A Light for Science

SHADOW

past, present and futue

Manuel Sánchez del Río (ESRF)

Franco Cerrina (U. Boston)

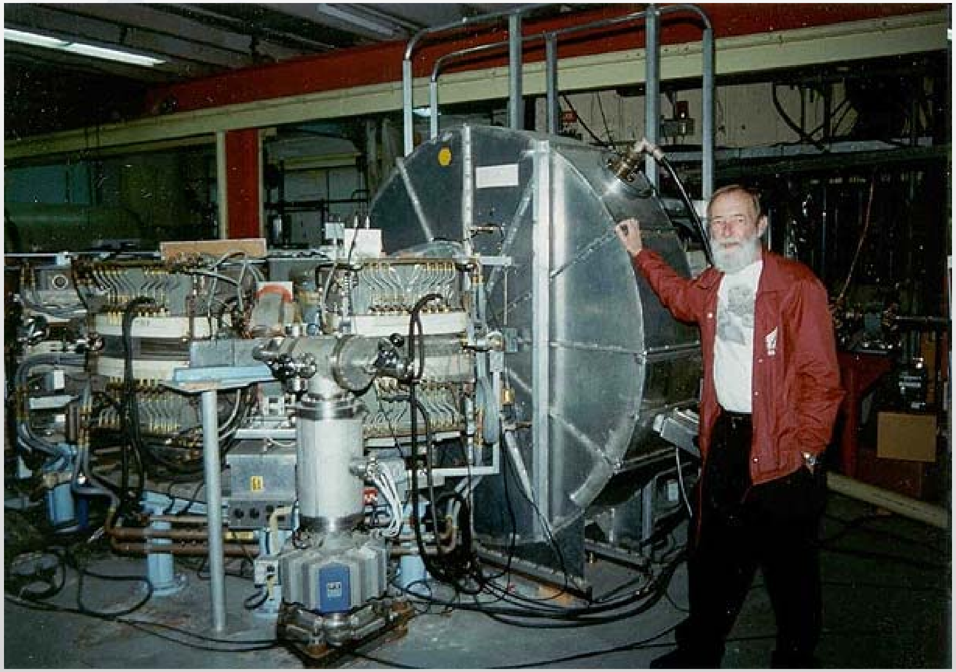
European Synchrotron Radiation Facility

Contents

- Past
  - History
  - Fundamental concepts
- Present
  - XOP and ShadowVUI
  - Some applications
  - Challenges
- Future
  - Requirements for Shadow 3.0
  - (Planning for Shadow 3.0 beta)

Synchrotron Radiation Center, U. Wisconsin

- At the University of Wisconsin during 1965 -1967, a team led by particle physicist Ednor Rowe built ***Tantalus***. He quickly adapted the machine to make synchrotron radiation available for use and soon the facility was crowded with experimentalists from all over the world
- In 1977 SRC began construction on its own facility focusing on a new and much larger SR source, ***Aladdin***. Ten years later, with Aladdin fully operational, Tantalus was decommissioned.



Ednor Rowe and Tantalus

Birth of SHADOW

- **Scientific motivation:**
  Grating monochromator design: TGM, ERG
  Toridal, spherical mirrors.

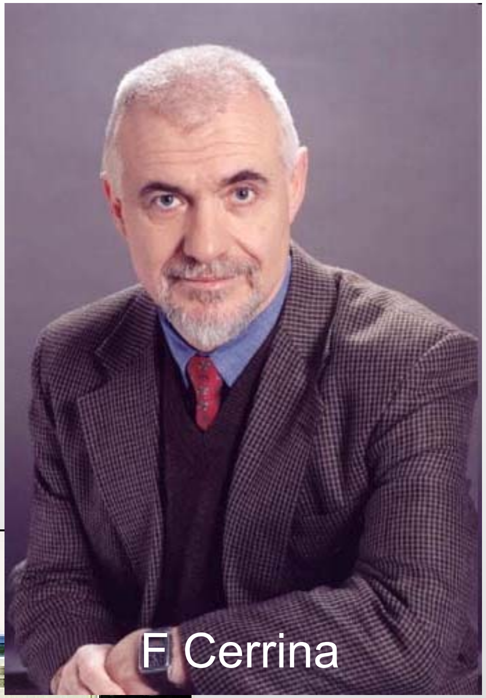
- **Monte Carlo ray tracing program *designed* to simulate X-ray optical systems**

- **Requirements**
  - **Accuracy and reliability**
  - **Easy to use (user interface, documentation)**
  - **Flexibility (it can model different beamlines)**
  - **Economy of computer resources (VAX-11 Computers)**

- **Efficient MC approach**
  - **Reduced number of rays**
  - **Exact simulation os SR sources**
  - **Vector calculus**
  - **Modular**
  - **Available to users**

- **Two years development**

- **Fortran 77+VAX/VMS extensions**



First publication (1984)

Ray tracing of recent VUV monochromator designs

F. Cerrina

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

Abstract

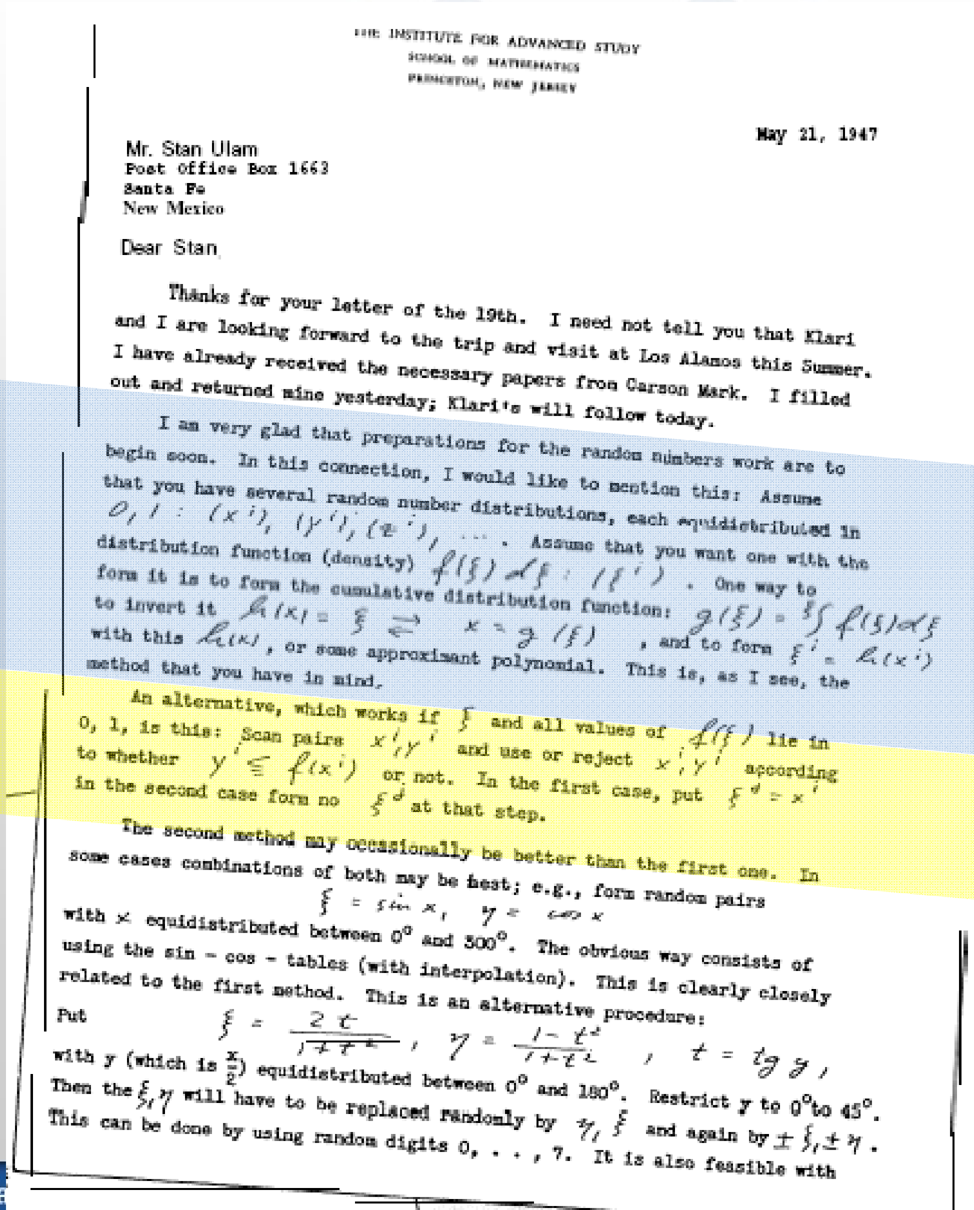
A new optical ray-tracing program is presented and some applications discussed. A Monte-Carlo modelling of several types of sources is implemented, and in particular the Synchrotron Radiation source is modelled exactly. The program is written specifically for grazing optics, although gaussian optics 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 to the Toroidal Grating Monochromator (TMG), Grating Crystal Monochromator (GCM), and Extended Range Grasshopper (ERG) are presented.

