

**A Light for Science**



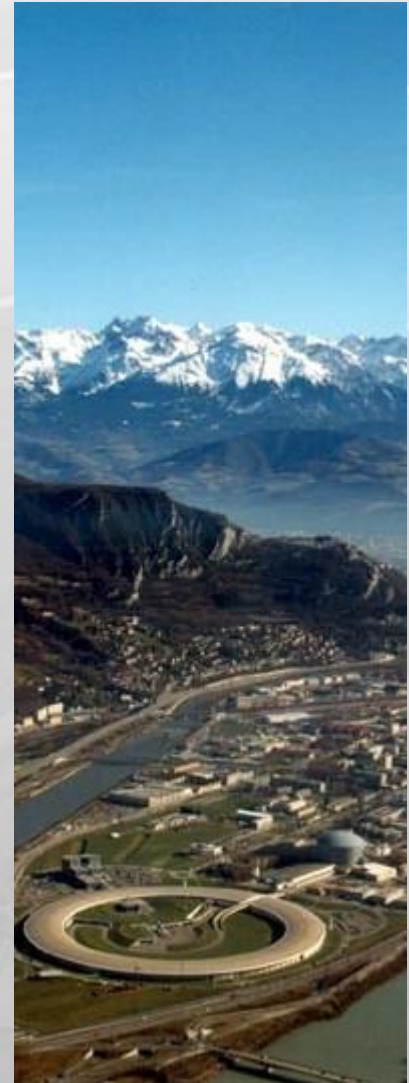
**European Synchrotron Radiation Facility**

# SHADOW (and related software)

Manuel Sánchez del Río

ESRF, BP 220, F-38043 Grenoble Cedex

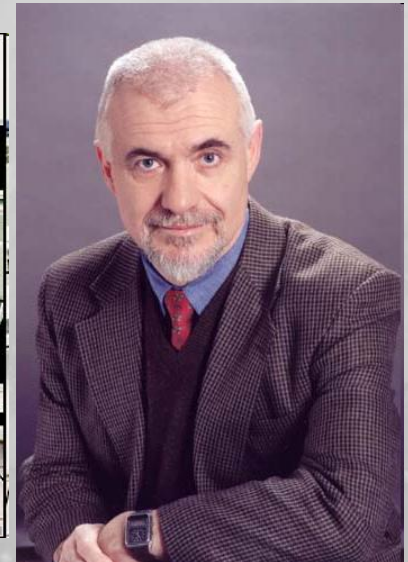
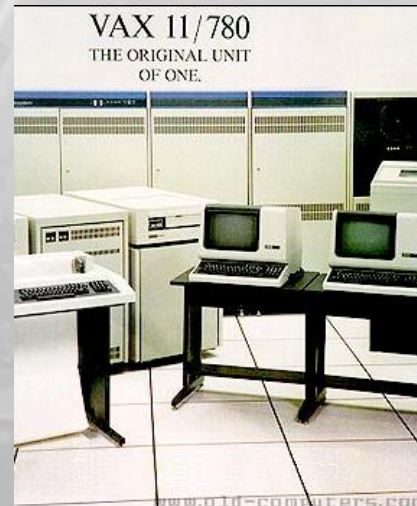
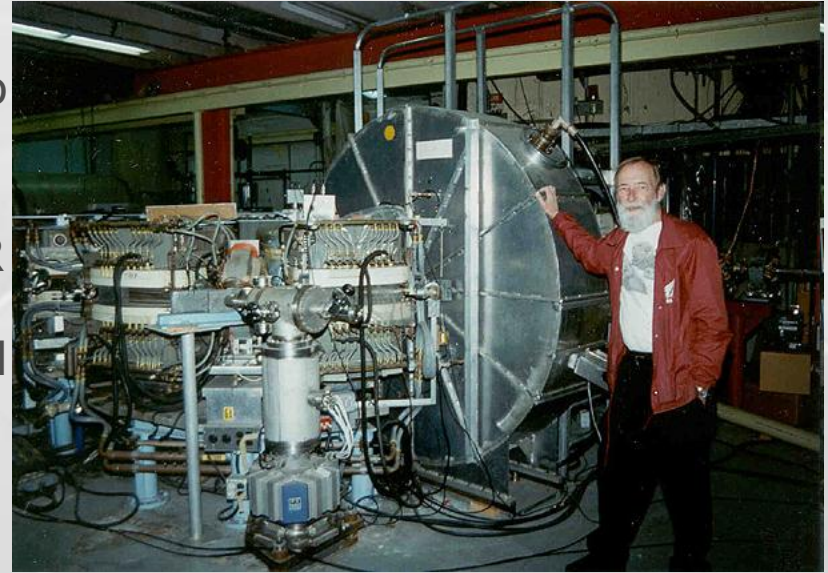
- Historical introduction
- What can SHADOW do? – functionality
- Examples
  - Classic
  - ESRF Upgrade
- New
- Future



# Historical introduction



- **1965 -1967** At the University of Wisconsin, a team led Ednor Rowe built ***Tantalus***, adapted to make synchrotron radiation available for experimentalists from all over the world
- **1977** SRC began construction on dedicated SR source, ***Aladdin***. Questions on grating monochromator design, TGM, toroidal, spherical mirrors.
- **1987** Tantalus decommissioned, Aladdin fully operational.
- **1984** Monte Carlo ray tracing program ***designed*** to simulate X-ray optical systems:
  - Two years development
  - Fortran 77+VAX/VMS extensions
  - Efficient MC approach
  - Reduced number of rays
  - Exact simulation of SR sources
  - Vector calculus
  - Modular
  - User-interface
  - Available to users



68 / SPIE Vol. 503 Application, Theory, and Fabrication of Periodic Structures (1984)

Ray tracing of recent VUV monochromator designs

F. Cerrina

Department of Electrical and Computer Engineering  
University of Wisconsin, Madison WI 53706

Abstract

A new optical ray-tracing program is presented and some applications discussed. A Monte-Carlo modelling of several types of sources is implemented, and in particular the Synchrotron Radiation source is modelled exactly. The program is written specifically for grazing optics, although gaussian optics can be treated as well. Diffraction from gratings, both ruled and holographic, is included as well as Bragg diffraction from crystals. The reflectivity of mirror surfaces and transmission of filters is treated exactly and locally, solving the Fresnel equations for each ray. The interactive nature of the program and its fast execution time allow the simulation of real-life situations quickly and efficiently.

Applications  
(GCM), and E

Nuclear Instruments and Methods in Physics Research A246 (1986) 337-341  
North-Holland, Amsterdam

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## **SHADOW: A SYNCHROTRON RADIATION RAY TRACING PROGRAM**

**B. LAI and F. CERRINA**

*Department of Electrical and Computer Engineering, University of Wisconsin, Madison, WI 53706, USA*

We present the new ray-tracing program SHADOW. The program was written specifically for the XUV optics range, but is now completely general. Its capabilities are discussed in terms of the physical basis on which the program is built, with particular emphasis on the synchrotron radiation applications.

Updated to include new models (several authors)

- Insertion devices (Wiggler and Undulators)
- First crystal model
- Multilayers

Documentation & Users support (C. Welnak)

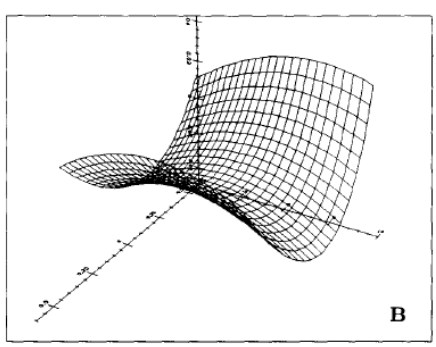
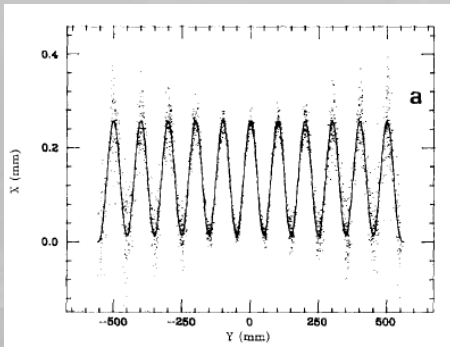


Fig. 1. Possible choices of toroidal surface regions.



544

Nuclear Instruments and Methods in Physics Research A266 (1988) 544-549  
North-Holland, Amsterdam

## SHADOW: NEW DEVELOPMENTS

B. LAI, K. CHAPMAN and F. CERRINA

*Department of Electrical and Computer Engineering, University of Wisconsin-Madison, Madison, WI 53706-1691, USA*

We describe the new extensions that we have implemented in our synchrotron radiation ray tracing code, SHADOW. The most important are the new angular source, the extension of 100 keV of the optical constant database, the novel power density calculations capabilities and the new optics case.

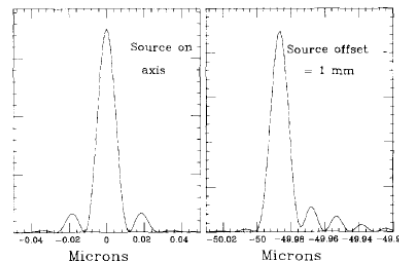
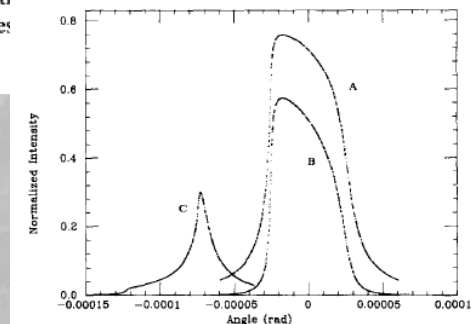


Fig. 7. Diffracted image formed by a Schwartzschild objective at 44 Å. All the physical parameters, such as phase shifts, multilayer reflectivities, and diffraction, are taken in account.

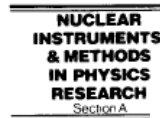




New machines enter in the scientific computing market. Unix workstations: Digital/Ultrix, Sun, HP.  
 UNIX version prepared by Mumit Khan  
 Other scattered developments  
 First version installed at ESRF (1991). Twofold development: Models and Software

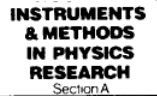
## Recent developments in SHADOW

Nuclear Instruments and Methods in Physics Research A 347 (1994) 344–347  
 North-Holland



A. Khan, S. Singh, and F. Cerrina  
*University of Wisconsin–Madison, 3731 Schneider Drive, Stoughton,*

Nuclear Instruments and Methods in Physics Research A 347 (1994) 407–411  
 North-Holland



### SHADOW: a synchrotron radiation and X-ray optics simulation tool

C. Welnak <sup>\*</sup>, G.J. Chen, F. Cerrina

*Center for X-ray Lithography, University of Wisconsin – Madison, 3731 Schneider Drive, Stoughton, WI 53589, USA*

### Ray-tracing of X-ray focusing capillaries

Guan-Jye Chen <sup>a,\*</sup>, F. Cerrina <sup>a</sup>, Karl F. Voss <sup>b</sup>, K. Hyde Kim <sup>b</sup>, Frederick C. Brown <sup>b</sup>

This article should be cited as *Rev. Sci. Instrum.* **67**, 3355 (1996).

### Multilayer roughness and image formation in the Schwarzschild objective

S. Singh, H. Solak, and F. Cerrina

*University of Wisconsin, 3731 Schneider Drive, Stoughton, WI 53589*

(Presented on 19 October 1995)



Nuclear Instruments and Methods in Physics Research A 347 (1994) 238–243  
 North-Holland

### Applications of faceted mirrors to X-ray lithography beamlines

Guan-Jye Chen, J.Z.Y. Guo, F. Cerrina

*Center for X-Ray Lithography and Department of Electrical and Computer Engineering, University of Wisconsin-Madison, 3731 Schneider Drive, Stoughton, WI 53589, USA*



## Asymmetrically cut crystals for synchrotron radiation monochromators

M. Sánchez del Río  
European Synchrotron Radiation Facility, B.P. 220, 38043 Grenoble Cedex, France

F. Cerrina  
Center for X-ray Lithography, 3731 Schneider Drive, Stoughton, Wisconsin 53589

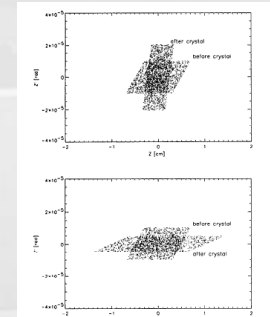


FIG. 3. Change in phase space of the photon beam of 8035 eV produced by an Si(111) asymmetrically cut crystal of  $\alpha = 5$  deg (top) and  $\alpha = -5$  deg (bottom). A linear and divergent source in Z direction has been considered.

936 Rev. Sci. Instrum. 63 (1), January 1992 0034-6748/92/010936-05\$02.00 © 1992 American Institute of Physics 936

Nuclear Instruments and Methods in Physics Research A 347 (1994) 338–343  
North-Holland

See: [ex23\\_crystal\\_laue.ws](http://ex23_crystal_laue.ws)

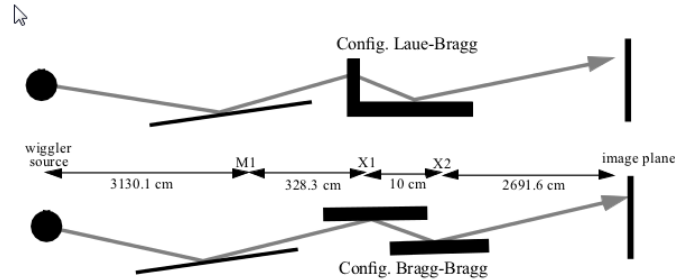
INSTRUMENTS  
& METHODS  
IN PHYSICS  
RESEARCH  
Section A

## Modeling perfect crystals in transmission geometry for synchrotron radiation monochromator design

M. Sánchez del Río <sup>a,\*</sup>, C. Ferrero <sup>a</sup>, G-J. Chen <sup>b</sup>, F. Cerrina <sup>b</sup>

<sup>a</sup> European Synchrotron Radiation Facility, BP 220, 30043 Grenoble Cedex, France

<sup>b</sup> Center for X-ray Lithography, 3731 Schneider Drive, Stoughton, WI 53589, USA



Nuclear Instruments and Methods in Physics Research A319 (1992) 170–177  
North-Holland

See: [ex20b\\_slopeerrors.ws](http://ex20b_slopeerrors.ws)

NUCLEAR  
INSTRUMENTS  
& METHODS  
IN PHYSICS  
RESEARCH  
Section A

## Waviness effects in ray-tracing of “real” optical surfaces

M. Sánchez del Río <sup>a</sup> and A. Marcelli <sup>b</sup>

<sup>a</sup> European Synchrotron Radiation Facility, B.P. 220, 38043 Grenoble Cedex, France

<sup>b</sup> INFN Laboratori Nazionali di Frascati, CP 13, 00044 Frascati, Italy

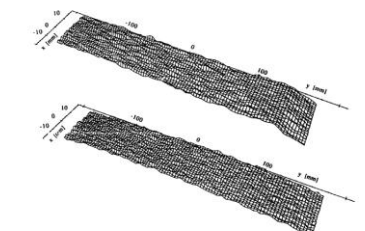
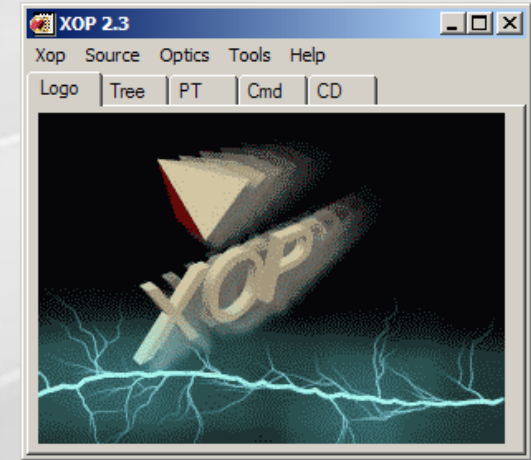


Fig. 3. Simulated waviness of optical surfaces with 0.4° slope error. The surface A has been generated considering  $n_{max} = 32$ ,  $C_x = 1$ ,  $C_y = 0$ , and  $f_x = 0.1$ ,  $f_y = 0$ . For surface B,  $n_{max} = 50$  and the eccentricity parameters were chosen in a more complicated way. The total length of each surface is 350 mm and the width is 30 mm. The vertical length is not scaled.

