchrotron radiation

J. Synchrotron Rad. (2011). **18**, 605–611

T. S. Toellner,* A. Alatas and A. H. Said



Element	HHLM	HRM 1st pair	HRM 2nd pair	HRM 3rd pair
Material	Diamond	Silicon	Silicon	Silicon
Reflection	1,1,1	3,1,1	15,11,9	2,2,0
Temperature factor	0.993	0.970	0.492	0.978
Asymmetry angle	0	-6.8	52.9 and -52.9	5.8



Crystal transmissions and Flux

$$F_f = F_i \frac{I_f}{I_i} \frac{\Delta E}{E} 1000, \quad F_i = 4 \times 10^{14} \frac{\text{photons}}{\text{s } 0.1\,\%\,\text{BW}}, \quad \Delta E = 10\text{ eV}, \quad E = 23\,725\text{ eV}$$

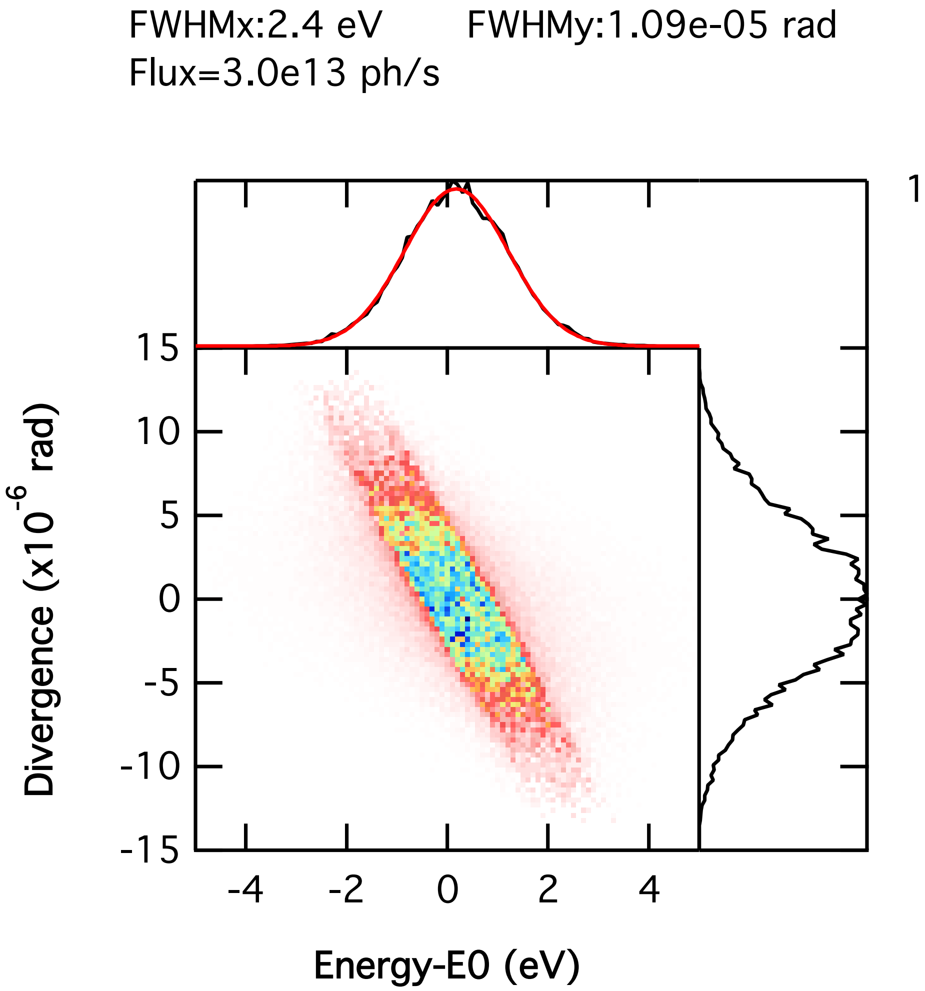
2.4 m long ID

E = 23.725 keV

Σx = 273 μm, Σy = 12 μm

$\Sigma' x$ = 11 μrad, $\Sigma' y$ = 4.7 μrad

C 1,1,1



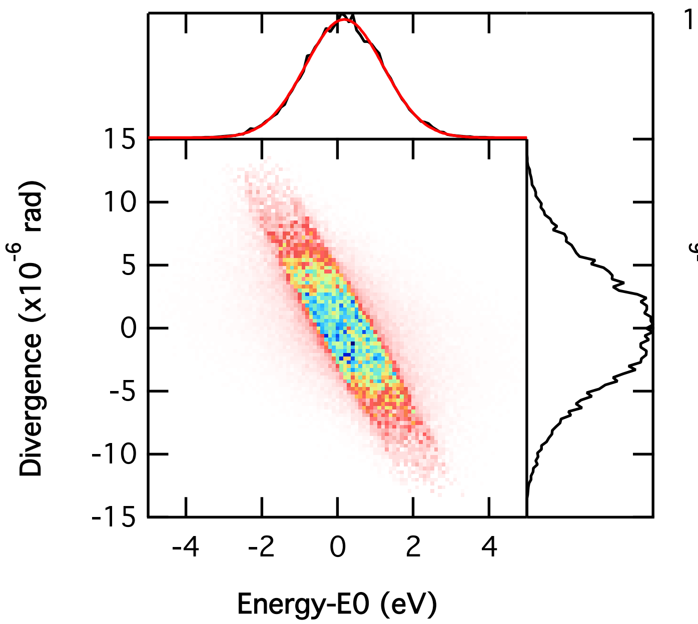
DuMond diagram

Crystal transmissions and Flux

$$F_f = F_i \frac{I_f}{I_i} \frac{\Delta E}{E} 1000, \quad F_i = 4 \times 10^{14} \frac{\text{photons}}{\text{s } 0.1\,\%\,\text{BW}}, \quad \Delta E = 10 \text{ eV}, \quad E = 23\,725 \text{ eV}$$