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

Monte Carlo (source model)

INVERSION

REJECTION


THE INSTITUTE FOR ADVANCED STUDY
SCHOOL OF MATHEMATICS
PRINCETON, NEW JERSEY

May 21, 1947

Mr. Stan Ulam
Post Office Box 1663
Santa Fe
New Mexico

Dear Stan,

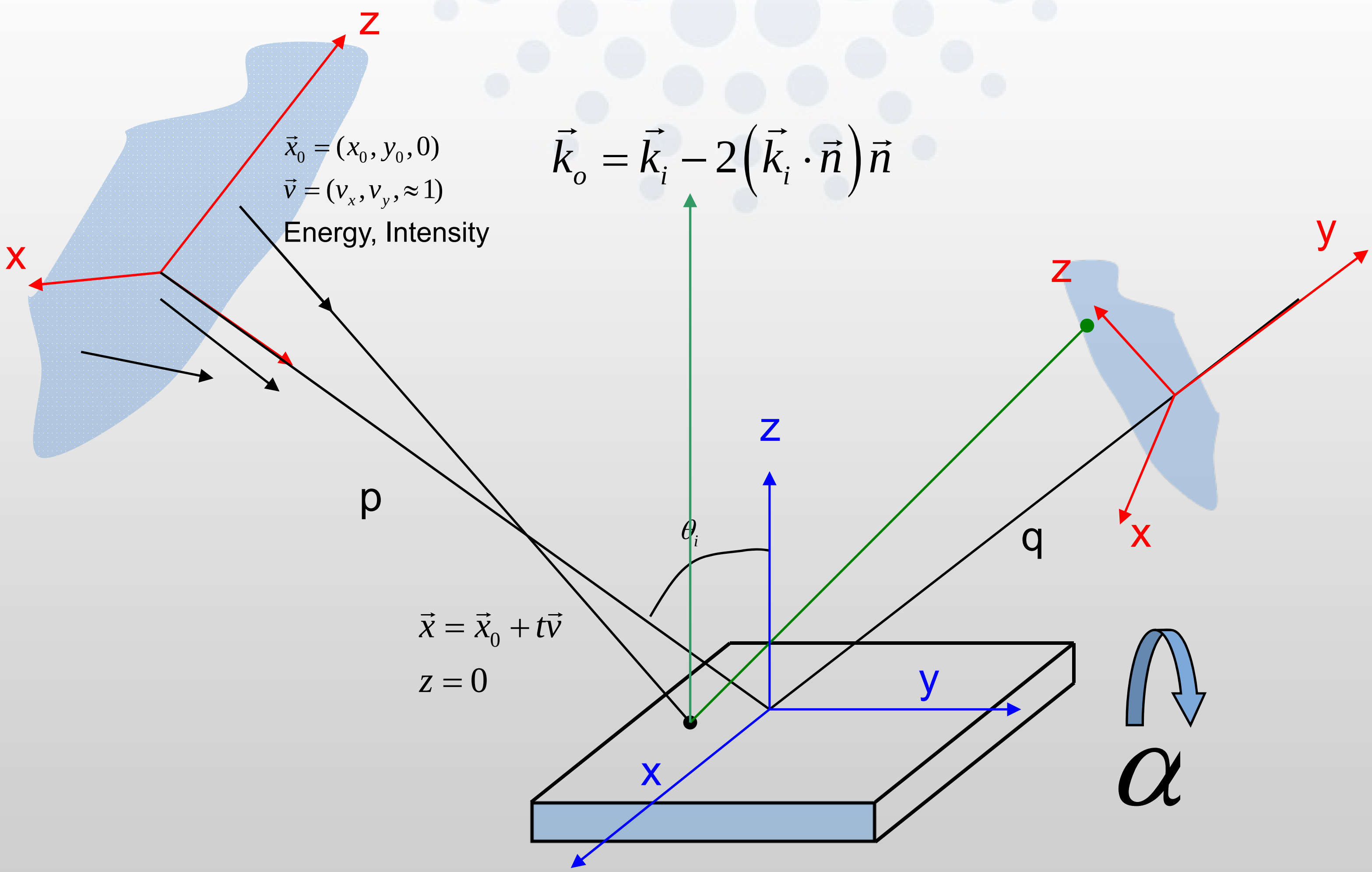
Thanks for your letter of the 19th. I need not tell you that Klari and I are looking forward to the trip and visit at Los Alamos this Summer. I have already received the necessary papers from Carson Mark. I filled out and returned mine yesterday; Klari's will follow today.

I am very glad that preparations for the random numbers work are to begin soon. In this connection, I would like to mention this: Assume that you have several random number distributions, each equidistributed in $0, 1$: (x^i), (y^i), (z^i), ... Assume that you want one with the distribution function (density) $f(\xi)\,d\xi$: (ξ^i) . One way to form it is to form the cumulative distribution function: $g(\xi) = \int^{\xi} f(\xi)\,d\xi$ to invert it $h(x) = \xi \rightleftarrows x = g(\xi)$, and to form $\xi^i = h(x^i)$ with this $h(x)$, or some approximant polynomial. This is, as I see, the method that you have in mind.

An alternative, which works if ξ and all values of $f(\xi)$ lie in 0, 1, is this: Scan pairs x^i, y^i and use or reject x^i, y^i according to whether $y^i \leq f(x^i)$ or not. In the first case, put $\xi^j = x^i$ in the second case form no ξ^j at that step.

The second method may occasionally be better than the first one. In some cases combinations of both may be best; e.g., form random pairs $\xi = \sin x$, $\eta = \cos x$ with x equidistributed between 0° and 360°. The obvious way consists of using the sin - cos - tables (with interpolation). This is clearly closely related to the first method. This is an alternative procedure:
Put $\xi = \frac{2t}{1+t^2}$, $\eta = \frac{1-t^2}{1+t^2}$, $t = tg\,y$, with y (which is $\frac{x}{2}$) equidistributed between 0° and 180°. Restrict y to 0° to 45°. Then the ξ, η will have to be replaced randomly by η, ξ and again by $\pm\xi, \pm\eta$. This can be done by using random digits 0, . . . , 7. It is also feasible with

Trace (the beamline)



What SHADOW is?