- Need of tools « before » using SHADOW => XOP

- XOP

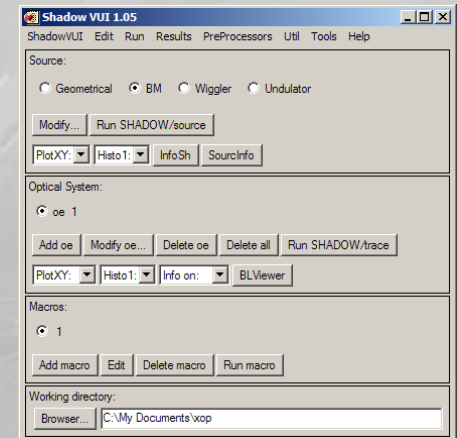
- quick calculations (synchrotron spectra, reflectivities, rocking curves, attenuation coeffs. etc.)
- generic data visualization and analysis
- specific applications (“extensions”)
- Collaboration work ESRF (M Sanchez del Rio)-APS (Roger Dejus)
- Freely available to users (>10 years)
- Large user community (>400 users in tens of laboratories)
- Multiplatform (Windows, Unix, MacOSX)
- Written in IDL (using Fortran and C modules). Embedded license



- Improve the « speed » of interaction with user (more than speed of calculation) => ShadowVUI
- Spreading the use of SHADOW and related tools at ESRF and outside
- SHADOW code « frozen », suffering from oldness

- ShadowVUI: interface that uses the standard SHADOW calculation engine

- “Easy” to use
- High performance graphics
- Macro language
- Tutorials
- BLViewer



- 1998-2008 Reduced interest in Optics simulations
- ESRF Upgrade programme 2008-2017
- Double implication
  - New trends in optics: CRL, transfocators, nanofocusing, partial coherence
  - Need to evolve following the new available computer environments
- Actions
  - Urgent renewal of SHADOW
  - Need of complementarities (other codes)
  - Consolidating collaborations
  - Software development programme

- Renew the internals
- Prepare the framework for the “new challenges”
- Fully compatible with existing version (only Kernel, no graphics, menu, etc.)
- Maintain Shadow’s flavor: SHADOW users will feel “comfortable” with it
- Remove present limitations in:
  - Dimensions (number of rays, optical elements, mesh points, etc.)
  - Old programming techniques (Common blocks, etc.)
- API (C, Python, IDL)
- Transform f77 to f95 and full use of modular structure
- Supported for Windows, Linux and MacOS
- Full compatibility of ShadowVUI
- New “basic” graphics (gnuplot)
- **In conclusion: first a lot of cleaning and modernisation of the code (mostly done, but still thinks to cleaned), then (on going), upgrade physical models)**

## research papers

Journal of  
Synchrotron  
Radiation  
ISSN 0909-0495

Received 14 January 2011  
Accepted 2 July 2011

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

Manuel Sanchez del Rio,<sup>a\*</sup> Niccolo Canestrari,<sup>b,a</sup> Fan Jiang<sup>c</sup> and Franco Cerrina<sup>c,t</sup>

<sup>a</sup>European Synchrotron Radiation Facility, 6 Jules Horowitz, 38000 Grenoble, France, <sup>b</sup>Institut Louis Néel, CNRS, Grenoble, France, and <sup>c</sup>Electrical and Computer Engineering, Boston University, 8 St Mary's Street, Boston, MA 02215, USA. E-mail: srio@esrf.eu



## shadow3

trace

gen\_source

shadow\_pre\_sync

shadow\_pre  
processors

shadow\_post  
processors

shadow\_synchrotron

shadow\_kernel

shadow\_variables

shadow\_beamio

shadow\_math

gfile

stringio

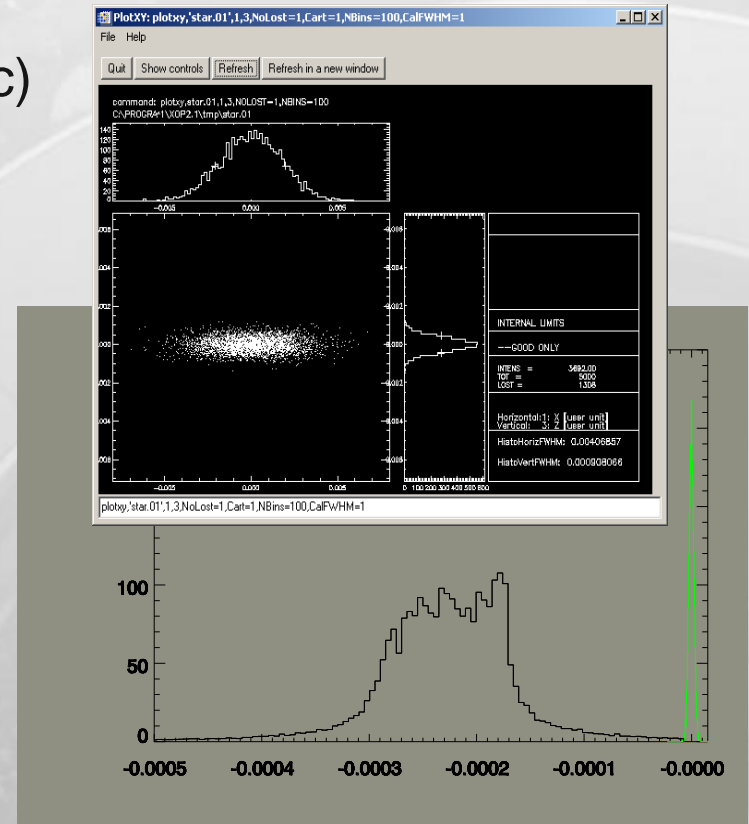
shadow\_globaldefinitions

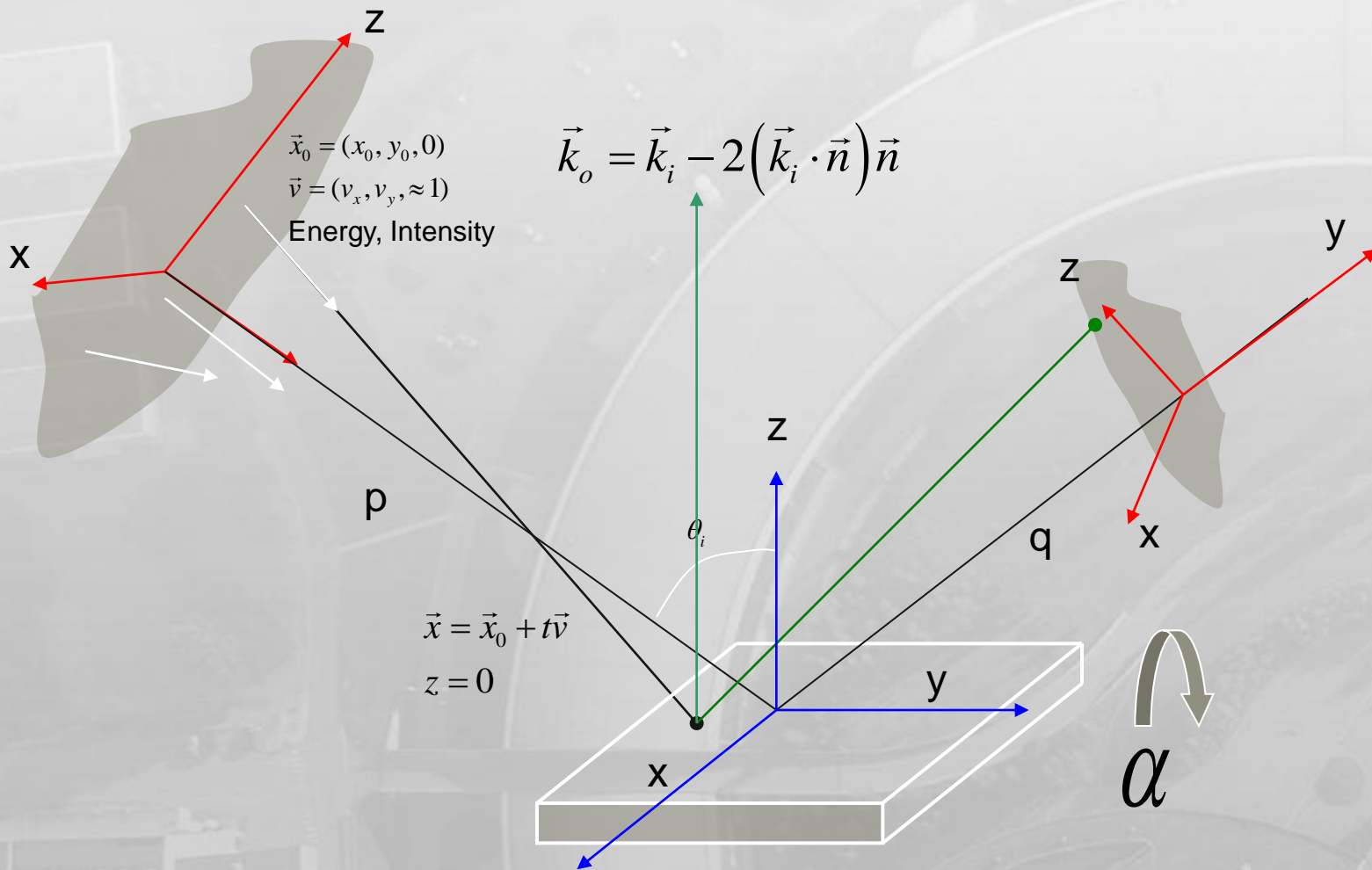


- Beam cross sections (focal spot, PSF, etc)
  - source characteristics (dimensions, depth, emittances)
  - vignetting (apertures, dimension of oe's)
  - effect of mirror shape: aberrations, errors...
  - effect of mirror imperfections (slope errors, roughness?)
  - dump of intensity because of reflectivity of elements

- Energy resolution

- Flux and power (number of photons at a given position, absorbed/transmitted power, etc)
- Other aspects? (polarization, coherence effects, etc.)



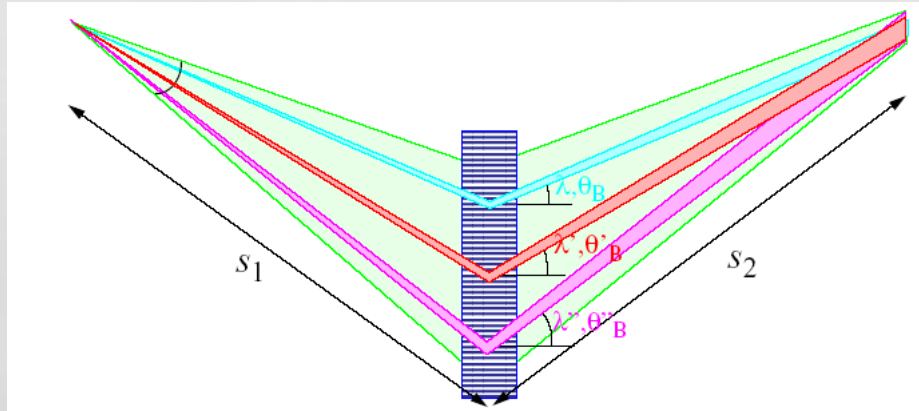


## Examples of applications

Crystals

Gratings

Mirrors



## Focusing characteristics of diamond crystal x-ray monochromators. An experimental and theoretical comparison <sup>a)</sup>

M. Sánchez del Río and G. Grübel  
European Synchrotron Radiation Facility, BP220 38043 Grenoble Cedex 9, France

J. Als-Nielsen  
European Synchrotron Radiation Facility, BP220 38043 Grenoble Cedex 9, France  
and Risø National Laboratory, Roskilde, Denmark

M. Nielsen  
Risø National Laboratory, Roskilde, Denmark

(Received 21 July 1994; accepted for publication)



ELSEVIER

Nuclear Instruments and Methods in Physics Research B 94 (1994) 306–318

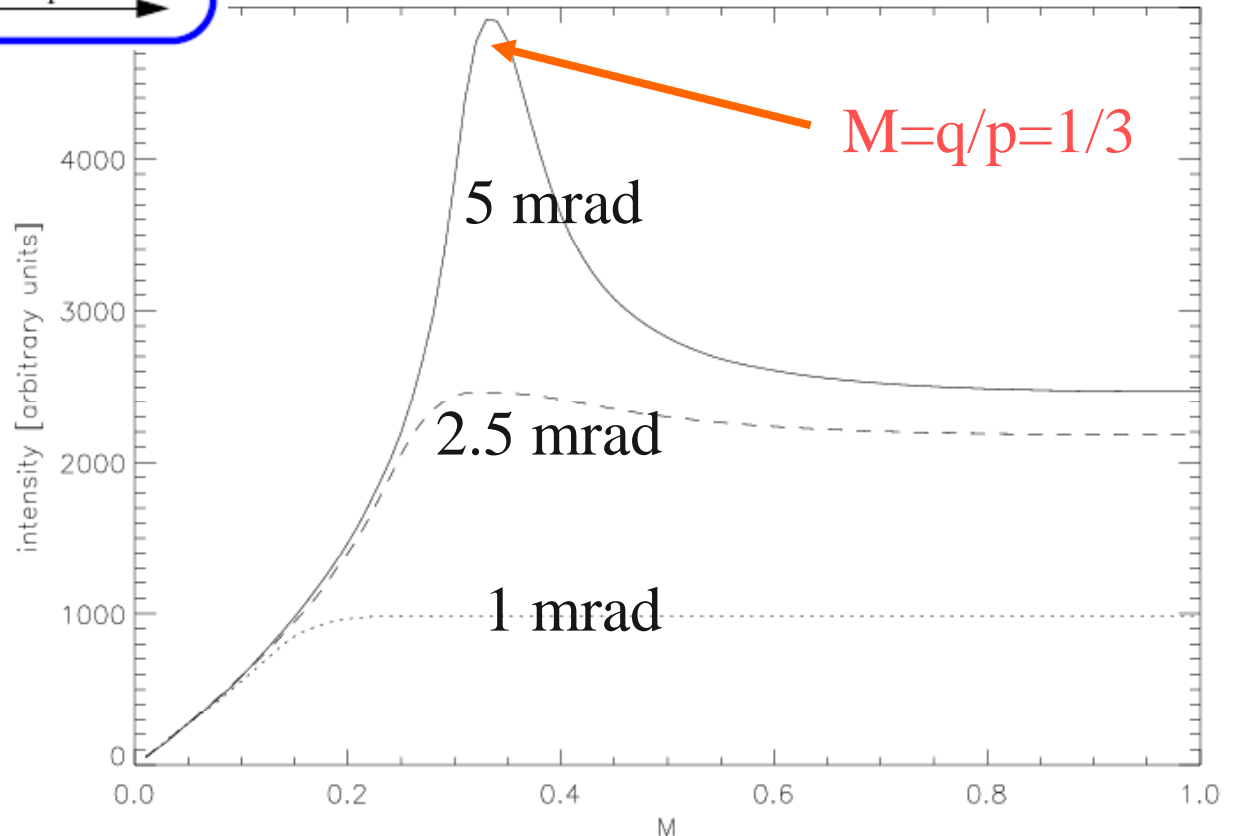
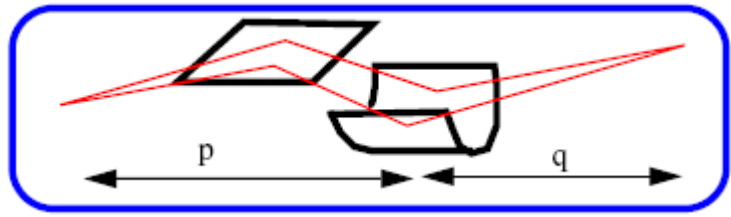


## Multiple station beamline at an undulator X-ray source

J. Als-Nielsen <sup>a,b,\*</sup>, A.K. Freund <sup>b</sup>, G. Grübel <sup>b</sup>, J. Linderholm <sup>a,b</sup>, M. Nielsen <sup>a</sup>,  
M. Sanchez del Rio <sup>b</sup>, J.P.F. Sellschop <sup>c</sup>

See: [ex23\\_crystal\\_laue.ws](#)





**Shape effects:**

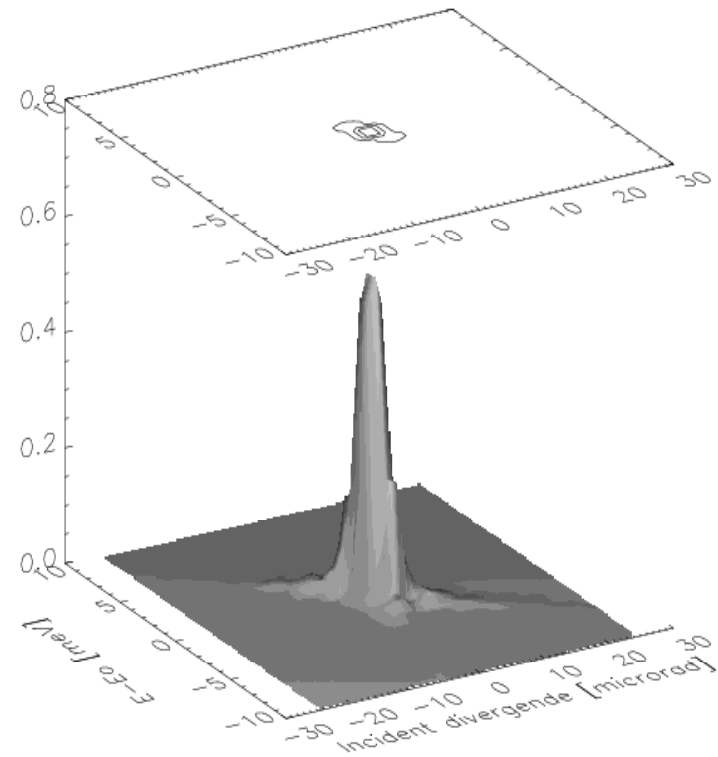
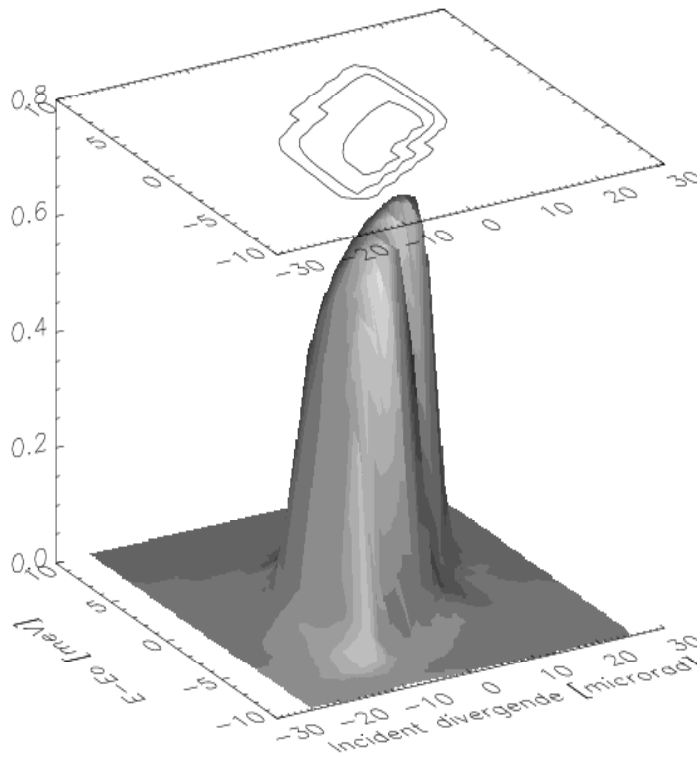
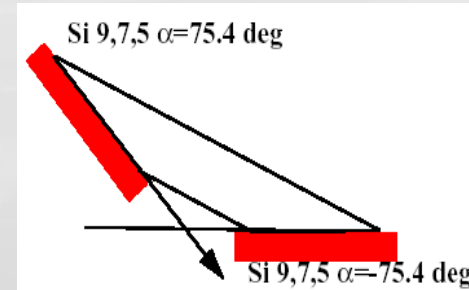
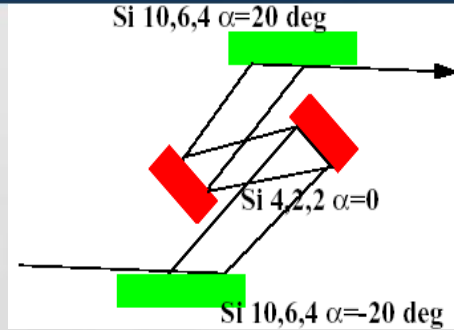
- Anticlastic curvature
- Cylindrical vs Conic

(Ice&Sparks, JOSA A11 (1994) 1265)

**Diffracted beam intensity vs accepted divergence:**

Sparks & Borie, NIM 172 (1980) 172

See: [ex18b\\_sagittalfocusing.ws](http://ex18b_sagittalfocusing.ws)



## X-Ray Bragg Diffraction in Asymmetric Backscattering Geometry

Yu. V. Shvyd'ko\*

Advanced Photon Source, Argonne National Laboratory, A

M. Lerche

University of Illinois at Urbana-Champaign, Urbana  
Advanced Photon Source, Argonne National Laboratory, A

U. Kuetgens

Physikalisch-Technische Bundesanstalt (PTB), Braunschweig

H. D. Rütter

Institut für Experimentalphysik, Universität Hamburg

A. Alatas and J. Zhao

Advanced Photon Source, Argonne National Laboratory, A  
(Received 9 May 2006; published 8 December 2006)

We observe three effects in the Bragg diffraction of x rays in asymmetrically cut crystals. First, exact Bragg backscattering takes place reflecting atomic planes. Second, a well-collimated ( $\approx 1 \mu\text{rad}$ ) beam is transformed into a strongly divergent beam ( $230 \mu\text{rad}$ ) with reflection angle effect of angular dispersion. The asymmetrically cut crystal thus behaves as an incident collimated polychromatic beam. The dispersion rate is  $\approx 230$  reflections accompanying Bragg backreflection are suppressed. These effects are for monochromatization of x rays not limited by the intrinsic width of the Bragg reflection.