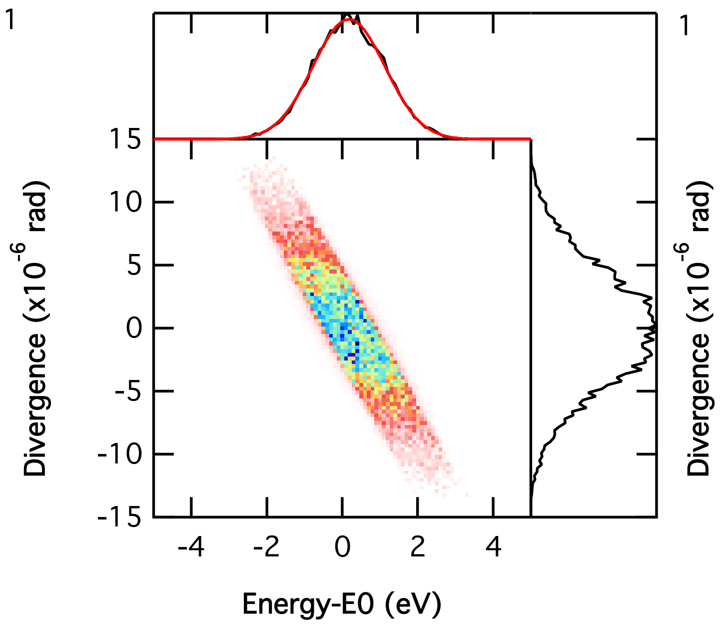
C 1,1,1

FWHMx:2.4 eV FWHMy:1.09e-05 rad
Flux=3.0e13 ph/s



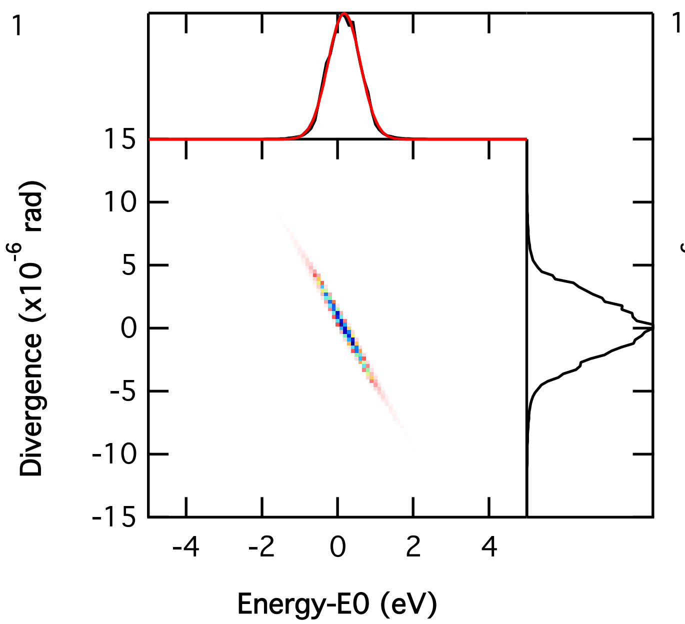
C 1,1,1

FWHMx:2.2 eV FWHMy:1.1e-05 rad
Flux=2.4 e13 ph/s



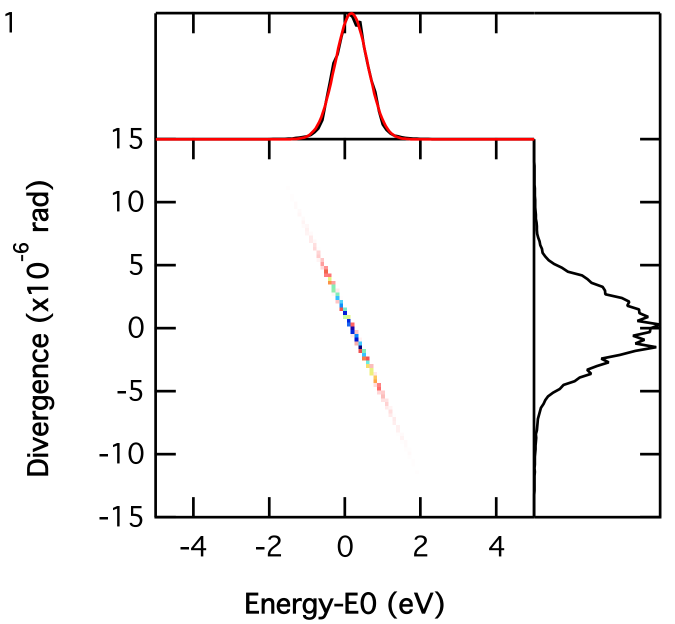
Si 3,1,1

FWHMx:1.0 eV FWHMy:5.51e-06 rad
Flux=1.1e13 ph/s

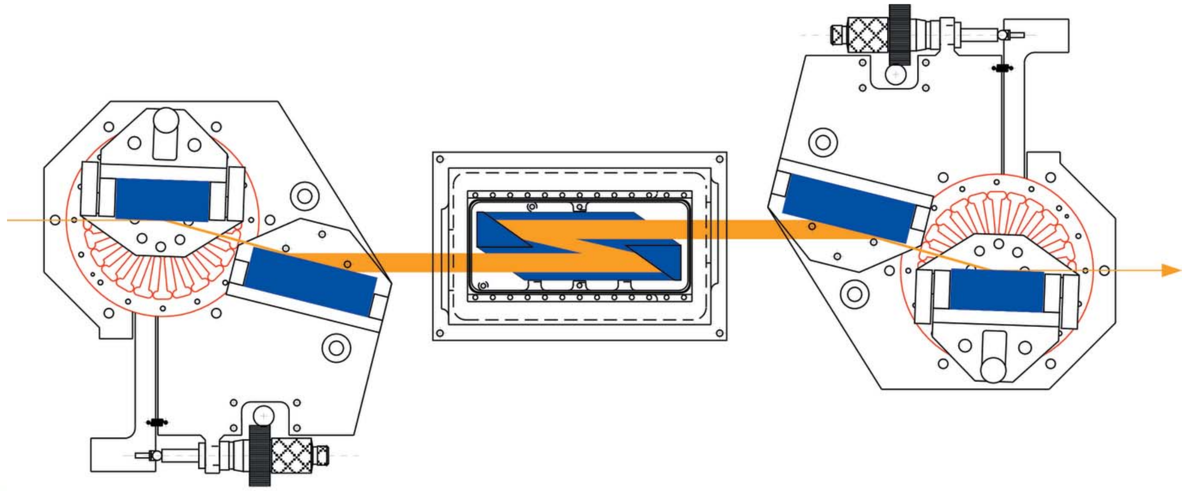


Si 3,1,1