- A ray-tracing code optimized for SR (>300 citations)
- Ray-tracing ≠ Geometric Optics
  Information on electric vectors, phases, polarization state:
  sometimes

JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 21, No. 2, April–June 2007

Applicability of Phase Ray-Tracing Method for Light Scattering from Rough Surfaces

H. J. Lee* and Z. M. Zhang†
Georgia Institute of Technology, Atlanta, Georgia 30332-0405

DOI: 10.2514/1.26191

The ray-tracing method based on geometric optics, in which the intensity of light is traced during scattering,

Wave-Optical Systems Engineering, Frank Wyrowski, Editor,
Proceedings of SPIE Vol. 4436 (2001) © 2001 SPIE · 0277-786X/01/$15.00

Anything optical rays cannot do?

Andrey Semichaevsky and Markus Testorf

University of Massachusetts, Dept. Elect. & Comp. Eng., Lowell, MA 01854, U.S.A.

ABSTRACT

The limits of ray optical methods to provide a valid model for describing the propagation of electromagnetic radiation are explored. We briefly review fundamentals of ray optics as well as various extensions. This review is partially intended to emphasize that existing ray based methods are able to address most, if not all, wave phenomena. In

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

1984-1990 The kingdom of Digital VAX/VMS

- Updated to include new models (several authors)
  - Insertion devices (Wiggler and Undulators)
- Users support (Chris Welnak)

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

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.

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 wiggler source, the extension of 100 keV of the optical constant database, the novel power density calculations capabilities and the inclusion of the full crystal and multilayer optics cases. Current work and future prospects will also be discussed.

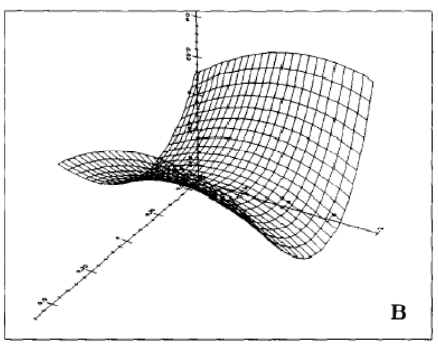
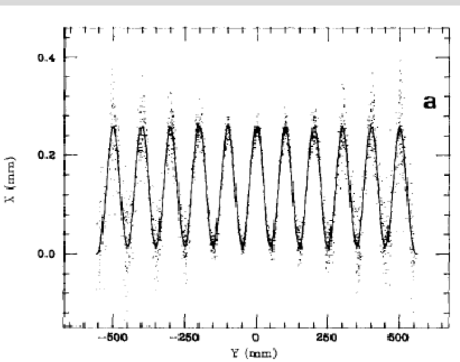
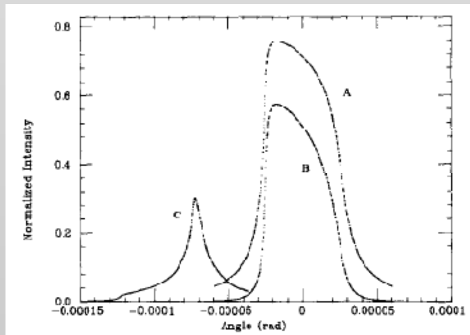


Fig. 1. Possible choices of toroidal surface regions.





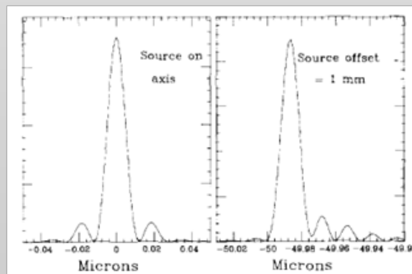


Fig. 7. Diffracted image formed by a Schwartzschild objective at 44 Å. All the physical parameters, such as phase shifts, multilayer reflectivities, and diffraction, are taken in account.

1990 The switch to UNIX

- New machines enter in the scientific computing market (Unix workstations: Digital/Ultrix, Sun, HP, …)
- UNIX version prepared by Mumit Khan
- First version installed at ESRF (1991)
- Simultaneaous development of new algorithms for crystal optics

Asymmetrically cut crystals for synchrotron radiation monochromators

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

(Presented on 22 July 1991)

936 Rev. Sci. Instrum. 63 (1), January 1992 0034-6748/92/010936-05$02.00 936

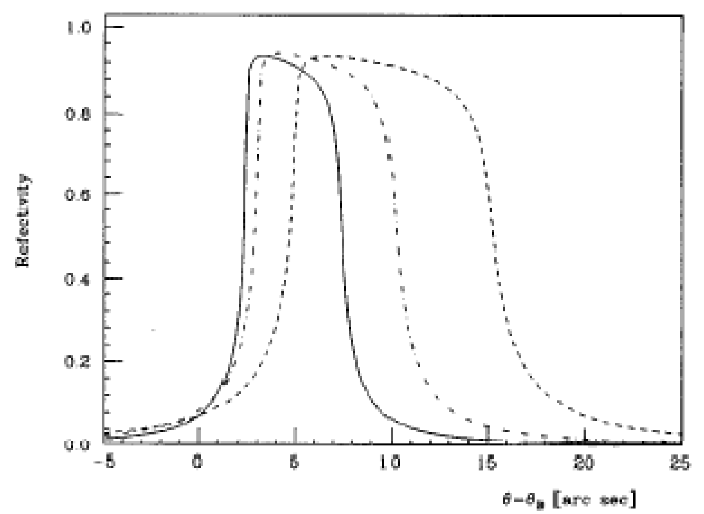

FIG. 2. Reflectivity curves for a silicon (111) crystal for symmetrical case (dot–dashed line) and for asymmetrical case with $\alpha = 5$ deg. For the asymmetrical case, the curves are plotted in function of the incoming (solid line) and outcoming (dashed line) beams.

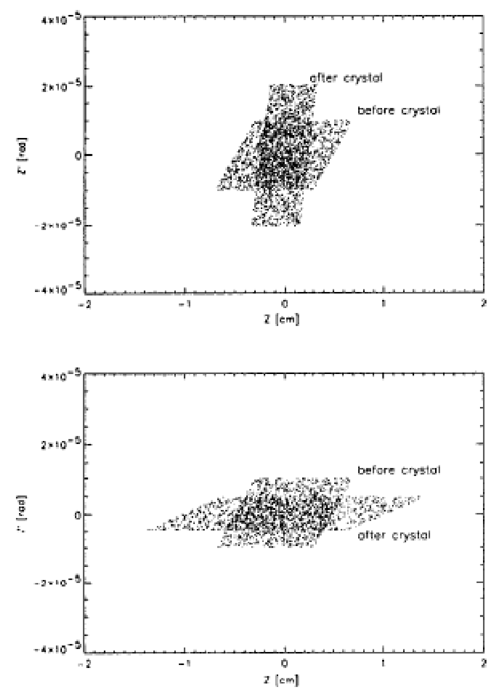

FIG. 3. Change in phase space of the photon beam of 8035 eV produced by an Si(111) asymmetrically cut crystal of $\alpha = 5$ deg (top) and $\alpha = -5$ deg (bottom). A linear and divergent source in Z direction has been considered.