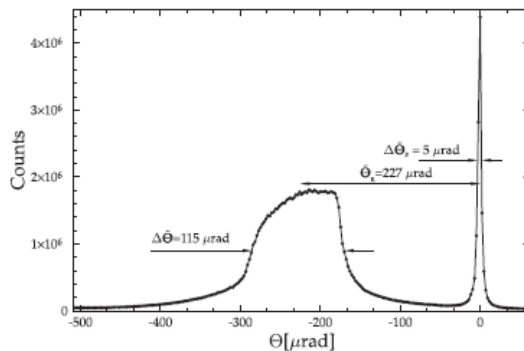
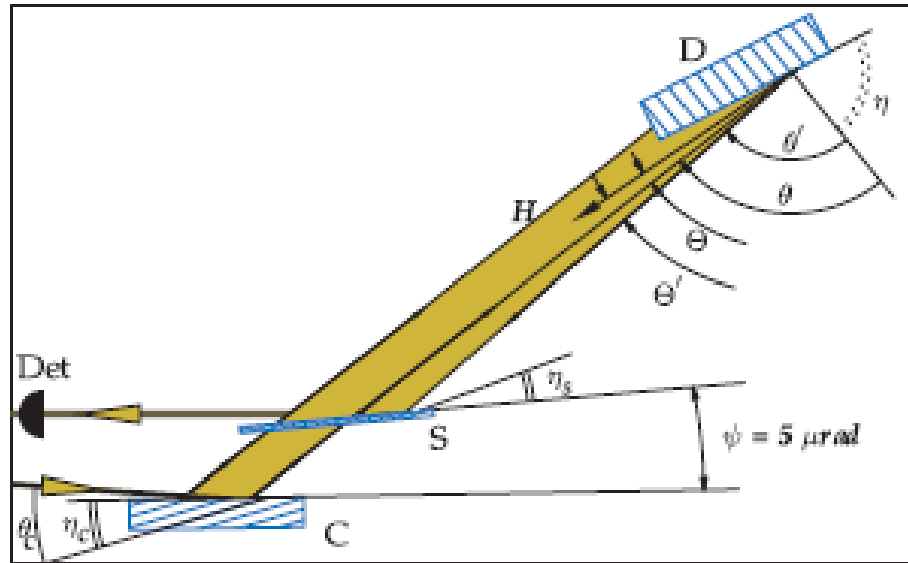
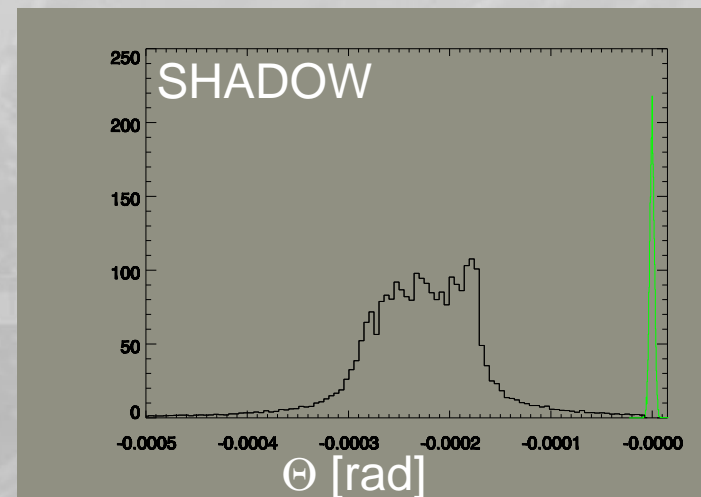
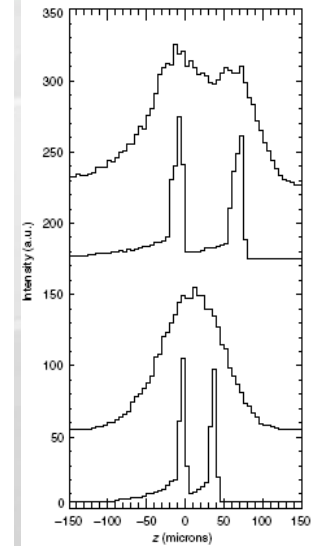
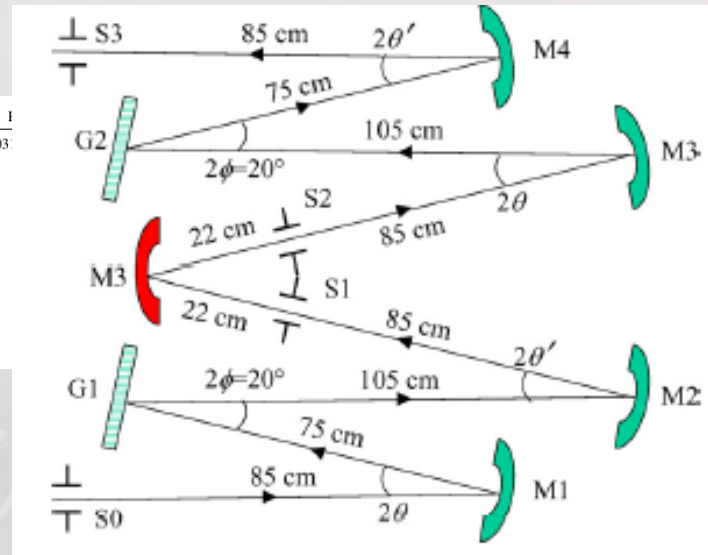


FIG. 4. Bragg reflectivity from crystal *D* of 9.1315 keV x rays, exactly backwards, as a function of the angle of incidence  $\Theta = \pi/2 - \theta$  to the reflecting atomic planes.



# Computer modelling of the optics of a dispersive Raman spectrometer

M Sánchez del Río<sup>1</sup>, E Haro-Poniatowski and M Picquart



Journal of Synchrotron

Spherical-grating monochromator

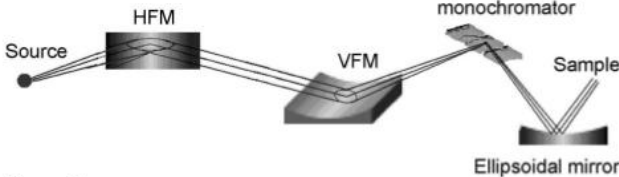
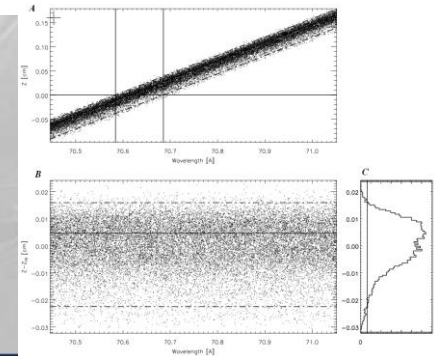


Figure 1 D09 beamline optical components layout.

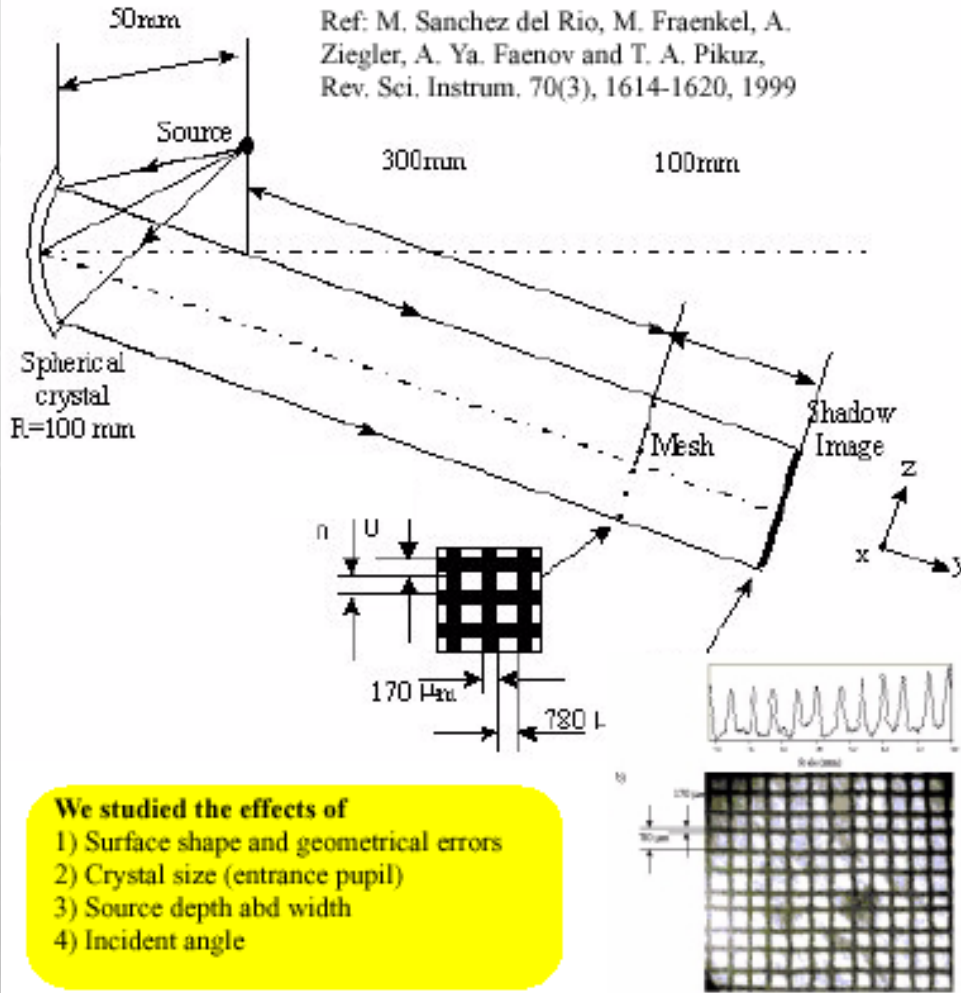
# Geometrical layout and optics modelling of the surface science beamline station at the SESAME synchrotron radiation facility

Wa'el Salah<sup>a,b,\*</sup> and Manuel Sanchez del Rio<sup>c</sup>



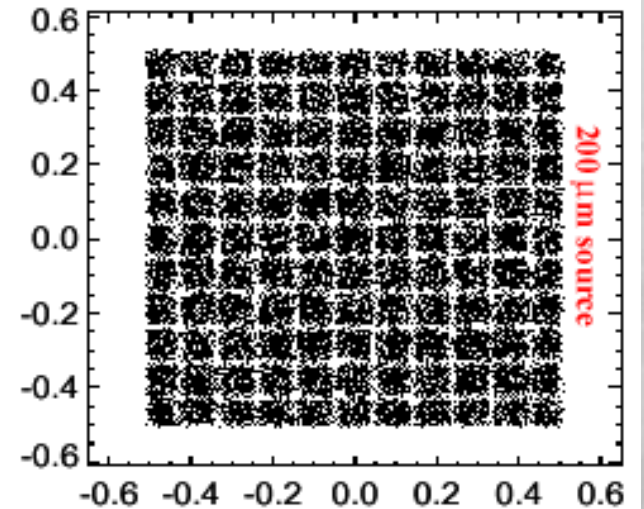
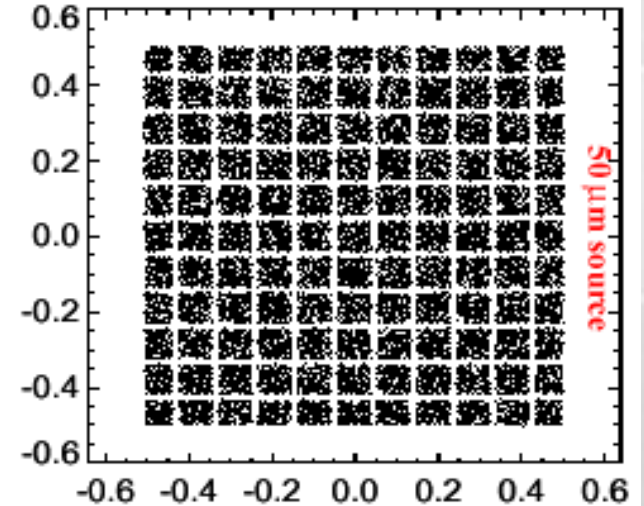
See: [example\\_respwer.ws](http://example_respwer.ws)





**We studied the effects of**

- 1) Surface shape and geometrical errors
- 2) Crystal size (entrance pupil)
- 3) Source depth and width
- 4) Incident angle



See: [example\\_grid\\_pattern.ws](#)

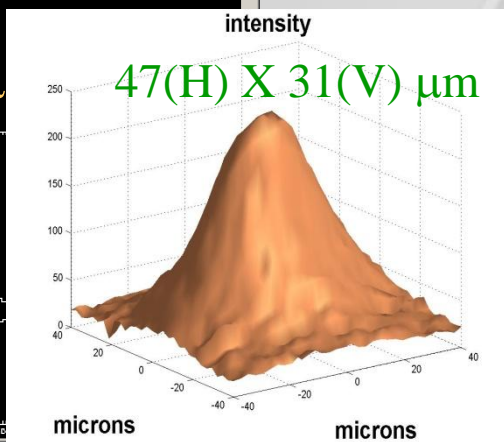
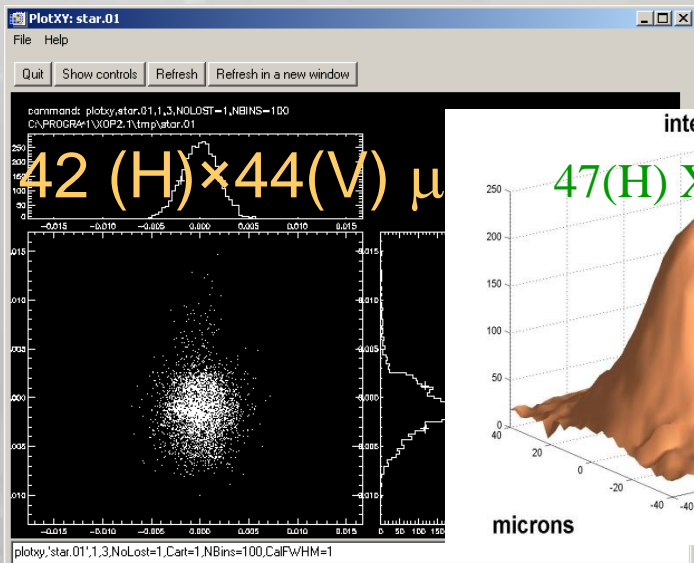
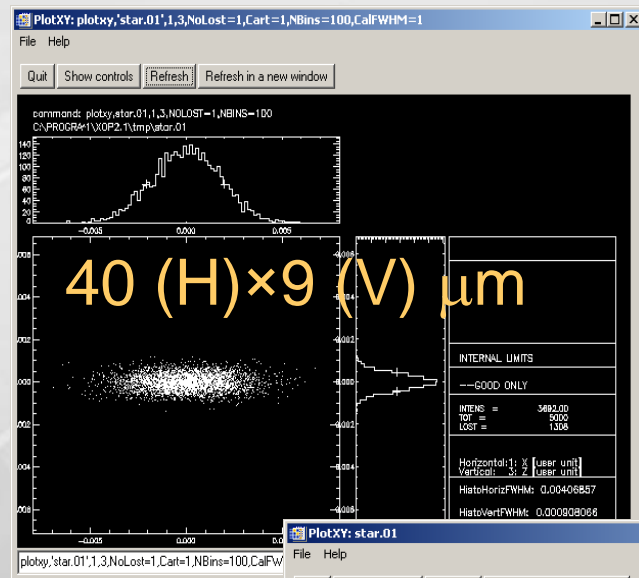
Toroidal mirror M~1/3 ( $p=31$  m,  $q=10$  m  $q=3.5$  mrad)

Gaussian source

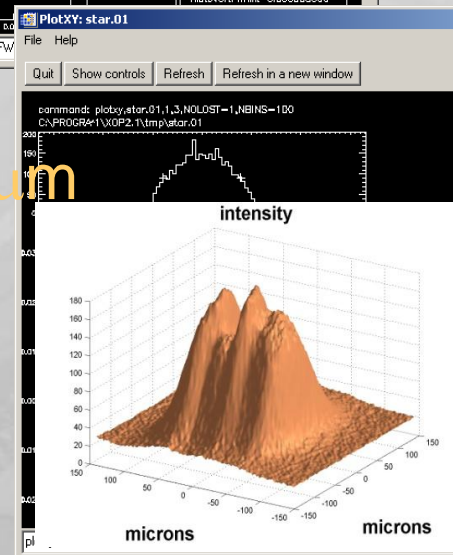
- Size: 134 (H) × 25 (V)  $\mu\text{m}^2$  FWHM
- Divergence: 6.8 (H) × 85.1 (V)  $\mu\text{rad}$  RMS

Expected:

- $134/3=45$  (H)  $\mu\text{m}^2$  FWHM
- $25/3=8.3$  (V)  $\mu\text{m}^2$  FWHM



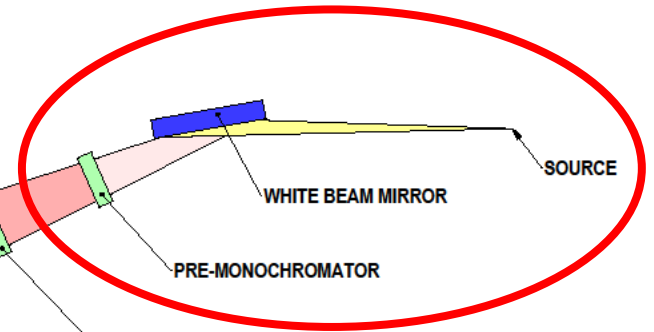
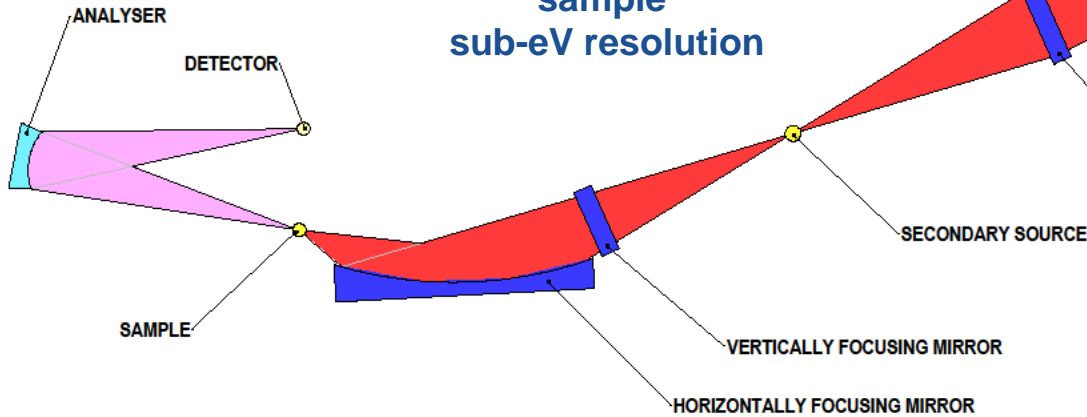
140 × 160  $\mu\text{m}$



See: [macro\\_metrology\\_mirror\\_profile.ws](#), [macro\\_metrology\\_hfm\\_slope.ws](#)

ESRF Upgrade – Examples  
Inelastic scattering UPBL6  
TEXAS ID24  
MASSIF  
Soft X-rays UPBL7

energy in the 5 - 20 keV range  
 focal spot size  $\leq 10 \mu\text{m}$   
 minimal beam losses  
 enough space (>20 cm) around the sample  
 sub-eV resolution



Use of secondary source  
 $(M=M1*M2 \quad M_A=3.1*16 \quad M_B=2.4*23)$   
 First High Power mirror  
 KB: good optical performance  
 Mirror optimisation:  
 (toroid  $M \sim 3$ , distances, astigmatism)  
 Slope errors ( $0.5\text{-}0.7 \mu\text{rad RMS}$ )  
 Power Load  
 Tolerances  
 Monochromator(s) optimization

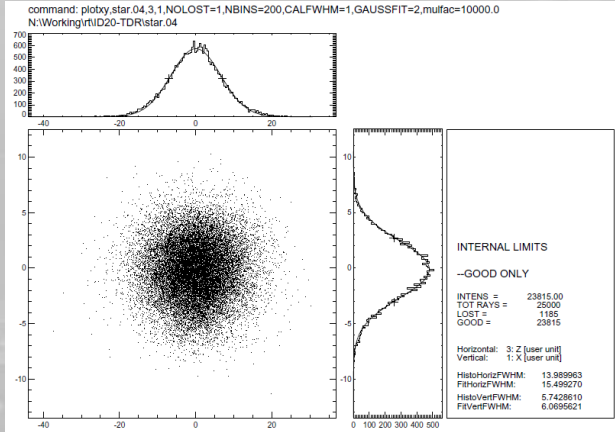
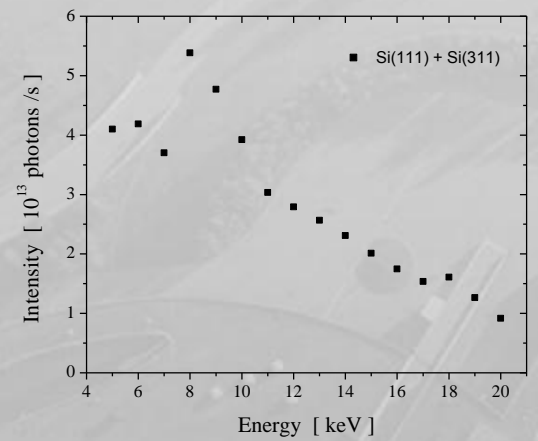
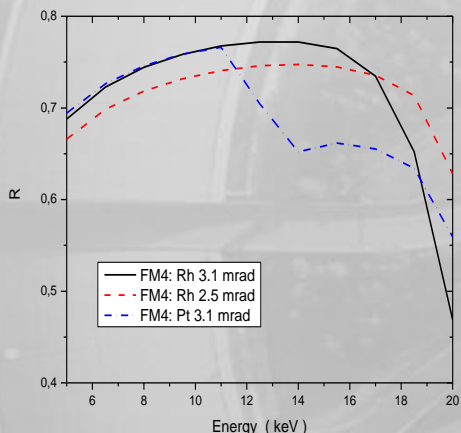
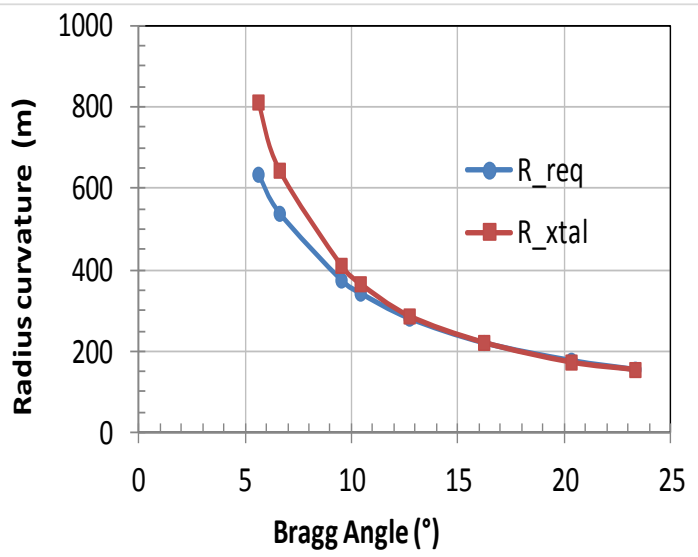
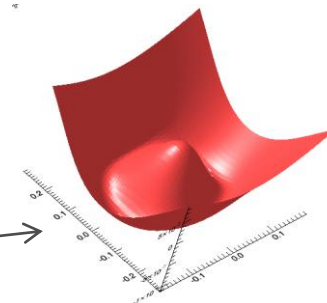
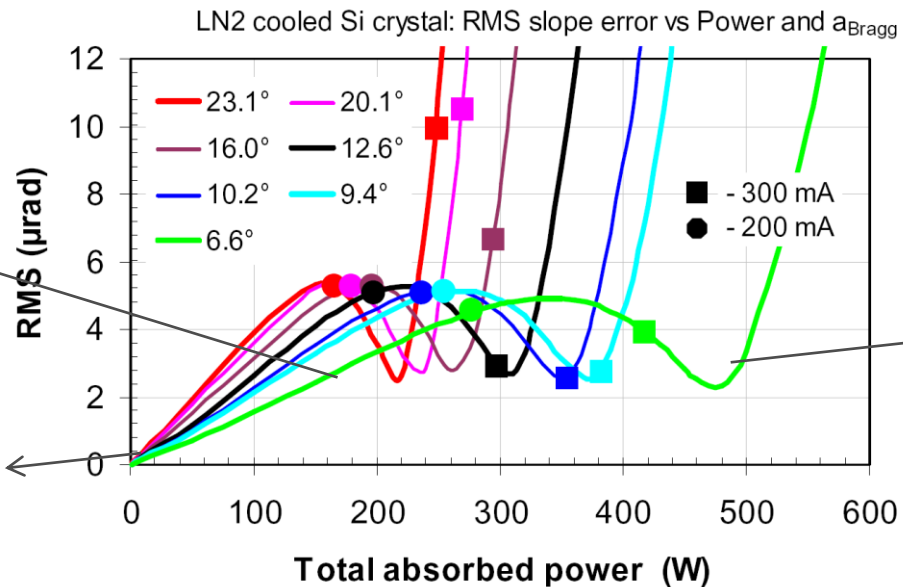
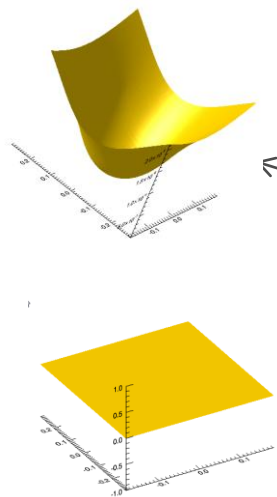
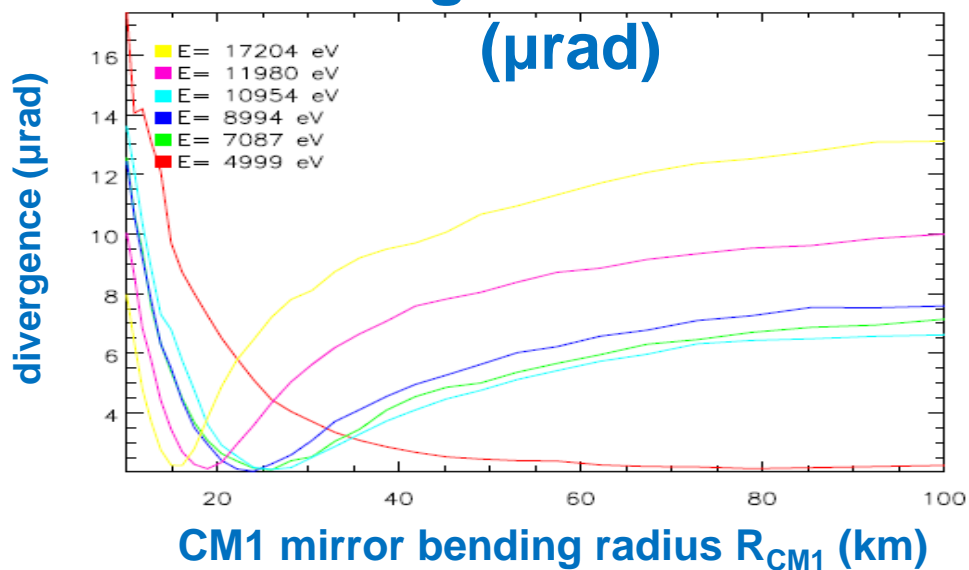


Figure 20: Geometrical contribution (including slope error effects) to the focal spot size at the sample position (optimized design option) on station UPBL06-A. FWHM =  $6 \times 15 \mu\text{m}^2$  V x H.





## Beam divergence before HRM





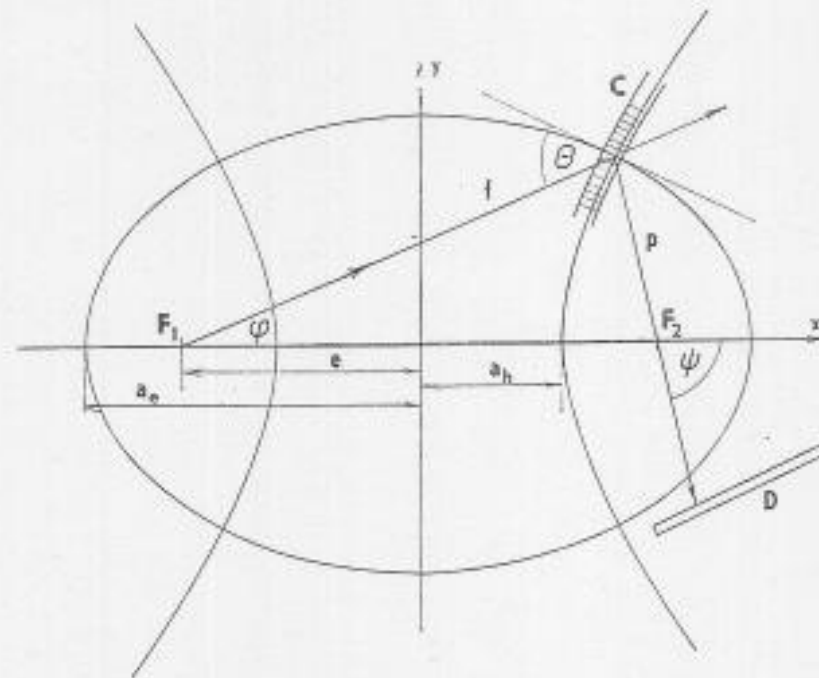


Fig. 1. A schematic drawing of the hyperbolic spectrograph. X-rays with the source in the focus  $F_1$  are, after diffraction on the crystal  $C$ , focused into the focus  $F_2$  and registered by the position sensitive detector  $D$ .

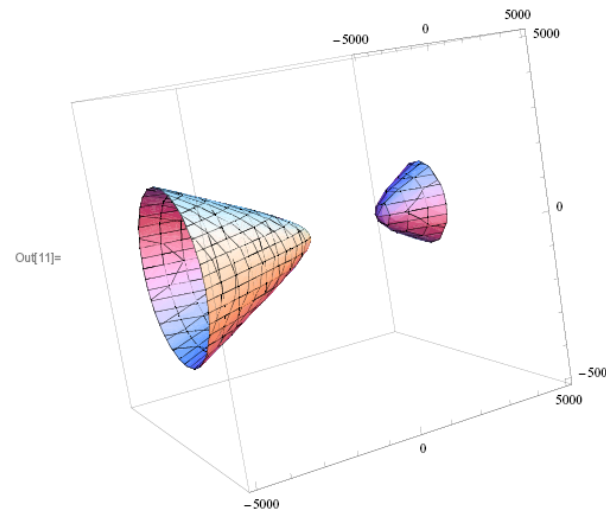
**Hrdy has shown that for focusing x-rays using a Laue crystal with atomic planes perpendicular to the crystal surface, the crystal surface must follow an hyperbola.**

Hrdy, J., 1990. POLYCHROMATIC FOCUSING OF X-RAYS IN LAUE-CASE DIFFRACTION - (HYPERBOLICAL SPECTROGRAPH). Czechoslovak Journal of Physics 40, 1086-1090.

$$c_0 x^2 + c_1 y^2 + c_2 z^2 + c_3 xy + c_4 yz + c_5 xz + c_6 x + c_7 y + c_8 z + c_9 = 0$$

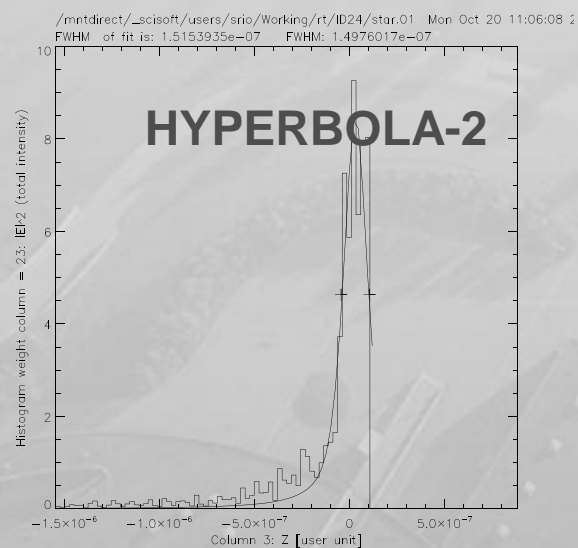
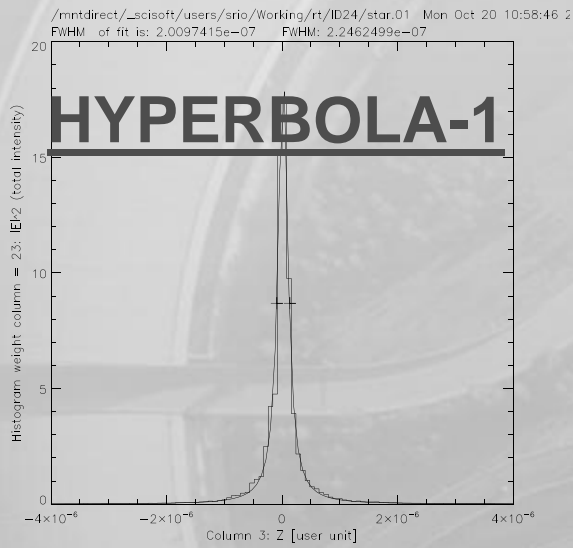
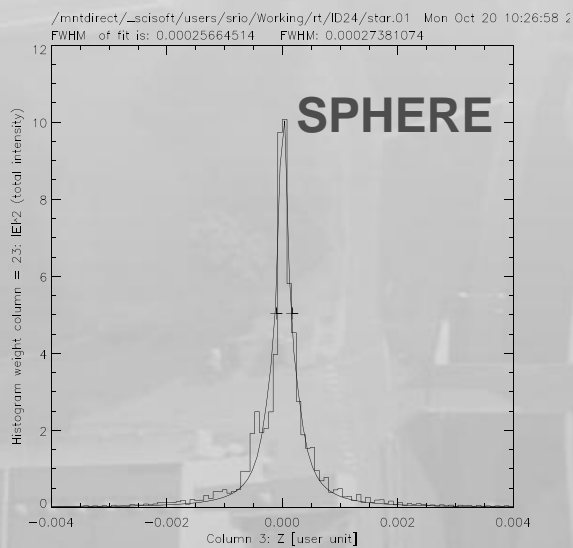
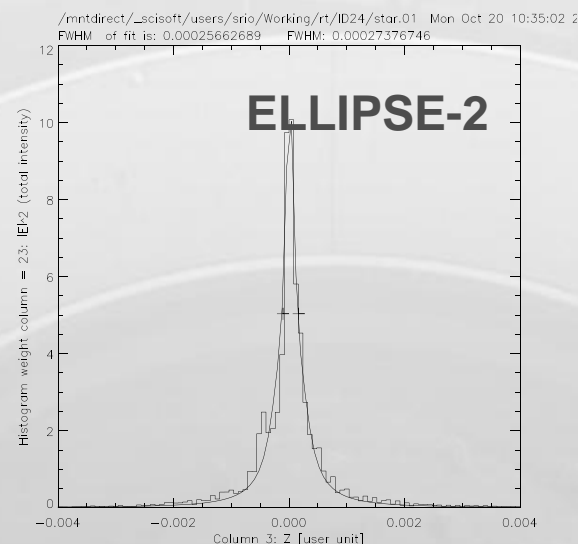
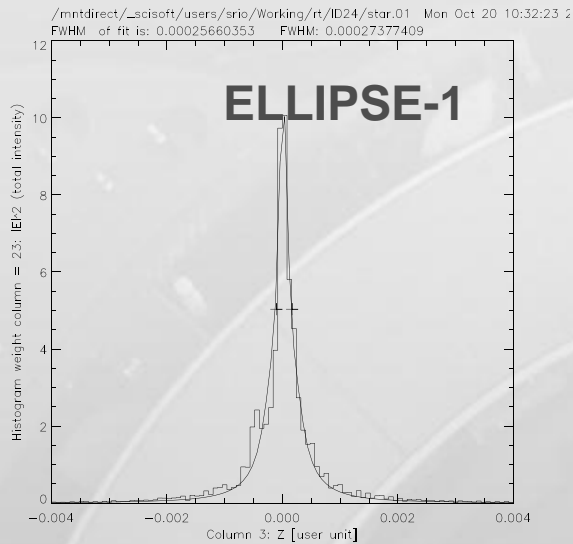
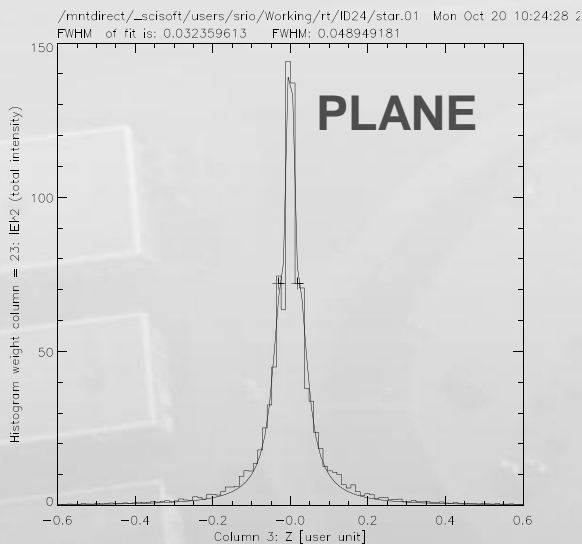
	plane	sphere	ellipse1	ellipse2	hyperbola1	hyperbola2
c0	0	1	2.99E-06	2.99E-06	-3E-06	-3E-06
c1	0	1	2.81E-06	2.81E-06	-2.8E-06	-2.8E-06
c2	0	1	6.01E-07	6.01E-07	3.1E-07	3.1E-07
c3	0	0	0	0	0	0
c4	0	0	-1.3E-06	1.32E-06	-1.6E-06	1.55E-06
c5	0	0	0	0	0	0
c6	0	0	0	0	0	0
c7	0	0	0	0	0	0
c8	-1	476.1324	0.001336	1.34E-03	-0.00145	-0.00145
c9	0	0	0	0	0	0