FWHMx:1.0 eV FWHMy:6.6e-06 rad
Flux: 1.1e13 ph/s



High heat load mono

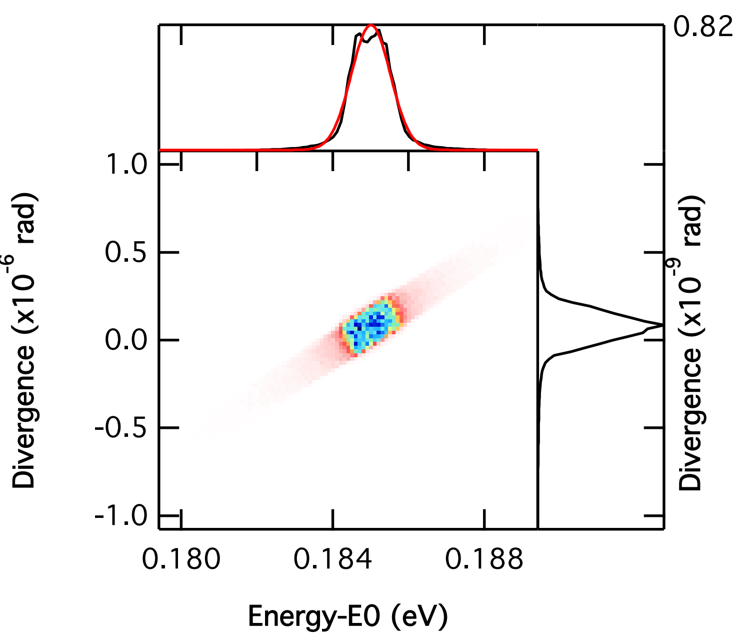


Crystal transmissions and Flux

$$F_f = F_i \frac{I_f}{I_i} \frac{\Delta E}{E} 1000, \quad F_i = 4 \times 10^{14} \frac{\mathrm{photons}}{\mathrm{s}\ 0.1\,\%\,\mathrm{BW}}, \quad \boxed{\Delta E = 10\ \mathrm{meV},} \quad E = 23\,725\ \mathrm{eV}$$