A conceptual model for ray tracing calculations with mosaic crystals

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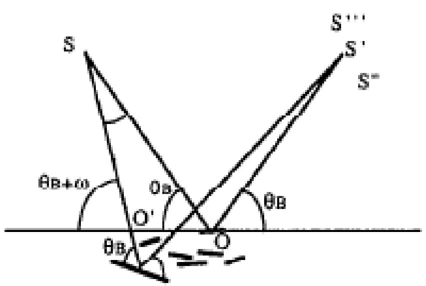
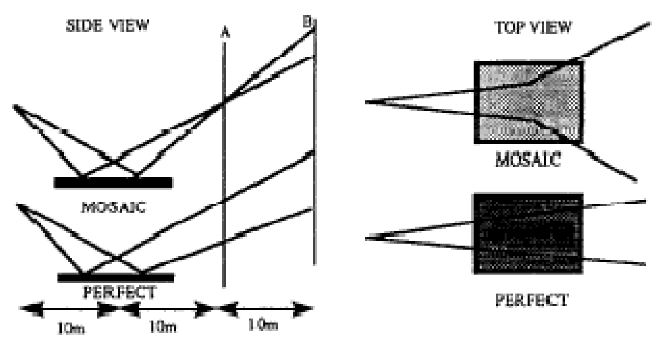
Center for X-ray Lithography, 3731 Schneider Drive, Stoughton, Wisconsin 53589

(Presented on 17 July 1991)

Rev. Sci. Instrum., Vol. 63, No. 1, January 1992 Synchrotron radiation





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Nuclear Instruments and Methods in Physics Research A 529 (2004) 231–233
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A
www.elsevier.com/locate/nima

A method for detailed simulations of neutron diffraction from imperfect crystals

L. Alianelli[a,b,*], N. Wilson[b], K.H. Andersen[b], M. Sánchez del Río[c], R. Felici[a]
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SCIENCE DIRECT
Physica B 350 (2004) e725–e729
PHYSICA B
www.elsevier.com/locate/physb

A novel Monte Carlo algorithm for simulating crystals with McStas

L. Alianelli[a,b,*], M. Sánchez del Río[c], R. Felici[a], K.H. Andersen[b], E. Farhi[b]
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Other developments

Recent developments in SHADOW

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

(Presented on 16 July 1991)

865 Rev. Sci. Instrum. 63 (1), January 1992 0034-6748/92/010865-04$02.00 © 1992 American Institute of Physics 865

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

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

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

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

INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

Ray-tracing of X-ray focusing capillaries

Guan-Jye Chen [a,*], F. Cerrina [a], Karl F. Voss [b], K. Hyde Kim [b], Frederick C. Brown [b]

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 535

(Presented on 19 October 1995)

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

IN PHYSICS RESEARCH Section A

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

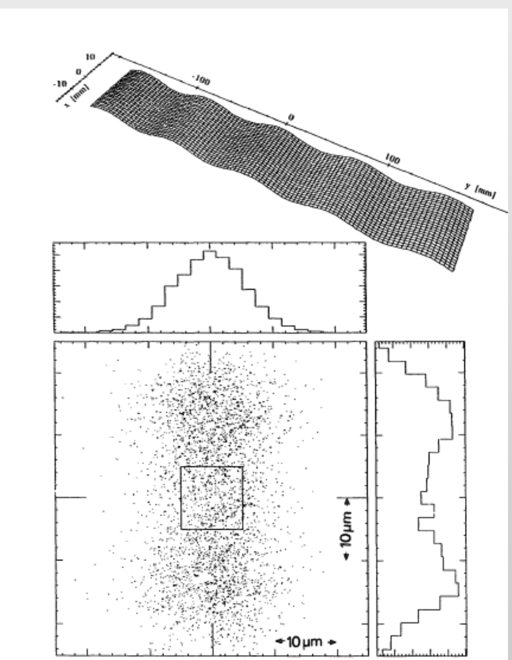
Nuclear Instruments and Methods in Physics Research A319 (1992) 170–177
North-Holland

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH
Section A

Waviness effects in ray-tracing of "real" optical surfaces

M. Sánchez del Río [a] and A. Marcelli [b]

[a] European Synchrotron Radiation Facility, B.P. 220, 38043 Grenoble Cedex, France
[b] INFN Laboratori Nazionali di Frascati, CP 13, 00044 Frascati, Italy



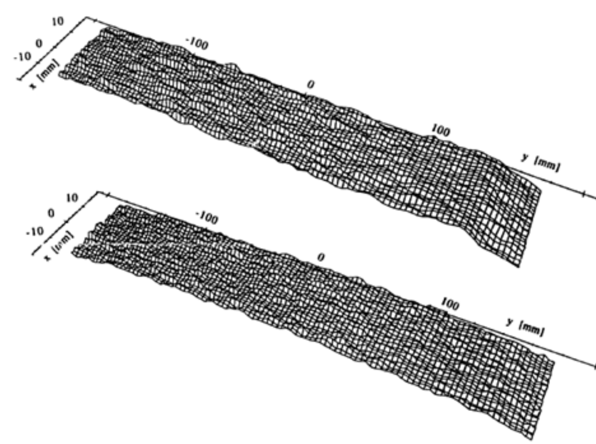
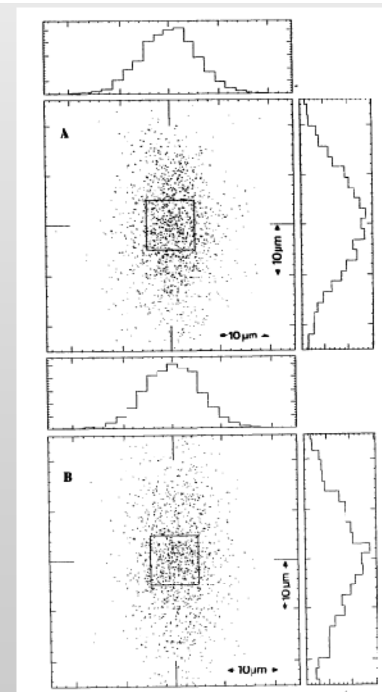


Fig. 3. Simulated waviness of optical surfaces with 0.4″ slope error. The surface A has been generated considering $n_{max} = 32$, $C_n = 1$, $y_n^0 = 0$, and $f_n = 0.1$, $f_0 = f_1 = 0$. For surface B, $n_{max} = 56$ and the remaining parameters have been changed in a more complicated way. The total length of each surface is 350 mm and the width is 30 mm. The vertical length is not scaled.



Laue crystals

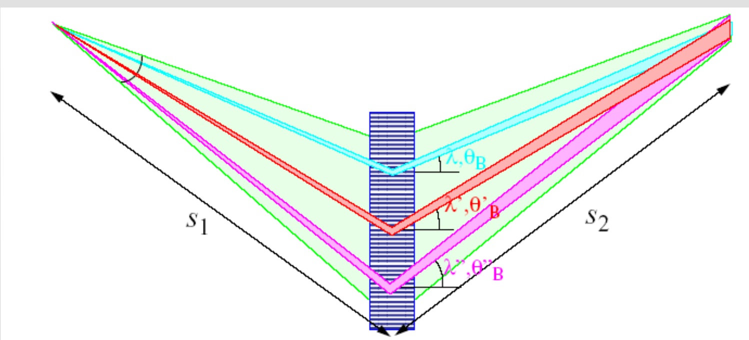
Nuclear Instruments and Methods in Physics Research A 347 (1994) 338–343
North-Holland

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

Modeling perfect crystals in transmission geometry for synchrotron radiation monochromator design

M. Sánchez del Río [a,*], C. Ferrero [a], G-J. Chen [b], F. Cerrina [b]

[a] *European Synchrotron Radiation Facility, BP 220, 30043 Grenoble Cedex, France*
[b] *Center for X-ray Lithography, 3731 Schneider Drive, Stoughton, WI 53589, USA*



Focusing characteristics of diamond crystal x-ray monochromators. An experimental and theoretical comparison [a)]

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 Risö National Laboratory, Roskilde, Denmark

M. Nielsen
Risö National Laboratory, Roskilde, Denmark

(Received 21 July 1994; accepted for publication 18 August 1995)