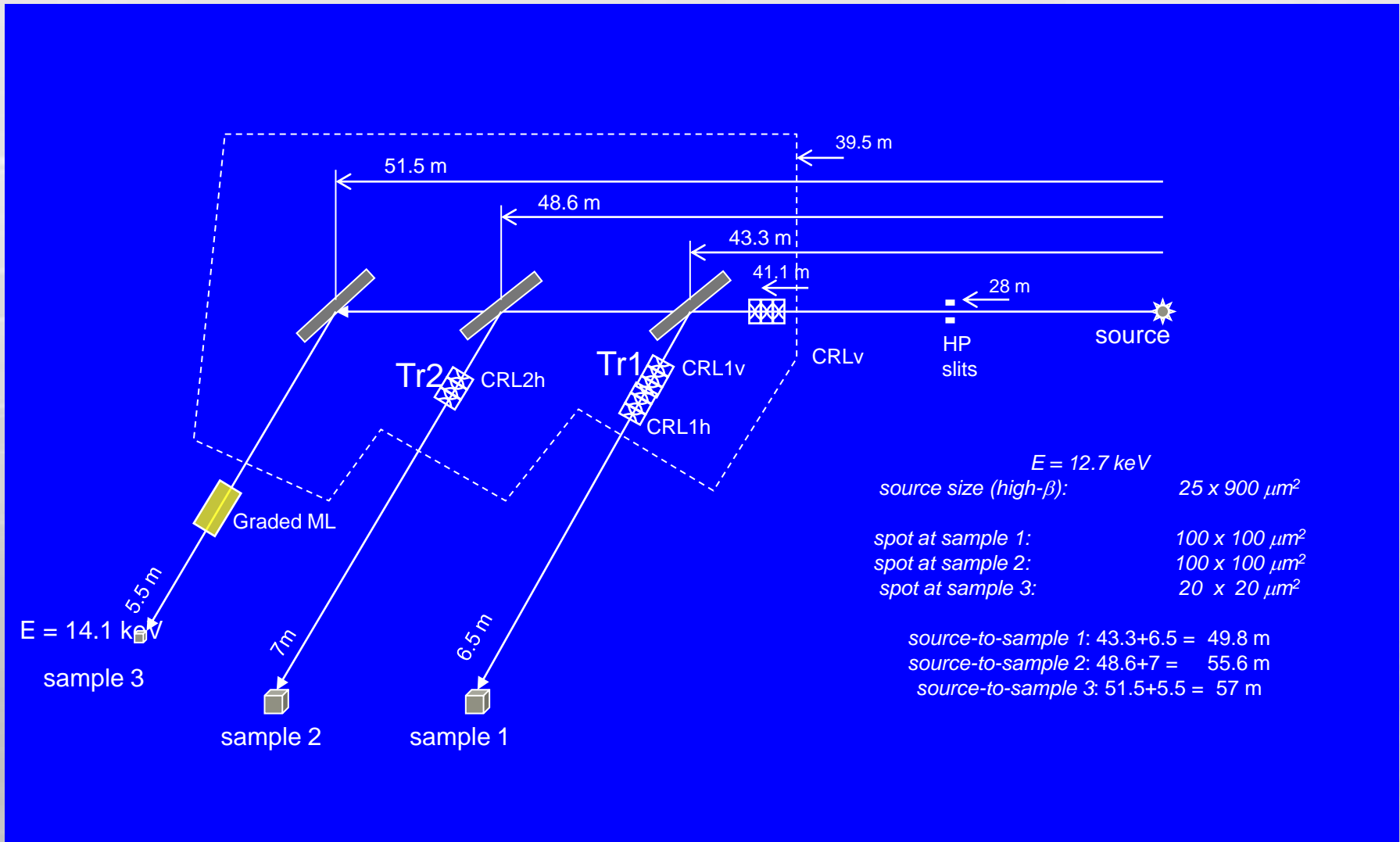
```
In[11]= ContourPlot3D[ccc1*x^2 + ccc2*y^2 + ccc3*z^2 + ccc4*x*y + ccc5*y*z + ccc6*x*z +
ccc7*x + ccc8*y + ccc9*z + ccc10 == 0, {x, -5000, 5000}, {y, -5000, 5000}, {z, -5000, 5000}]
```

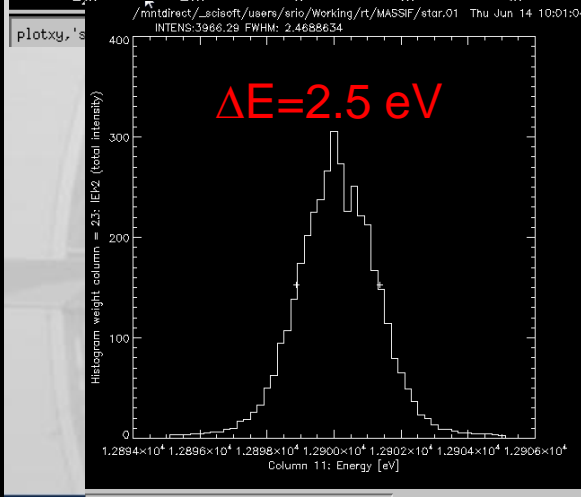
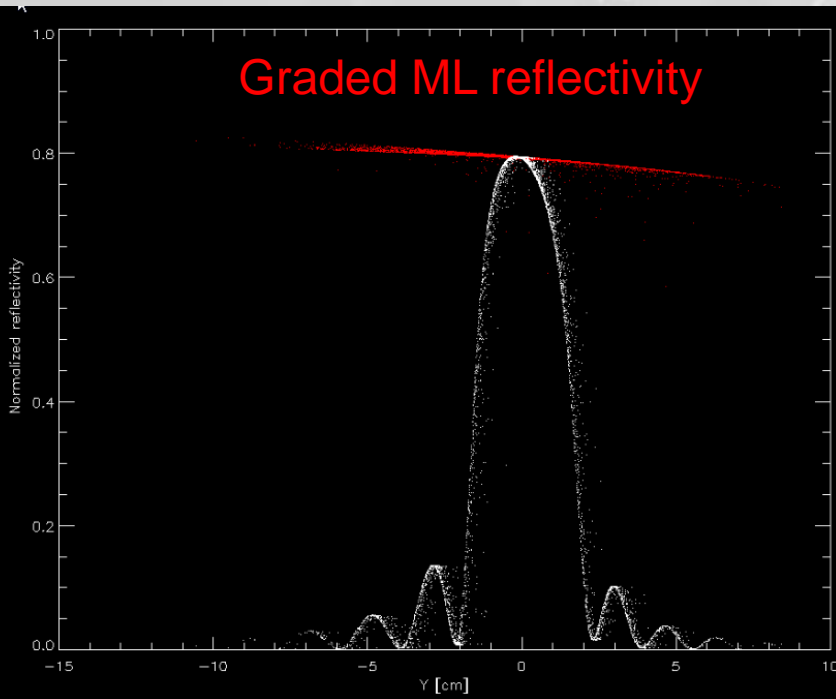
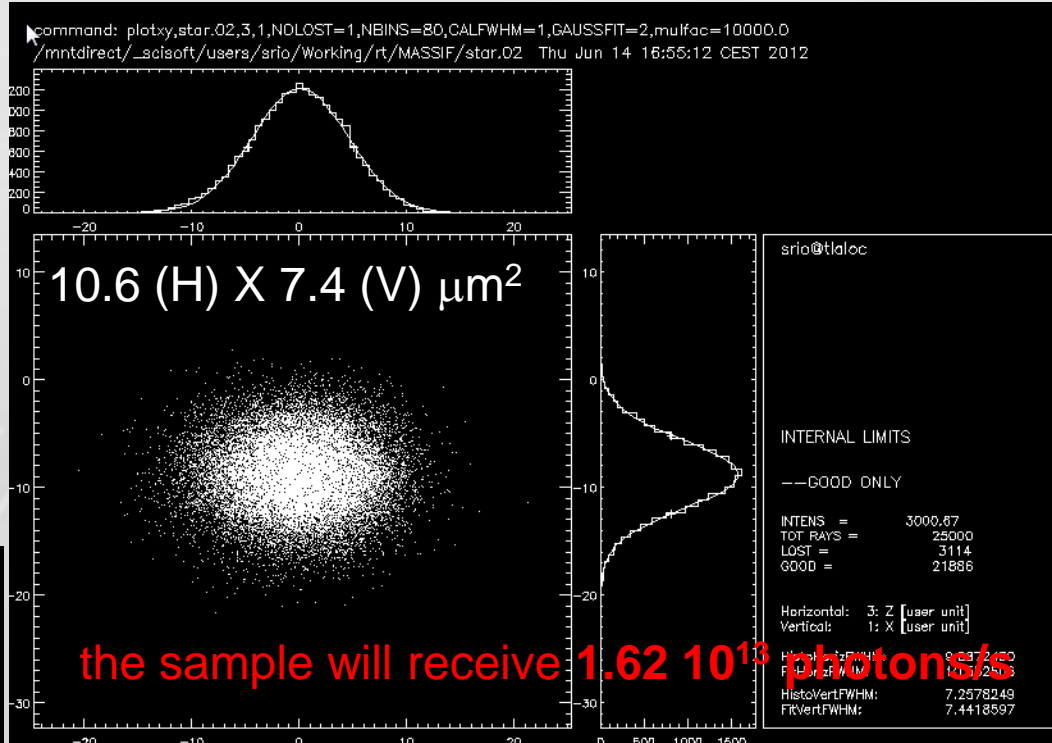
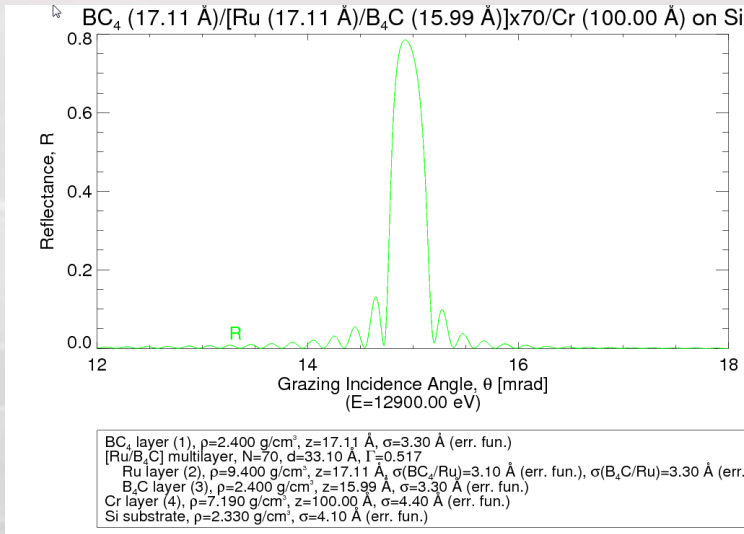


**p=2790, q=120 and  $\theta_B=14.3\text{deg}$ .**

Ellipse2 (Hyperbola2) is obtained from ellipse1 (Ellipse1) by symmetry with respect to the (x,z) plane (i.e.,  $y \rightarrow -y$ ).