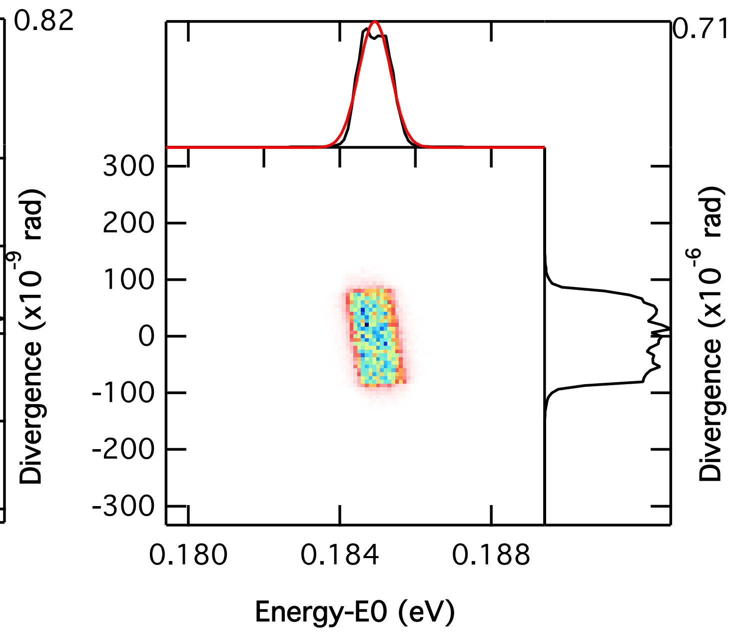
Si 15,11,9

FWHMx:1.2 meV FWHMy:2.1e-07 rad
Flux: 1.2e10 ph/s



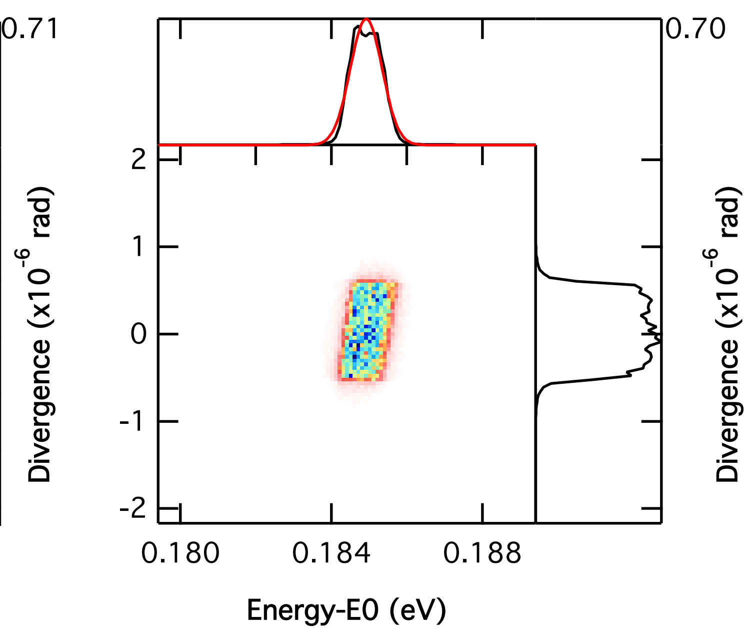
Si 15,11,9

FWHMx:1 meV FWHMy:1.4e-07 rad