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

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NIM B Beam Interactions with Materials & Atoms

Multiple station beamline at an undulator X-ray source

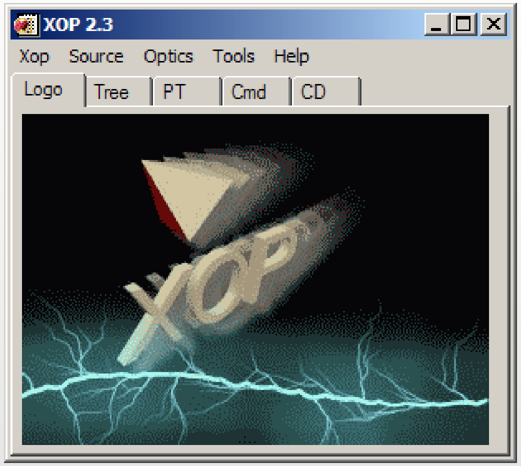
J. Als-Nielsen [a,b,*], A.K. Freund [b], G. Grübel [b], J. Linderholm [a,b], M. Nielsen [a], M. Sanchez del Rio [b], J.P.F. Sellschop [c]

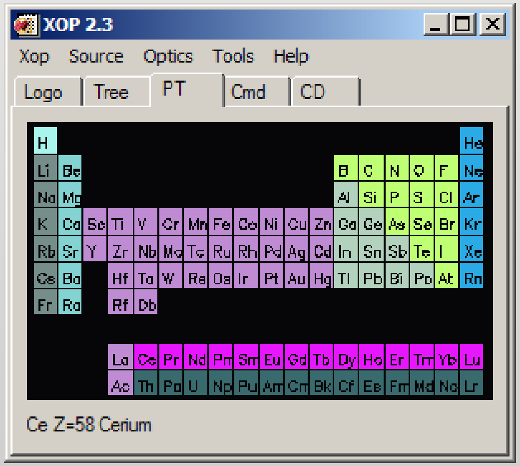
PRESENT

XOP

- A user-friendly platform for
  - quick calculations (synchrotron spectra, reflectivities, rocking curves, attenuation coeffs. etc.)
  - generic data visualization and analysis
  - specific applications (“extensions”)

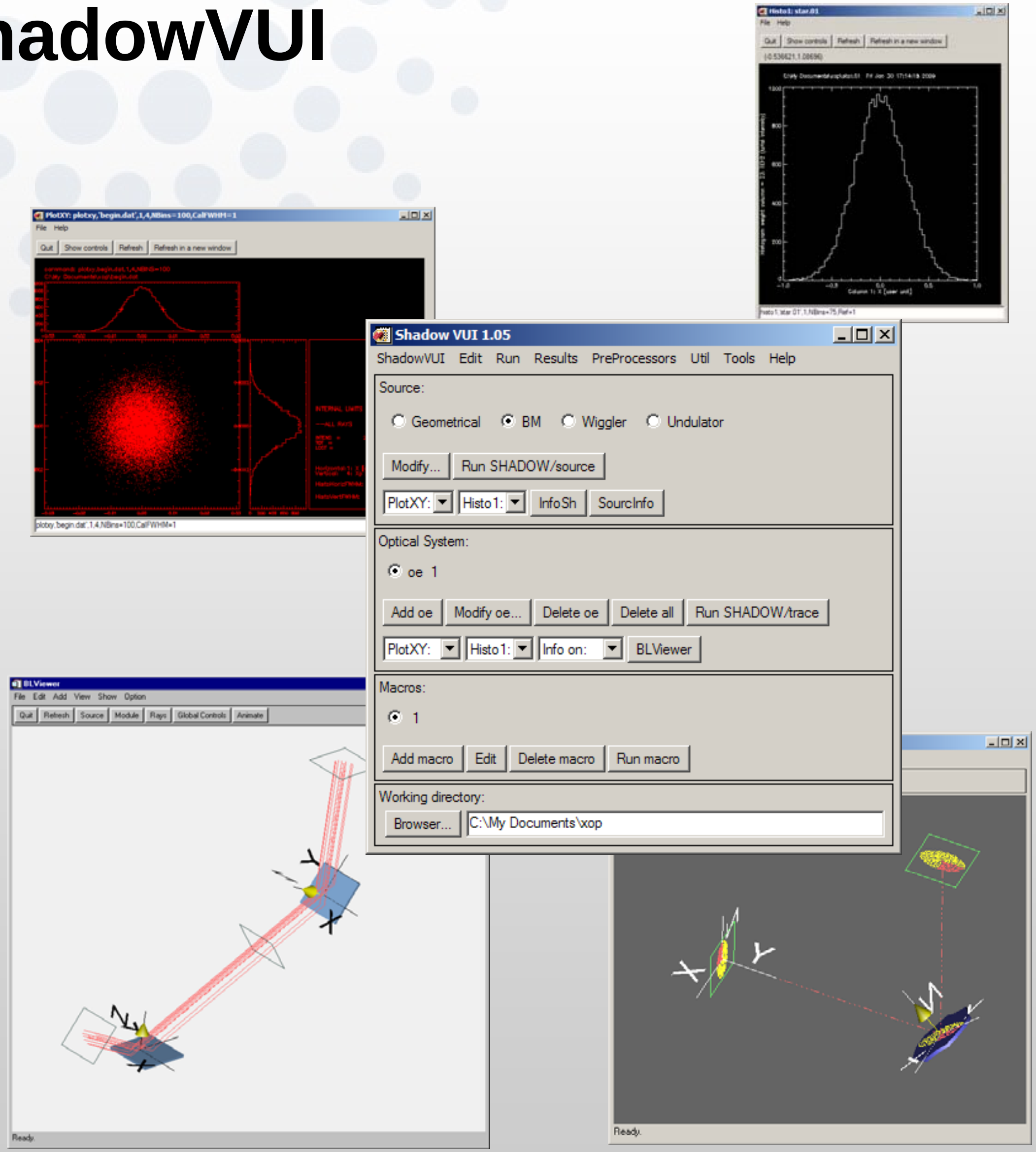
- Characteristics
  - Long history (>10 years)
  - Large user community (>400 users in tens of laboratories)
  - Multiplatform (Windows, Unix, MacOSX)
  - Freely distributed to users
  - Collaboration work ESRF (M Sanchez del Rio)-APS (Roger Dejus)
  - Written in IDL (using Fortran and C modules). Embedded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





ShadowVUI

- Entirely new interface that uses the standard SHADOW calculation engine
- High performance graphics
- Macro language
- Tutorials
- Beamline viewer – 3D graphics



Applications (examples)

Gratings

INSTITUTE OF PHYSICS PUBLISHING PHYSICA SCRIPTA
Phys. Scr. 73 (2006) 499–505 doi:10.1088/0031-8949/73/5/014

Computer modelling of the optics of a dispersive Raman spectrometer

M Sánchez del Río[1], E Haro-Poniatowski and M Picquart

Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Apdo. postal 55-534, México DF 09340, Mexico