the sample will receive  $1.62 \cdot 10^{13}$  photons/s



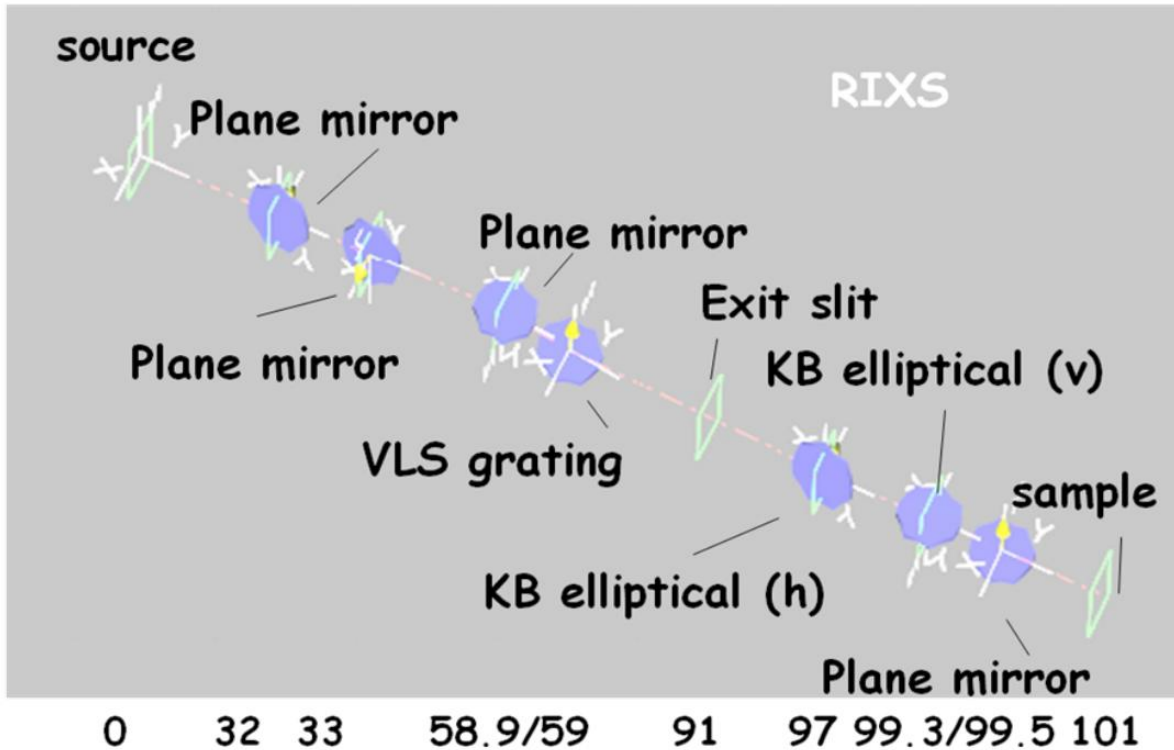


Figure 18: Optical layout with a horizontal monochromator exit arm

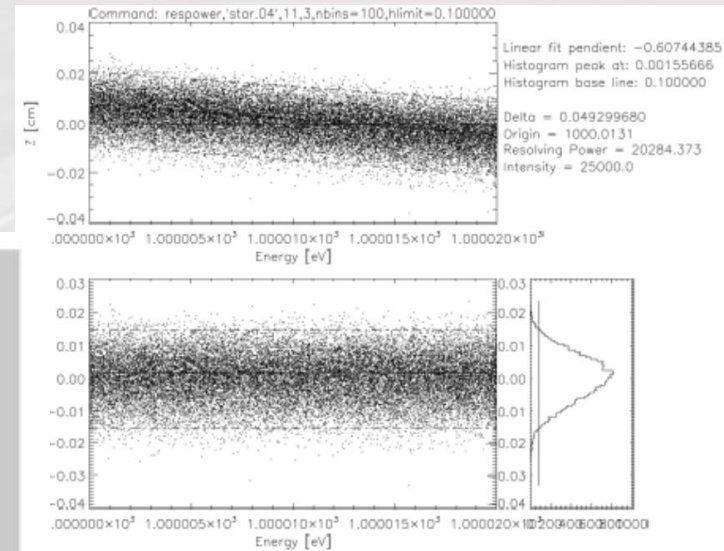


Figure 28: Ultimate resolution with a 1000 l/mm grating

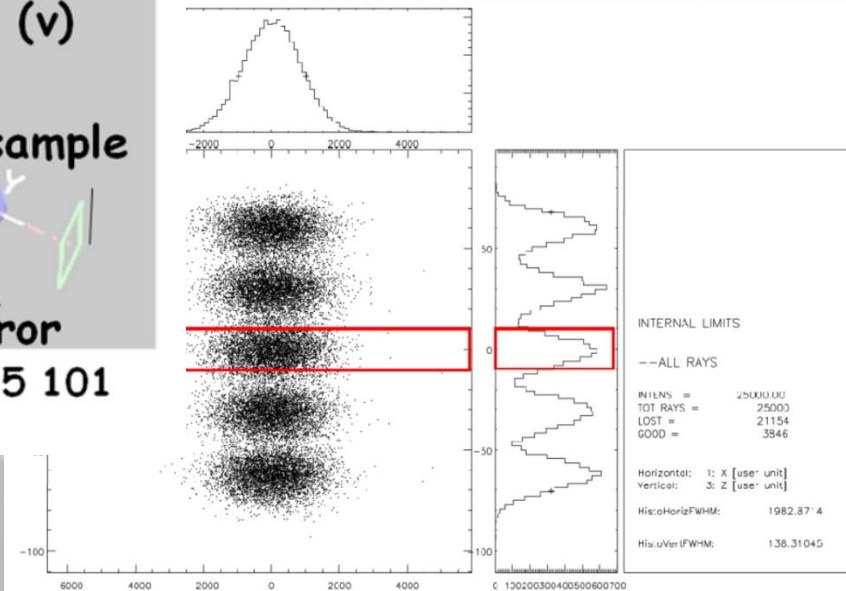
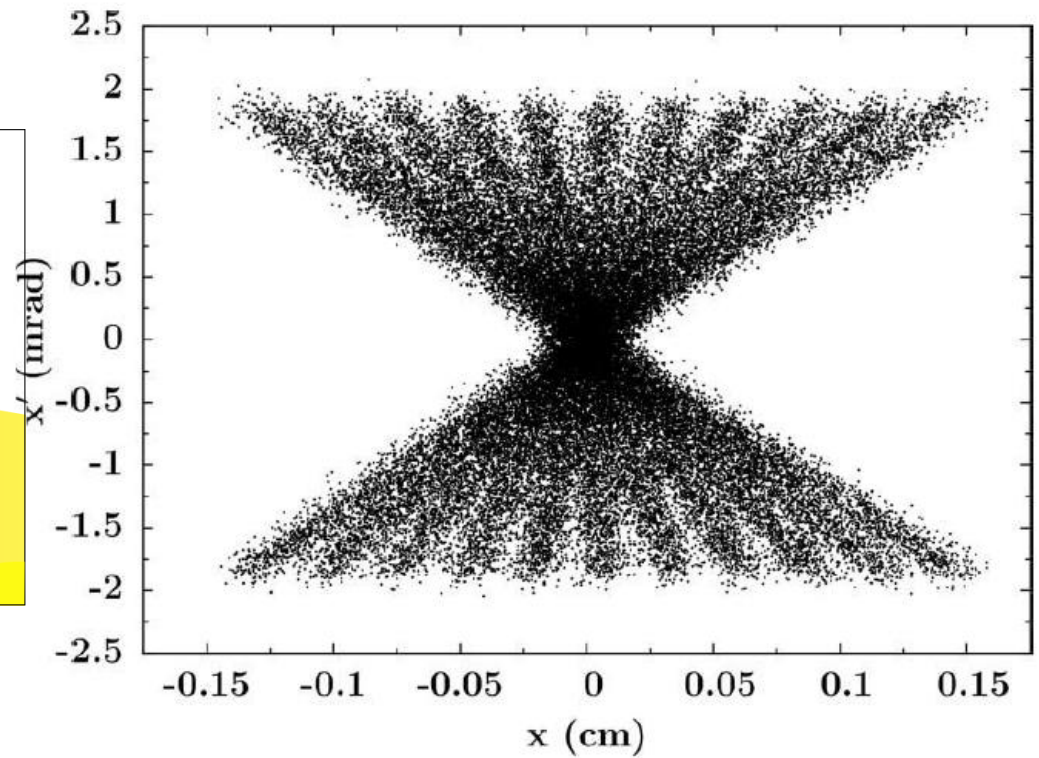
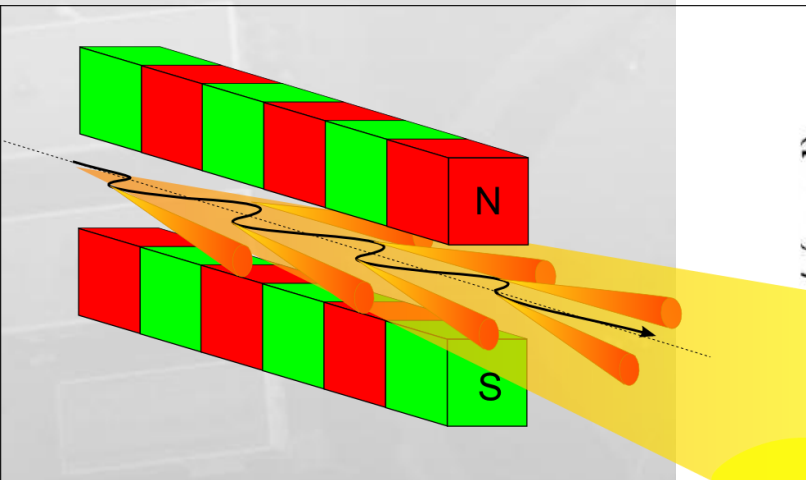


Figure 29: Energy separation of lines. The red rectangle represents the exit slit (20 μm)

# On-going developments



**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.

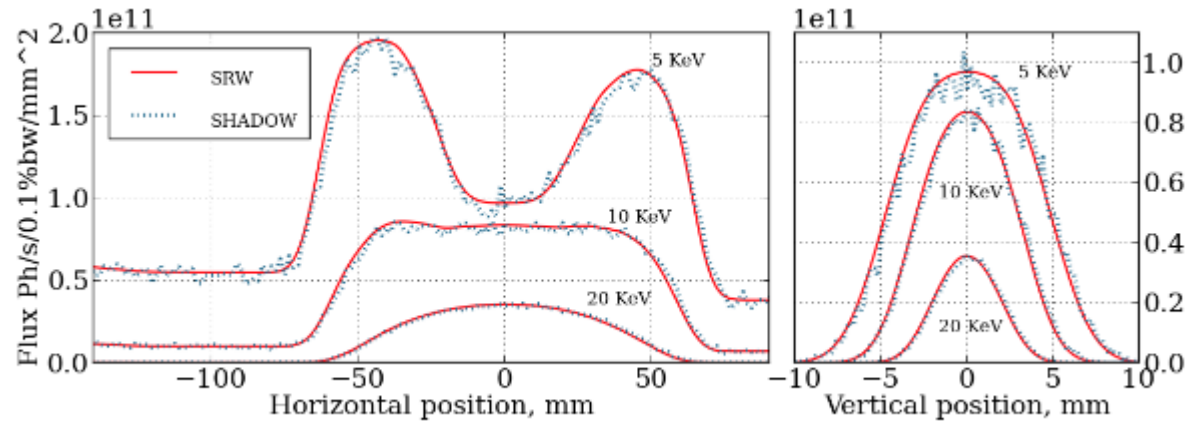
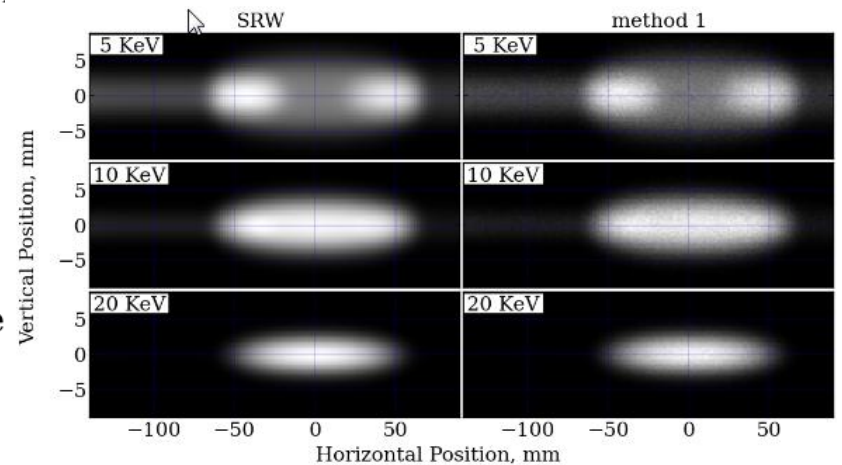
See: [macro\\_source\\_spectrum.ws](#)

## Improved models for synchrotron radiation source in SHADOW

Niccolo Canestrari<sup>1,2</sup>, Oleg Chubar<sup>1</sup>, Manuel Sanchez del Rio<sup>2</sup>




<sup>1</sup> Brookhaven National Laboratory, Upton, NY 11973

<sup>2</sup> European Synchrotron Radiation Facility, Grenoble, France 38043



See:  
[shadow3/README\\_PYTHON.txt](#)  
[shadow3/SRW2SHADOW\\_Example01.py](#)



	$n_1 < n_2$	$n_1 > n_2$
Collimated to convergent 	Ellipse c)	Hyperbola a)
Convergent to collimated 	Hyperbola	Ellipse
Divergent to convergent 	Cartesian oval d)	Cartesian oval b)

Journal of  
Synchrotron  
Radiation

ISSN 0909-0495

Received 1 May 2011

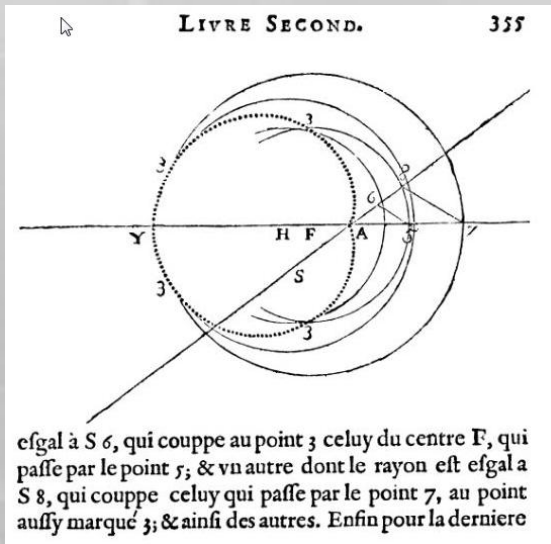
Accepted 24 January 2012

## Aspherical lens shapes for focusing synchrotron beams

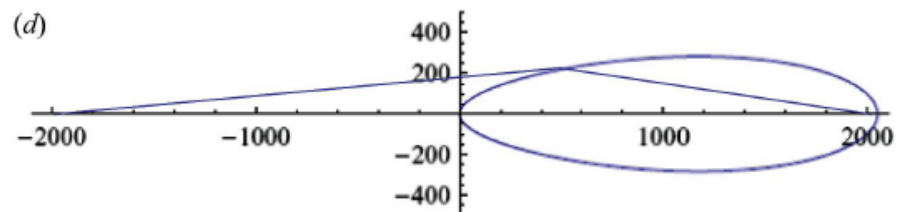
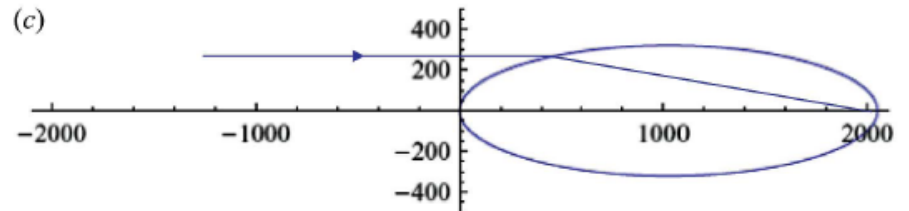
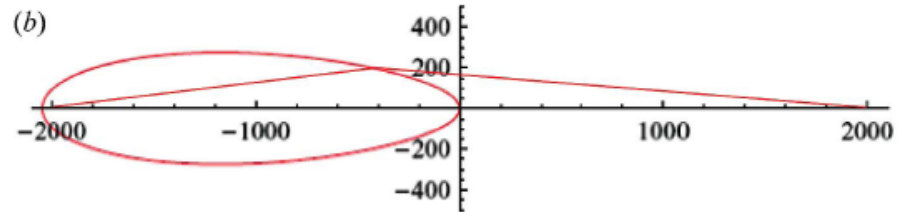
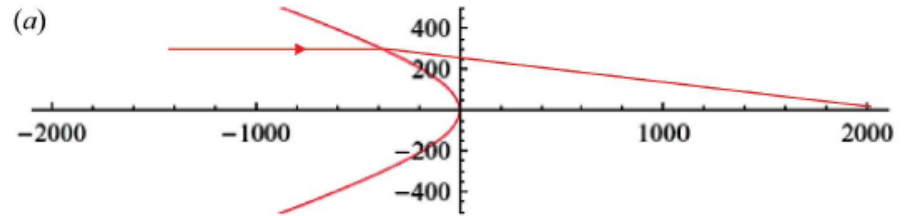
Manuel Sanchez del Rio<sup>a\*</sup> and Lucia Alianelli<sup>b</sup>

<sup>a</sup>European Synchrotron Radiation Facility, France, and <sup>b</sup>Diamond Light Source Ltd, UK.

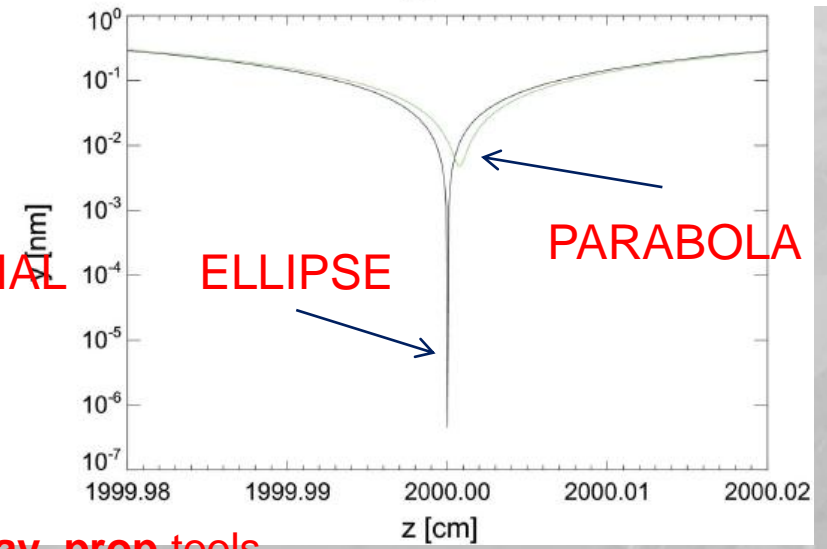
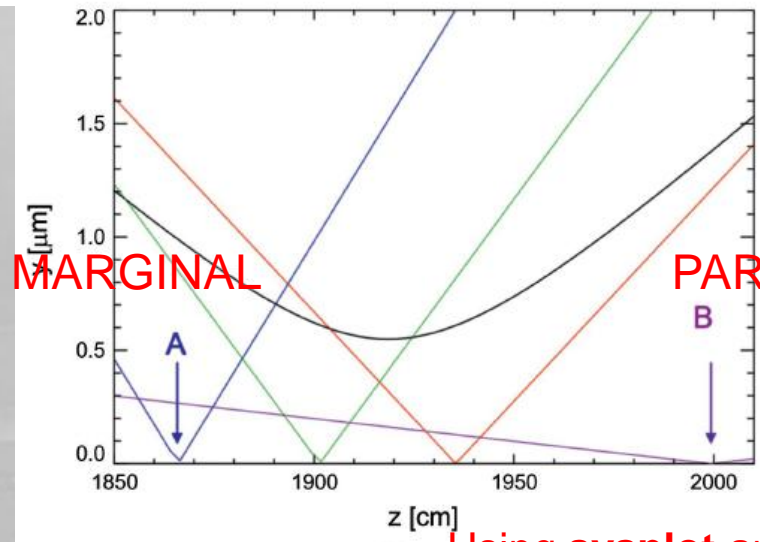
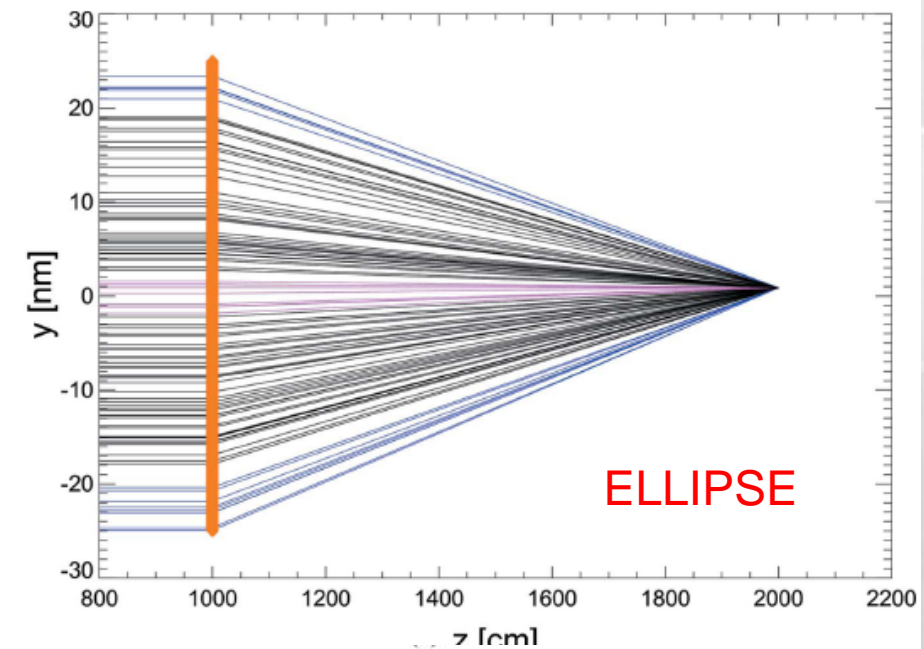
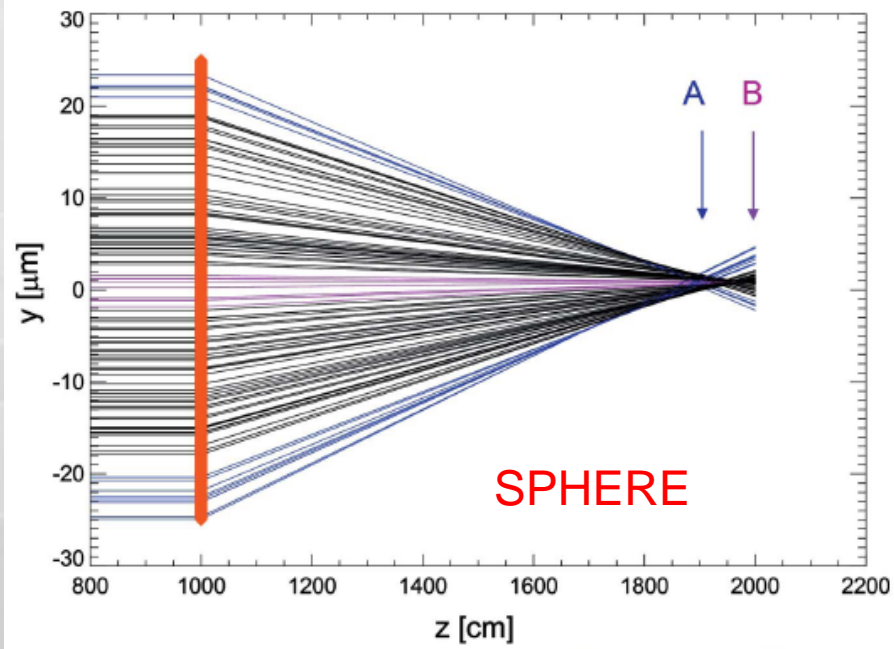
Figure 4  
Ideal surface shape for different focusing conditions.