Flux: 7.7e9 ph/s



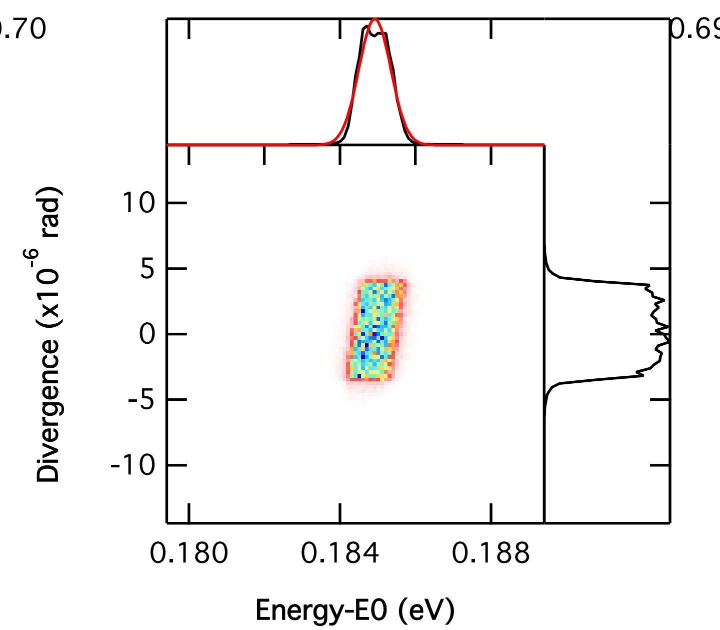
Si 2,2,0

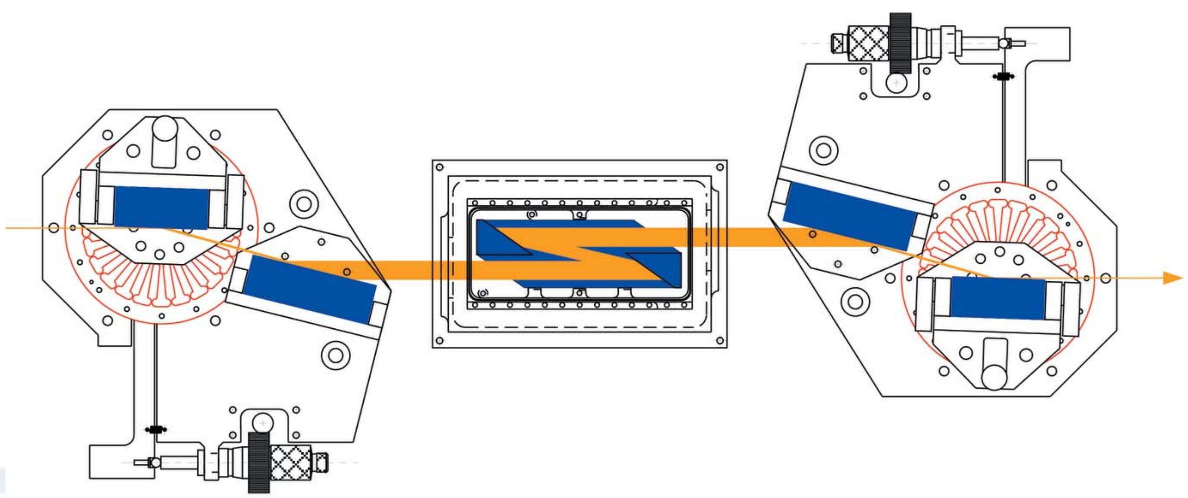
FWHMx:1 meV FWHMy:9.6e-07 rad
Flux=7.6e9 ph/s