M Sánchez del Río *et al*

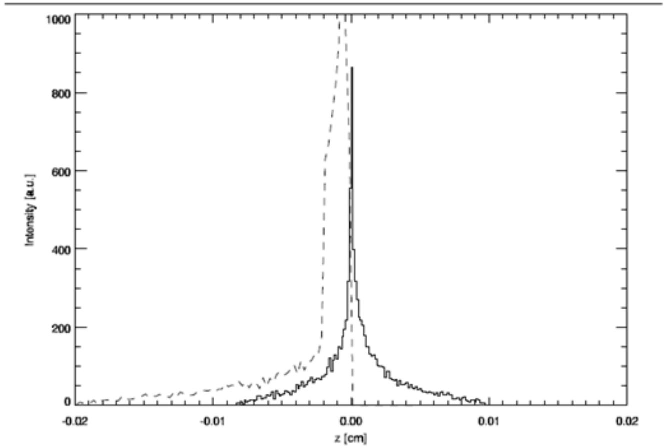
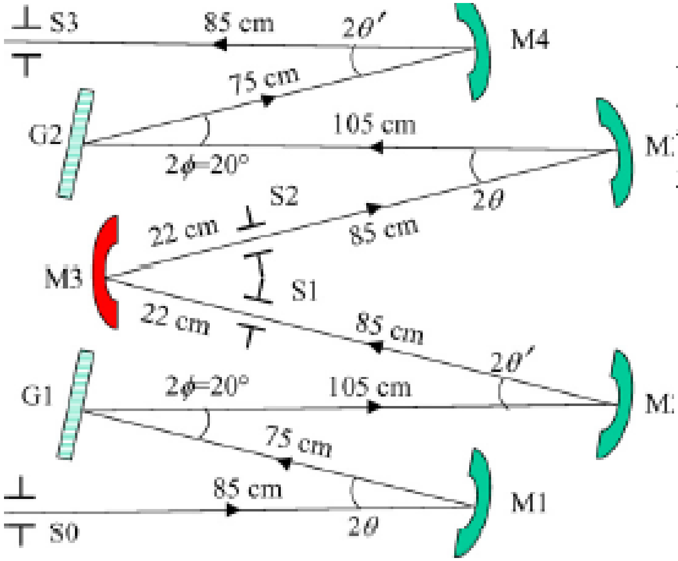
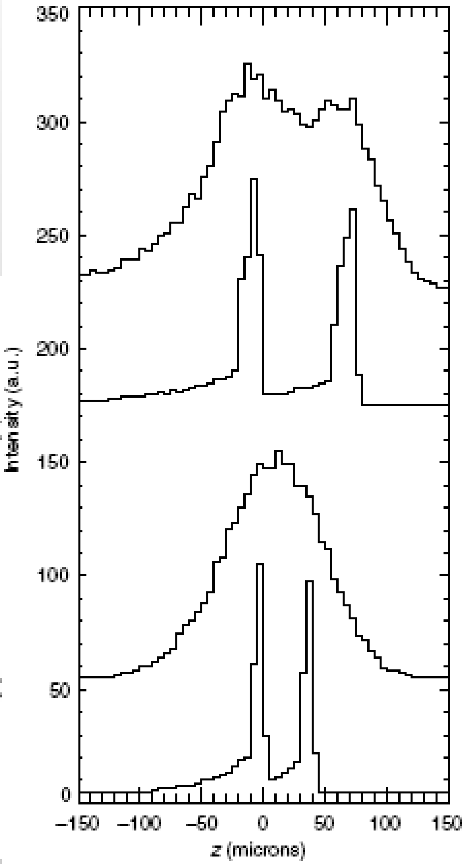


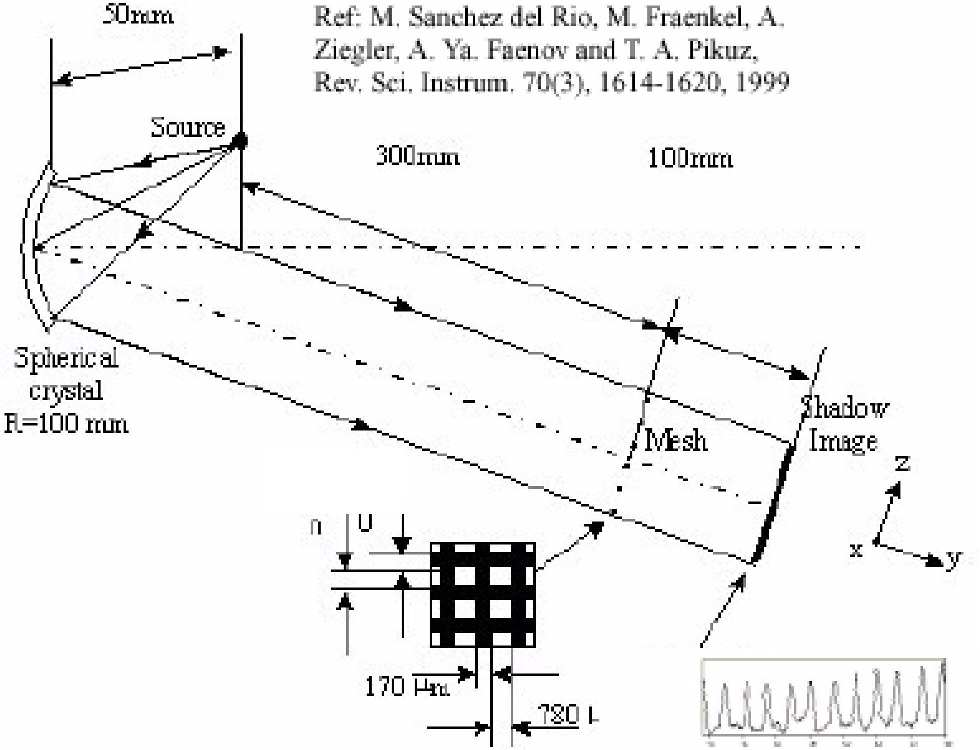
Figure 5. Spectrometer instrumental line functions for a typical case (dashed line: $\theta = 5°$ for M1, M2, M4 and M6) and the optimized case (solid line: $\theta = 5°$ for M1 and M4, and $\theta = 3.7°$ for M2 and M5).

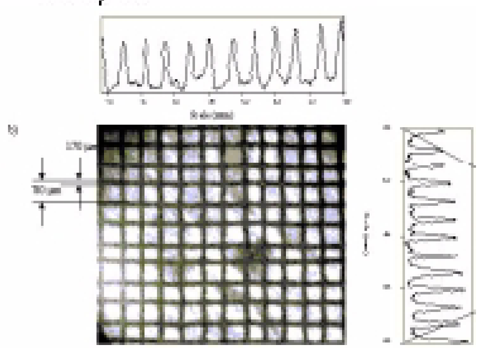


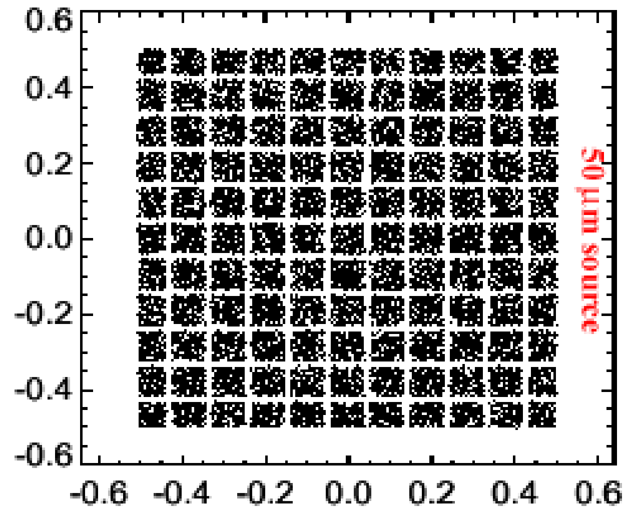


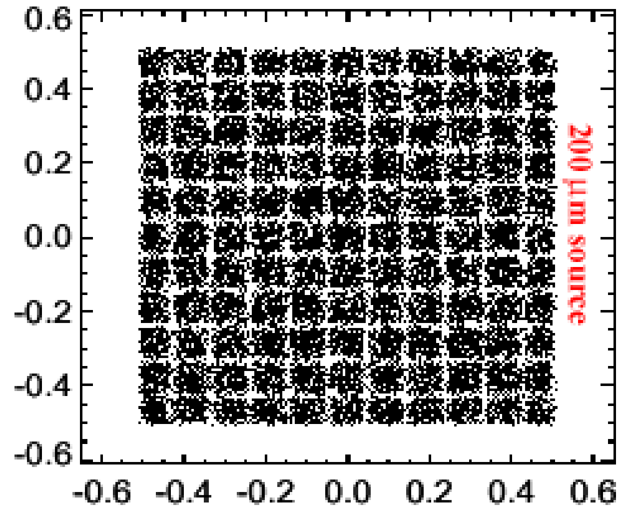
Vignetting/Spatial resolution (grid_pattern.ws)