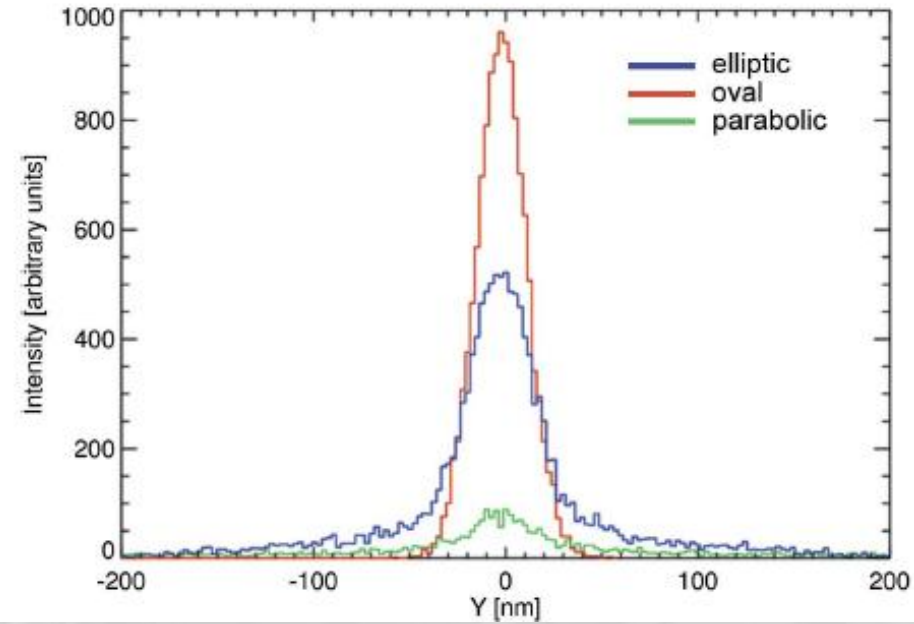
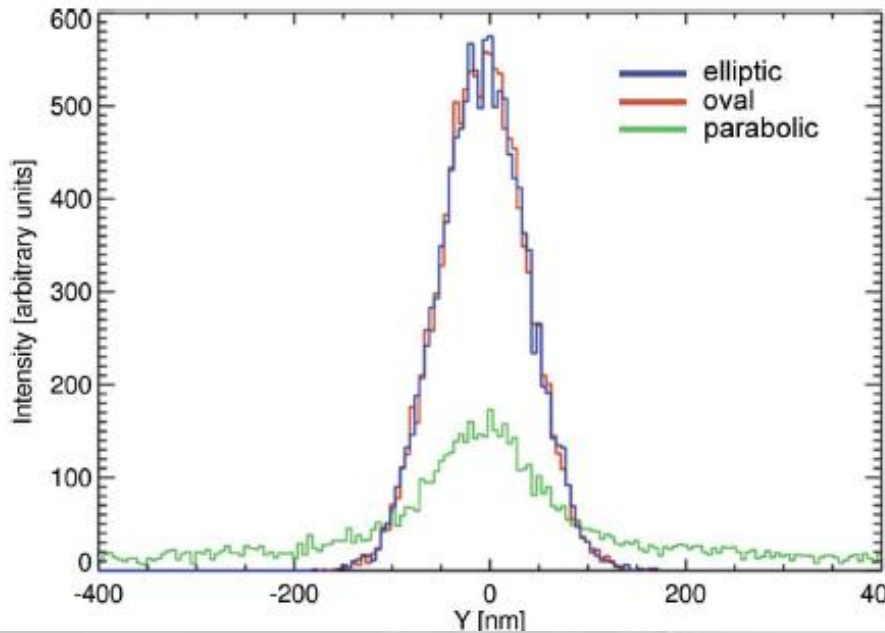
Descartes 1637







Using **sysplot** and **ray\_prop** tools



E=8 keV  
Si Lens  
p=47 m  
h=0.3 mm

q=30 cm  
M=157

q=10 cm  
M=470

We may need in the future to shape lenses following the Cartesian oval...

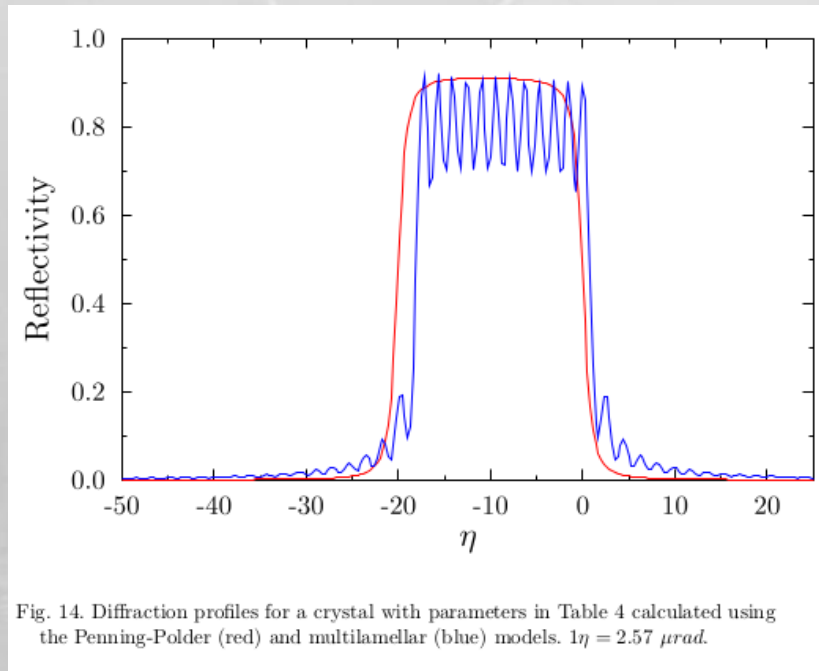


See:  
[shadow3/README\\_CRL.txt](#)  
[lens\\_single\\_sysplot.ws](#)  
[lens\\_chromatic\\_aberrations.ws](#)  
[crl\\_snigirev1996.ws](#)

```
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
```

- Allow any crystal structure (e.g., quartz)
- Calculate diffraction profiles for bent crystals (ML & PP)
- Allow the possibility to use external diffraction profiles
- X-ray polarisers (changes in phase)
- UPBL2 High energy X-rays



See: [macro\\_crystal\\_with\\_external\\_diffraction\\_profile.ws](#)

- Current limitations
  - The current data is quite old (new tabulations are available)
  - Only covers 30eV-100keV
  - It does not include Compton scattering (important in many cases)
- Good points
  - SHADOW optic library is decoupled from the kernel
  - Re-write the preprocessors with using your preferred data
- Ideas
  - Rebuild the existing database with new data and perhaps more points
  - Use xraylib

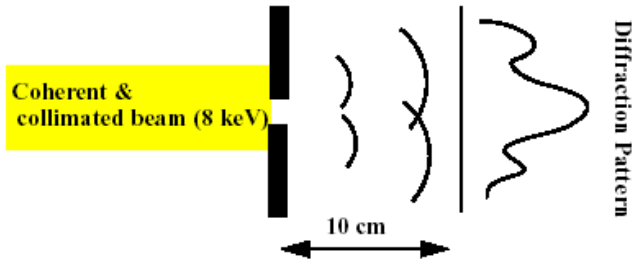
See:

[shadow3/README\\_PYTHON.txt](#)

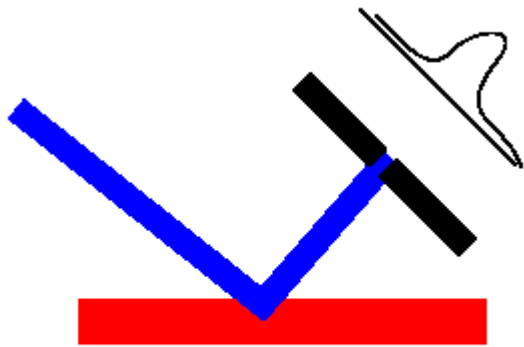
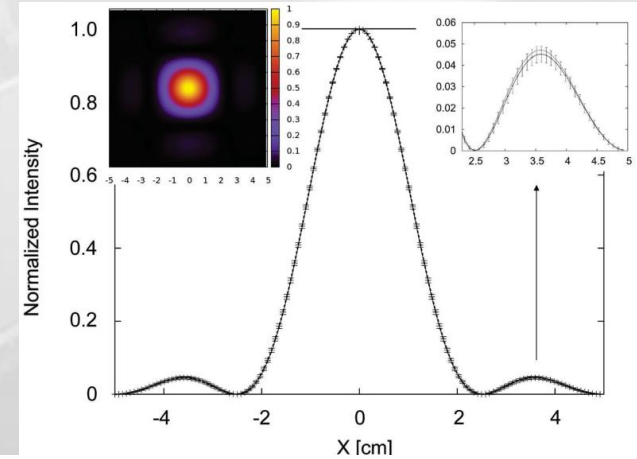
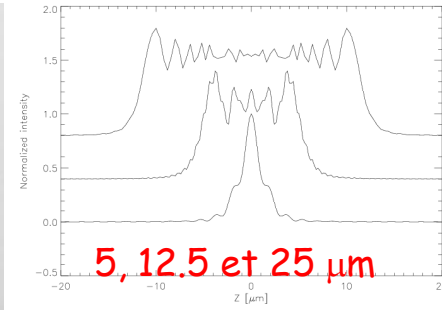
[shadow3/ShadowPreprocessorsXraylib.py](#)



$$u(\mathbf{x}) = \frac{ikI}{4\pi} \int_A u_{\text{inc}}(\mathbf{r}) \frac{e^{iks}}{s} dS$$

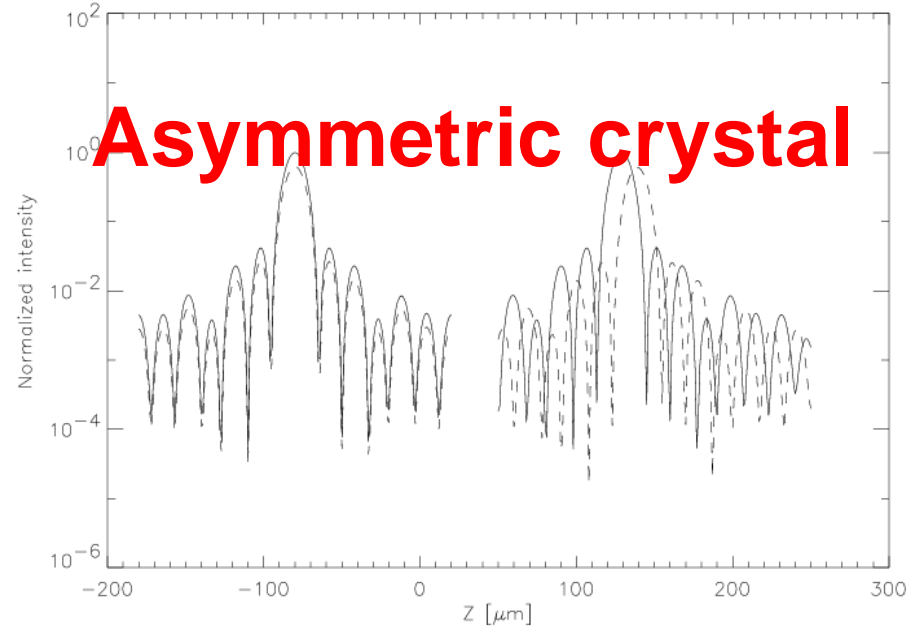


Fraunhofer Diffraction by a slit



Si 111,  $\alpha=0$ ,  $\alpha=0.15$  deg

8 keV,  $\Delta E \sim 1$  eV



# Two slits experiment

## Coherence by propagation

Thomson & Wolf, JOSA 47, 895 (1957)

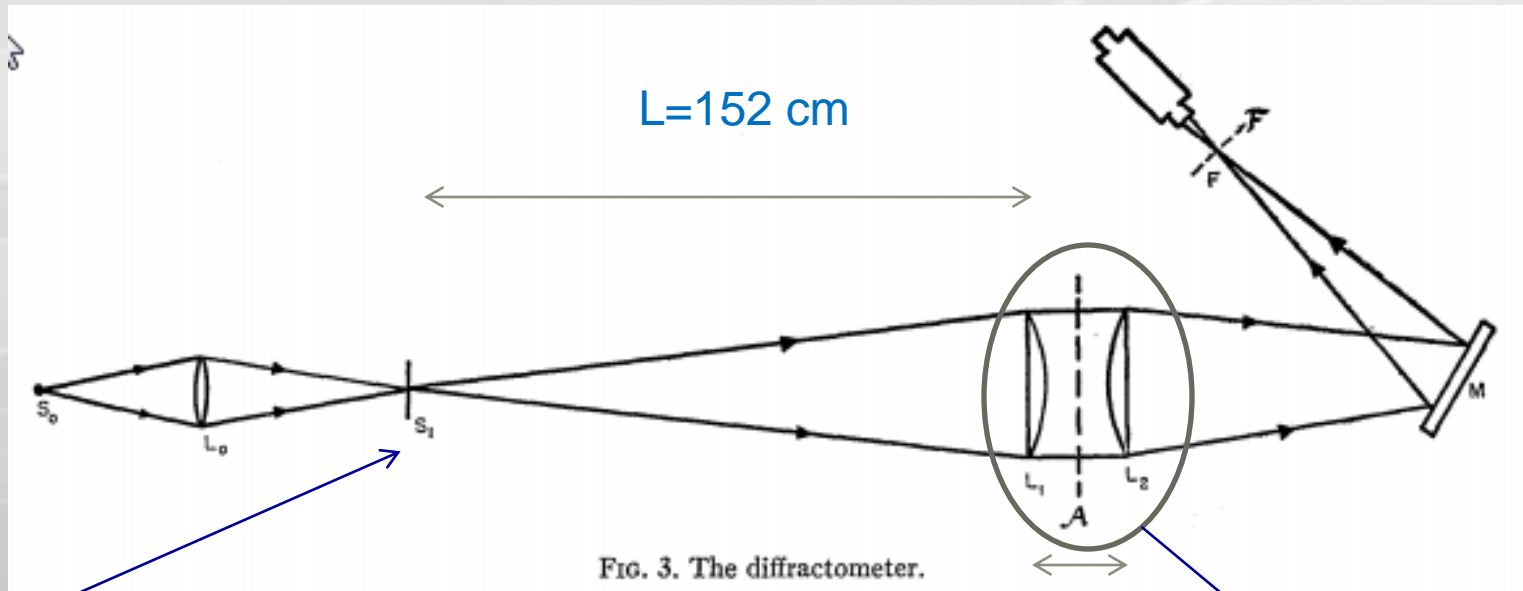
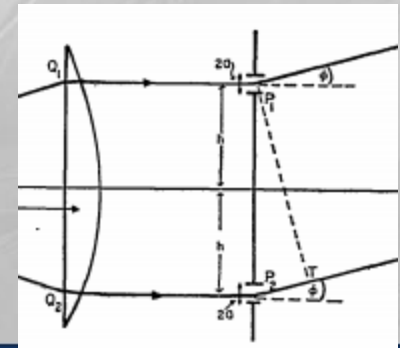


FIG. 3. The diffractometer.