Si 2,2,0

FWHMx:0.99 meV FWHMy:6.4e-06 rad
Flux=7.5e9 ph/s

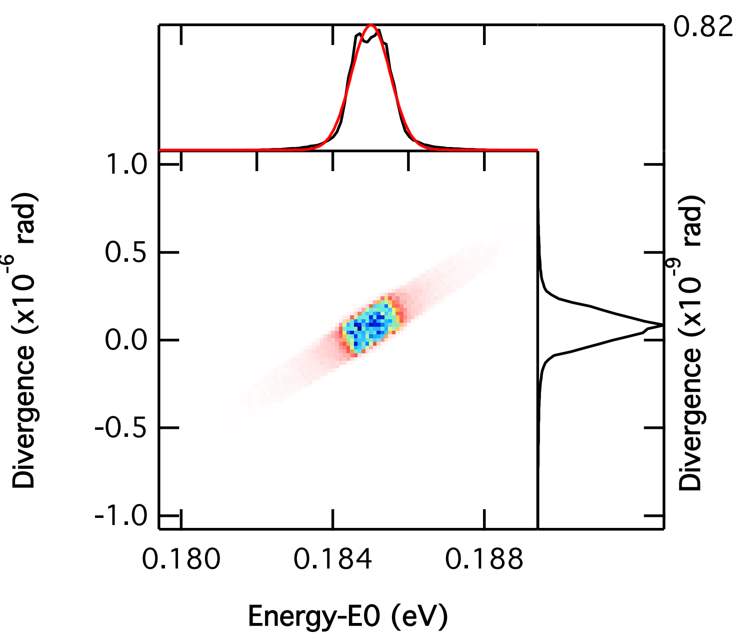


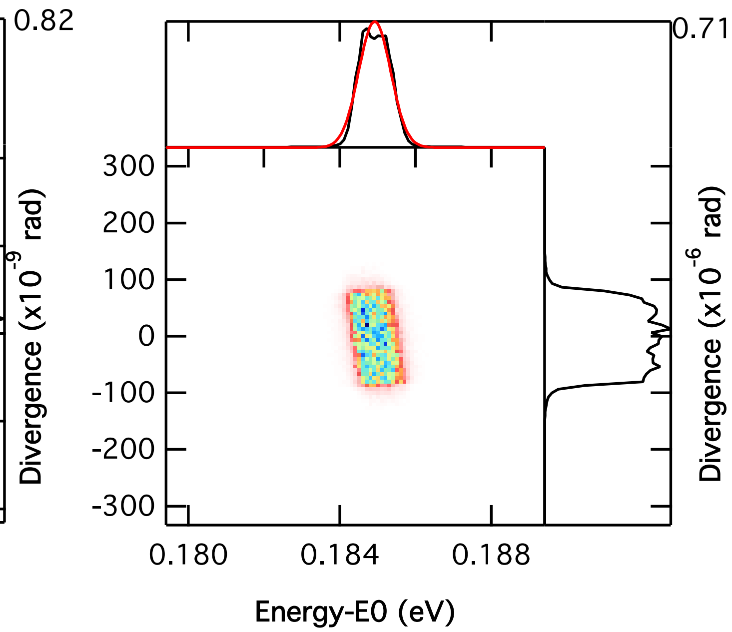


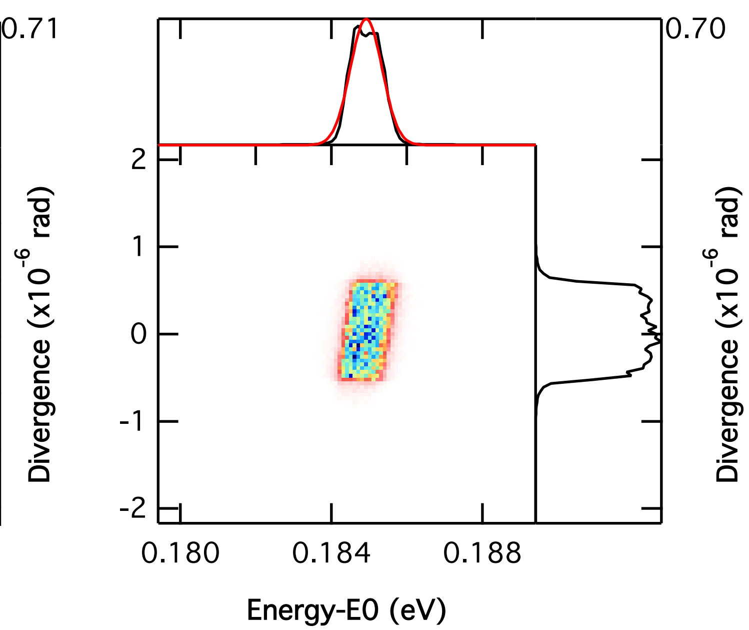
Crystal transmissions and Flux

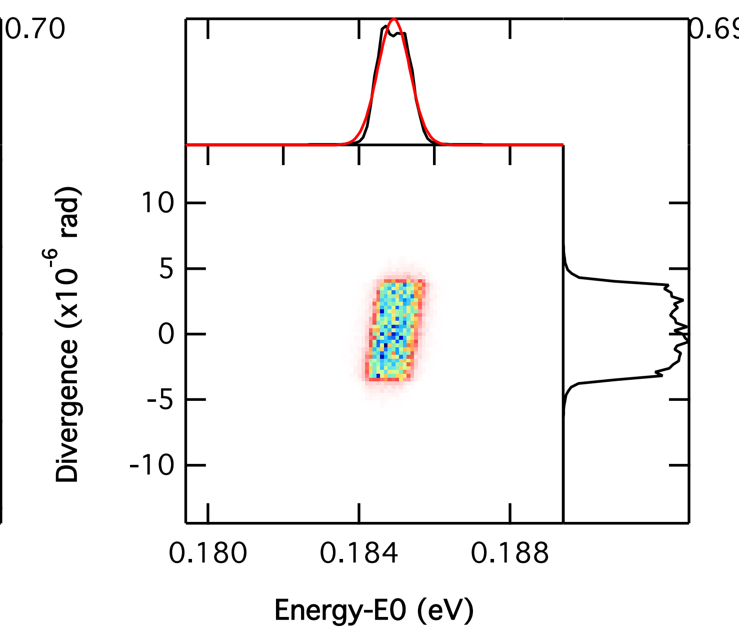
$$F_f = F_i \frac{I_f}{I_i} \frac{\Delta E}{E} 1000, \quad F_i = 4 \times 10^{14} \frac{\text{photons}}{\text{s } 0.1\,\%\,\text{BW}}, \quad \boxed{\Delta E = 10\ \text{meV},} \quad E = 23\,725\ \text{eV}$$

Si 15,11,9	Si 15,11,9	Si 2,2,0	Si 2,2,0
FWHMx:1.2 meV FWHMy:2.1e-07 rad	FWHMx:1 meV FWHMy:1.4e-07 rad	FWHMx:1 meV FWHMy:9.6e-07 rad	FWHMx:0.99 meV FWHMy:6.4e-06 rad
Flux: 1.2e10 ph/s	Flux: 7.7e9 ph/s	Flux=7.6e9 ph/s	Flux=7.5e9 ph/s









RP: 23,725,000