Ref: M. Sanchez del Rio, M. Fraenkel, A. Ziegler, A. Ya. Faenov and T. A. Pikuz, Rev. Sci. Instrum. 70(3), 1614-1620, 1999





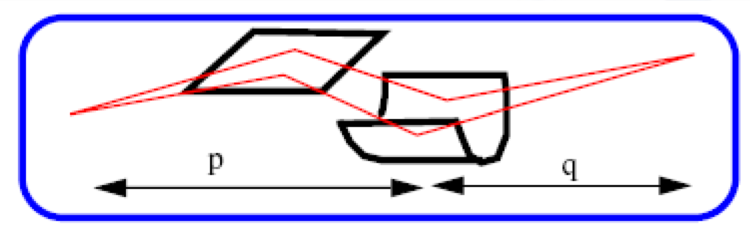




We studied the effects of

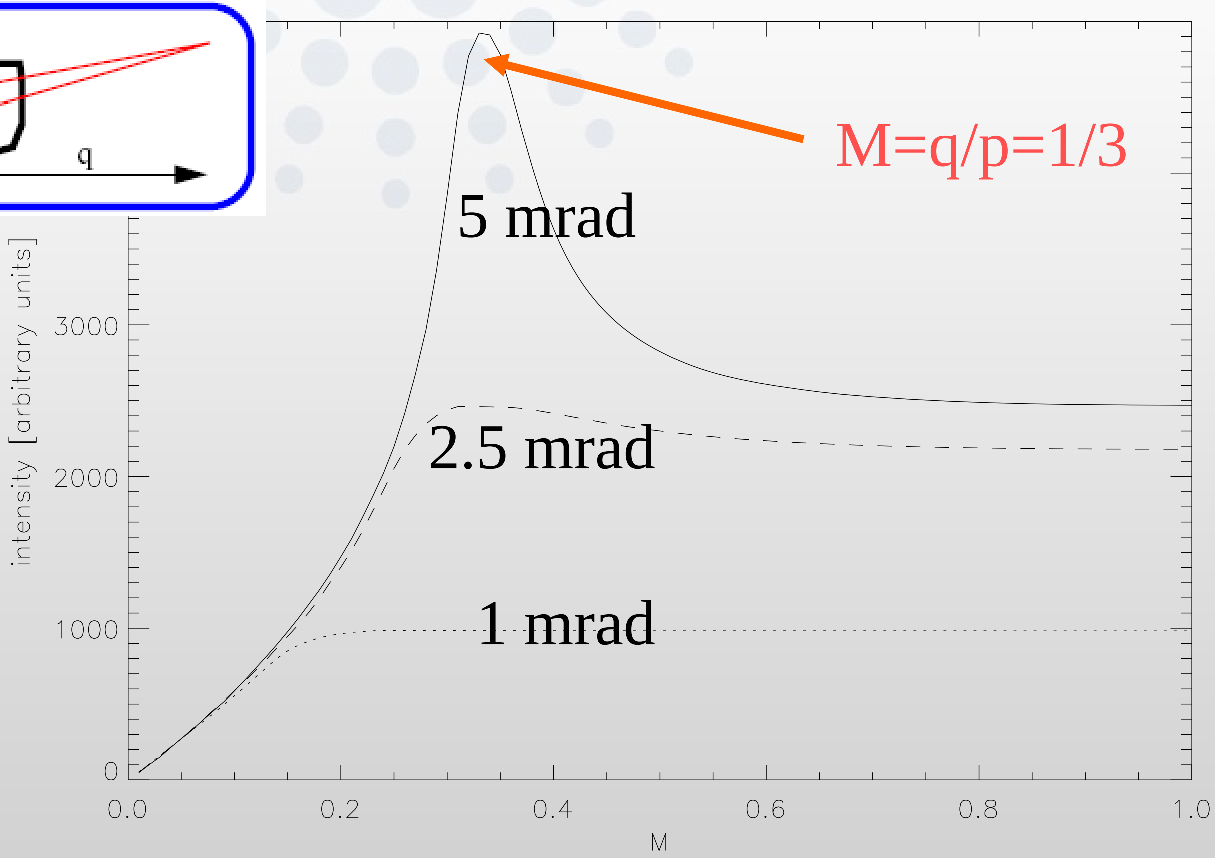
1) Surface shape and geometrical errors
2) Crystal size (entrance pupil)
3) Source depth abd width
4) Incident angle