- $S_1$  INCOHERENT source ( $90 \mu\text{m}$ )
- $\lambda=579$  nm

$L_1-L_2=14$  cm

- 2xPinhole  $\varnothing=0.14$  cm
- $2h=0.6-2.5$  cm



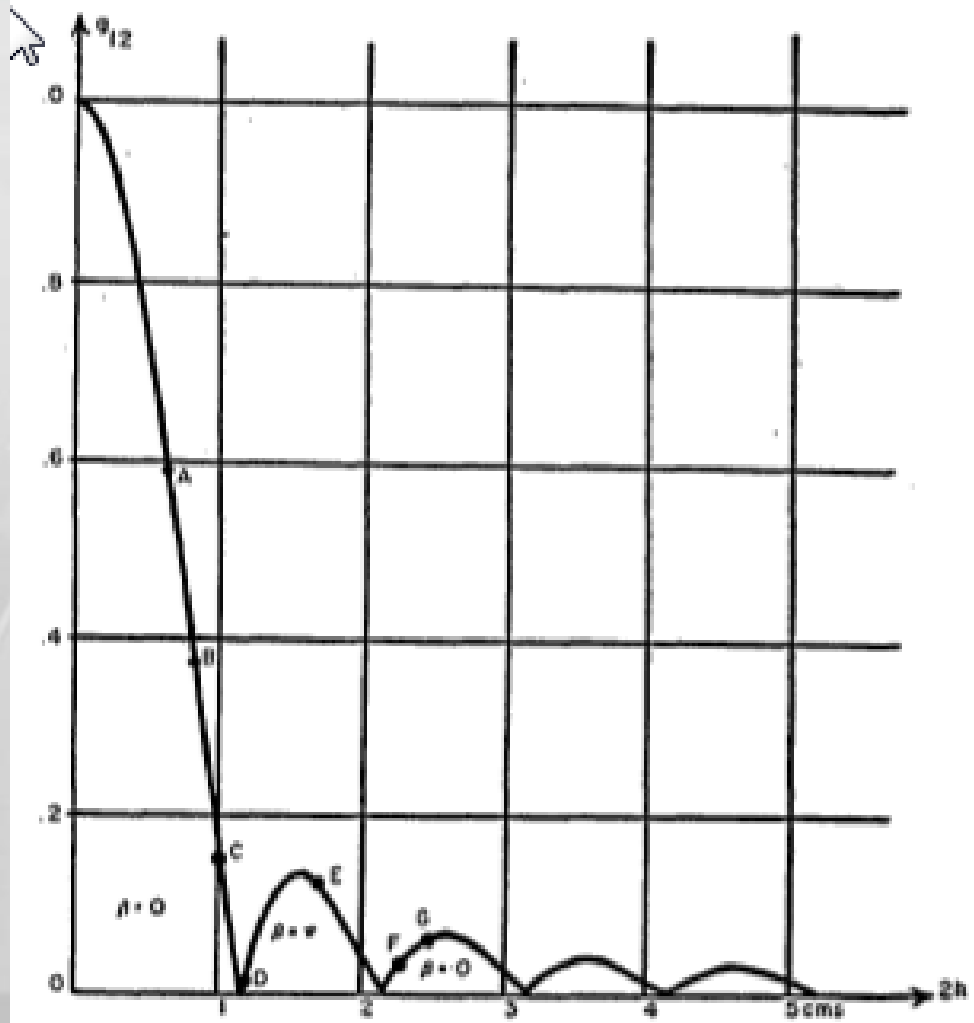
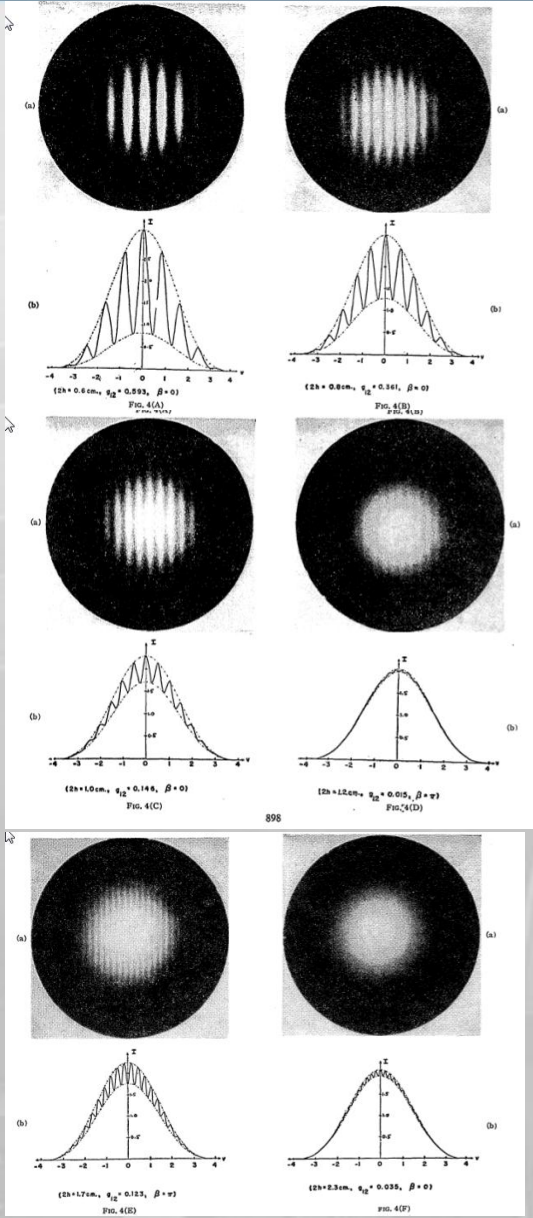
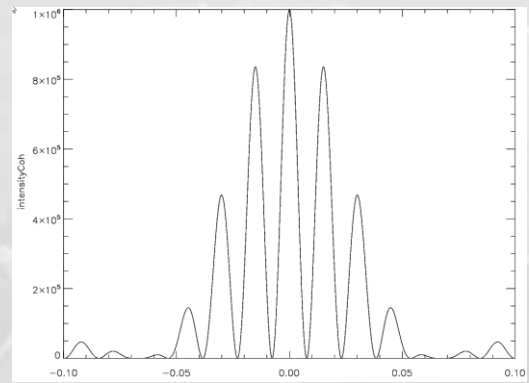
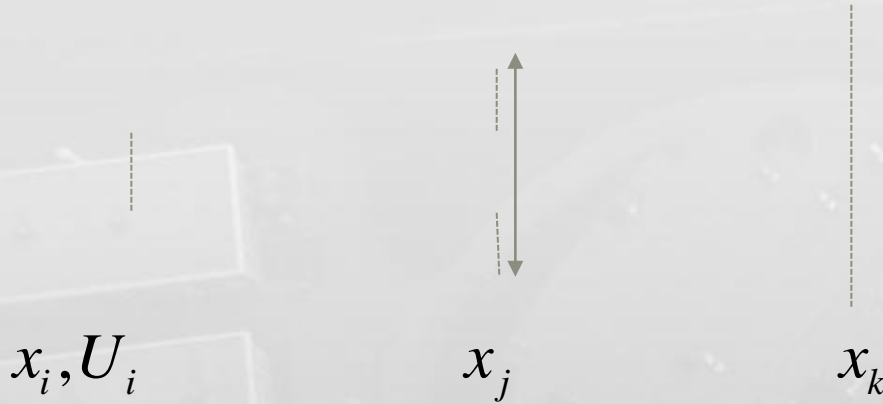


FIG. 6. The degree of coherence, as function of the separation  $2h$  of the apertures at  $P_1$  and  $P_2$ .



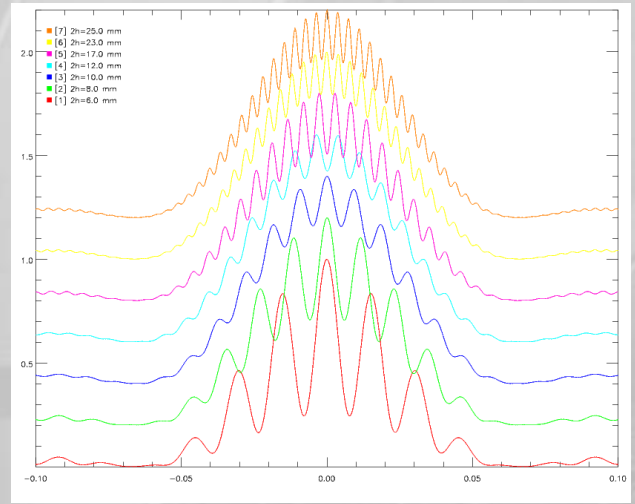
Coherent:  $U_i = 1$

$$r_{mn} = \sqrt{(x_m - x_n)^2 + y_{mn}^2}$$

$$M_{nm} = e^{i k r_{nm}}$$

$$U_k = U_i (M_{ij} M_{jk})$$

$$I_k = |U_k|^2$$



Fully incoherent:  
Use ensemble average

$$U_i = e^{i2\pi\zeta} \quad \zeta = \text{random}$$

$$I_k = \sum_{\rho \in \text{realisations}} |U_k^\rho|^2$$

## Double pinhole diffraction of white synchrotron radiation

W. Leitenberger<sup>a,\*</sup>, H. Wendrock<sup>b</sup>, L. Bischoff<sup>c</sup>, T. Panzner<sup>a</sup>, U. Pietsch<sup>a</sup>,  
J. Grenzer<sup>a</sup>, A. Pucher<sup>a</sup>

<sup>a</sup> Institut für Physik, Universität Potsdam, Am Neuen Palais 10, D-14469 Potsdam, Germany

<sup>b</sup> Institut für Festkörper- und Werkstofforschung, P.O. Box 270016, D-01171 Dresden, Germany

<sup>c</sup> Forschungszentrum Rossendorf e.V., P.O.B. 51 01 19, D-01314 Dresden, Germany

Received 26 September 2002; accepted 12 December 2002

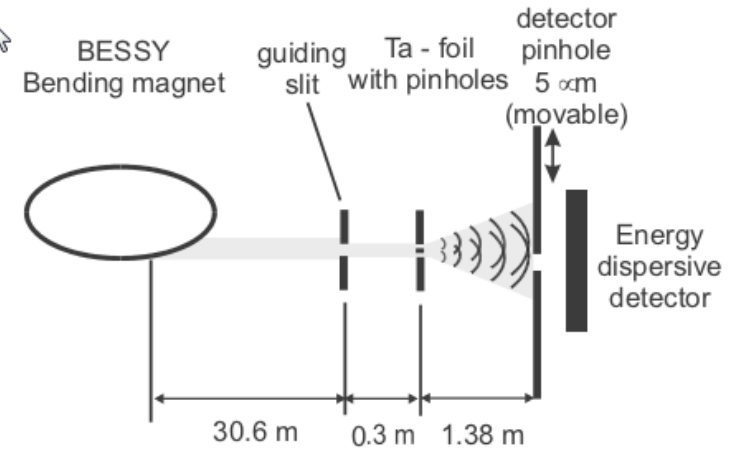


Fig. 1. Experimental set-up at the EDR-beamline at BESSY II.

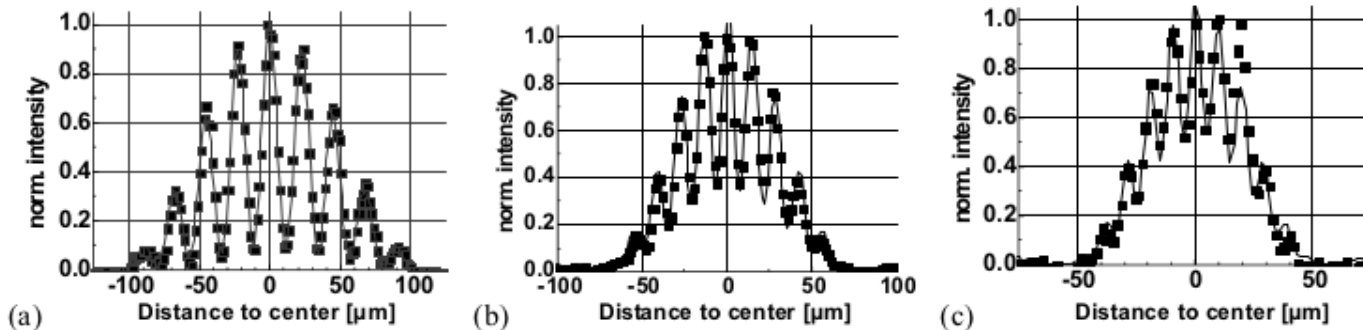
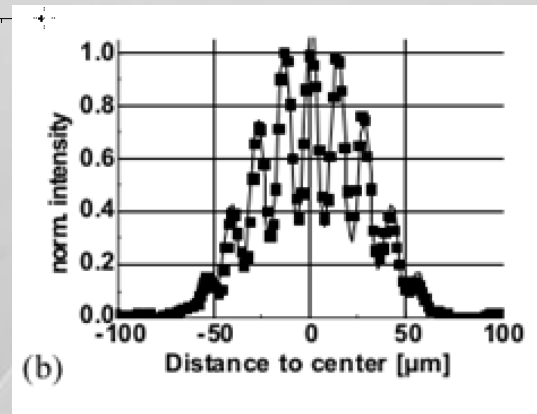
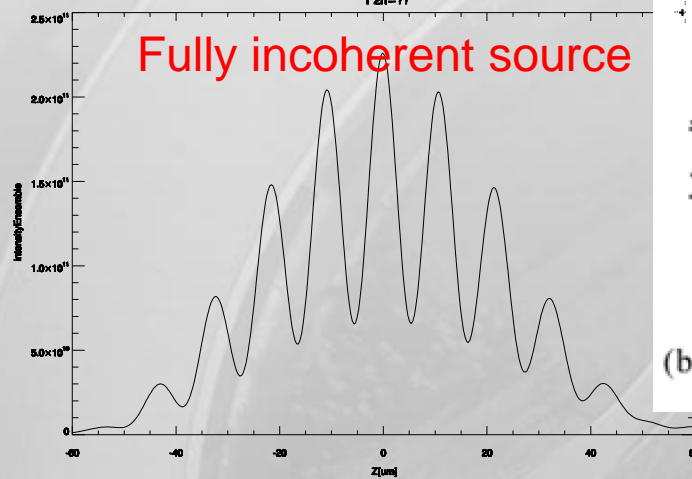
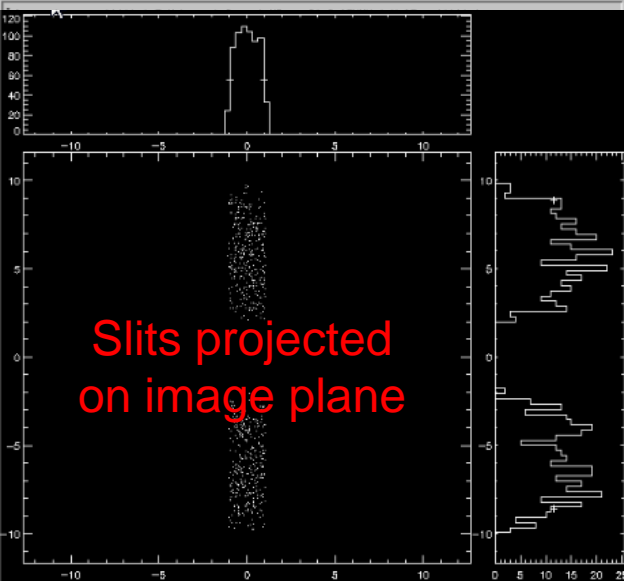
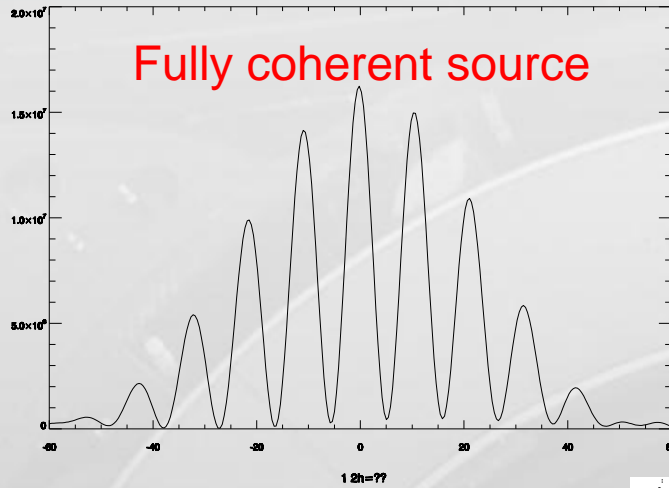
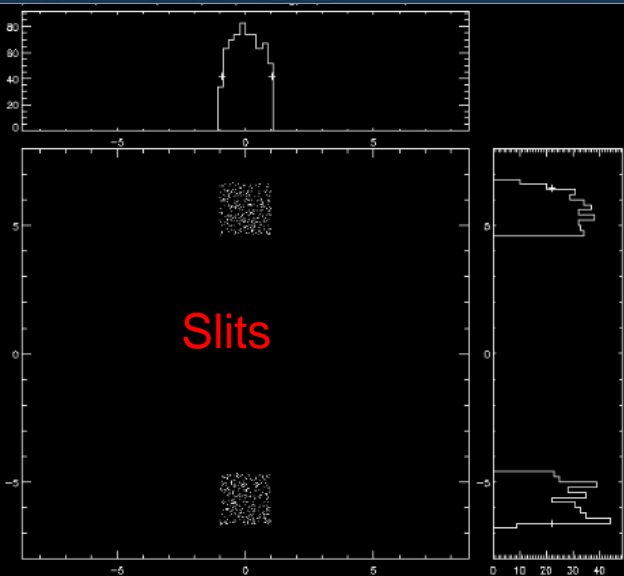


Fig. 4. Normalized interference fringes obtained with the double pinhole at three different energies (a)–(c) 6 keV, 10 keV and 14 keV. The squares indicate the measured data from Fig. 3 and the lines indicate the results of the best fit of Eq. (1).





=> Use ray tracing for *gridding*, and a postprocessor for calculating  $M$  matrices and the ensemble average over many source realisations

- SHADOW
  - Compound Refractive Lenses and Transfocators
  - Crystals
  - Optical constants
  - Partial Coherence
  - Global optimization
  - Model samples
- Towards a new hybrid (ray-tracing+wave-optics) optics toolbox?
  - SPIE Conference 2011 (to be followed...)
  - Collaborative work
    - NSLS-II
      - Cross talk SHADOW-SRW
      - API in python for ray tracing and wave optics (python)
  - Switch Ray optics <-> Wave optics
  - New GUI
  - McXtrace

### Beamline Experiment Chain

Storage Ring  
( $e^-$  optics)



Radiation devices  
( $e^- \rightarrow \gamma$ )



Beamline  
( $\gamma$  optics)



Sample  
( $\gamma$  - matter interactions)

At-Collab

SRW

Codes in use at ESRF

SHADOW

XOP

McXtrace

At-Collab

SRW

NEW TOOLBOX

SHADOW

OTHER

- Timing:

- Alpha1 Version: Defining basic tools, making the skeleton, prototype an XOP clone
- Alpha2 Version: Define SHADOW+SRW inputs, basic use of them
- Alpha3 Version: Allow to use most SHADOW+SRW functionality, advanced visualization tools, beta test version

- Tools (dependencies): based on python, Qt4 and many other tools to be defined
- Personnel: MSR+PhD+SE (2 y.)+collaborators
- Document in preparation

## NEW TOOLBOX

### Physics engines

SRW

SHADOW

Plugin-  
runner

OTHER

### Tools

I/O

FF

DB

### Graphics

Widget  
-app  
editor

1D

2D

3D

Thank you

(more tomorrow)