sagittal focusing



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

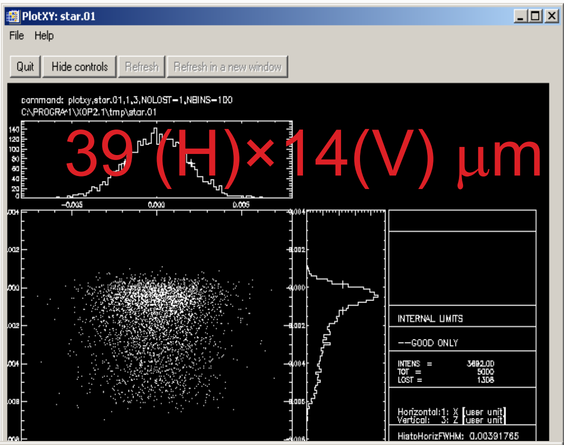
Beam transmission vs angular divergence

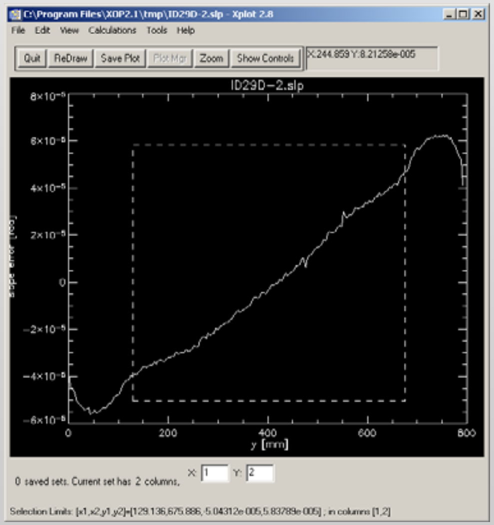


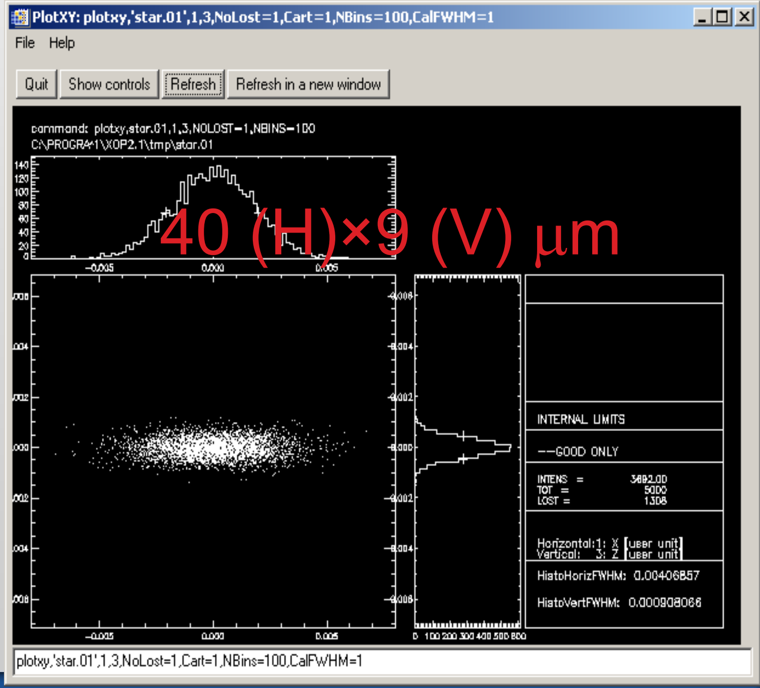
Intensity (in arbitrary units) versus magnification factor M for monochromatic (E=20 keV) point source placed at 30 m from the sagittaly bent crystal.
We clearly observe the maximum of the transmission at M=0.33, as predicted by the theory
(C. J. Sparks, Jr. and B. S. Borie Nuclear Instruments and Methods,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

Example of using LTP profile

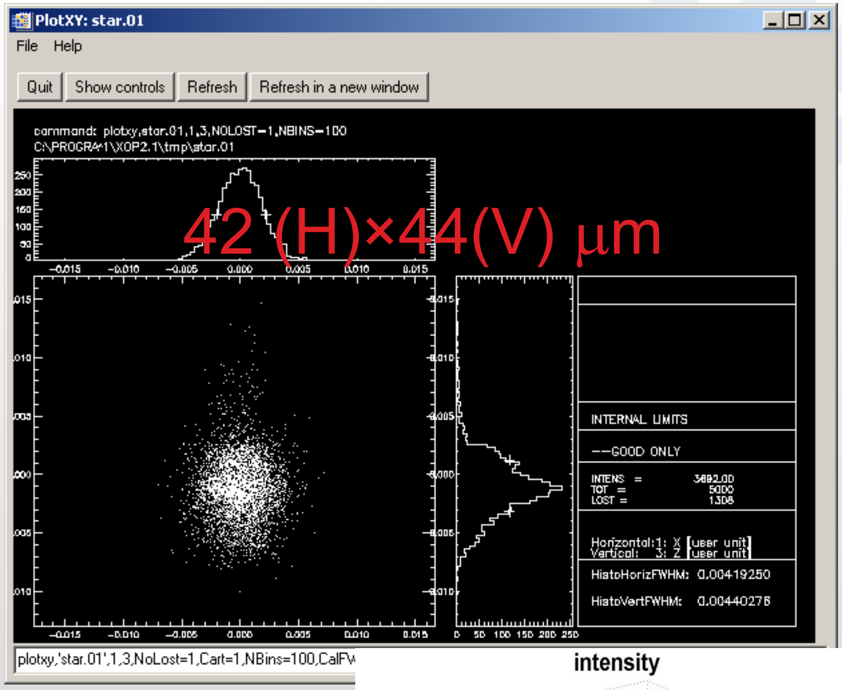
- Toroidal mirror M~1/3 (p=31 m, q=10 m q=3.5 mrad)
- Gaussian source
  - Size: 134 (H) × 25 (V) µm² FWHM
  - Divergence: 6.8 (H) × 85.1 (V) µrad RMS
- Expected:
  - 134/3=45 (H) µm² FWHM
  - 25/3=8.3 (V) µm² FWHM



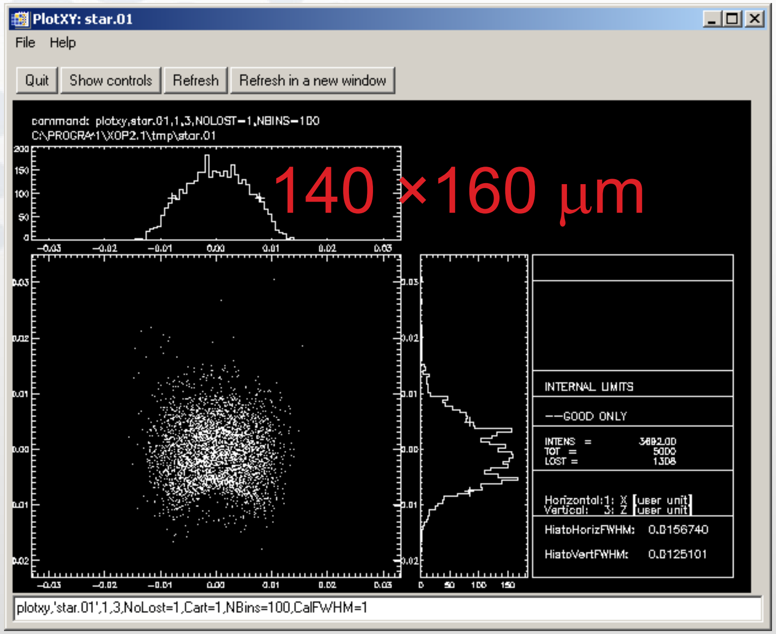




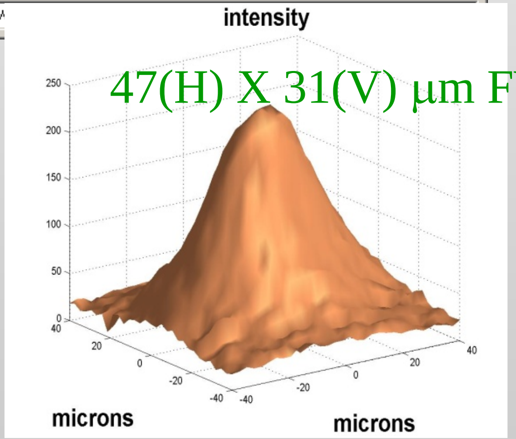
Focal plane



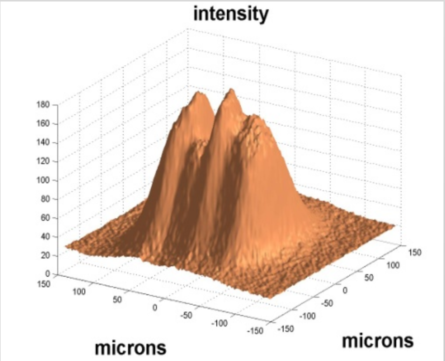
42 (H)×44(V) μm



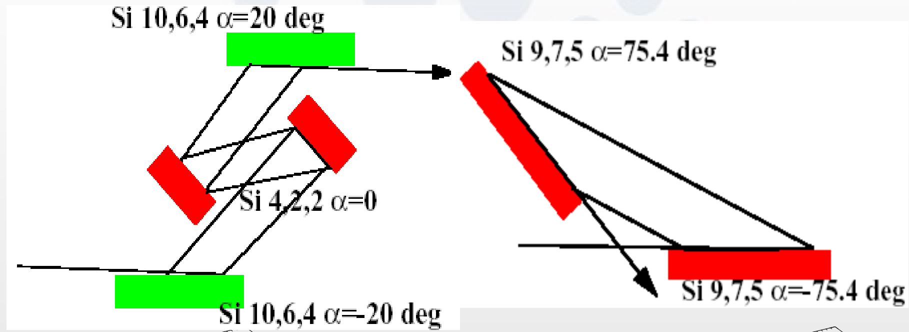
140 ×160 μm

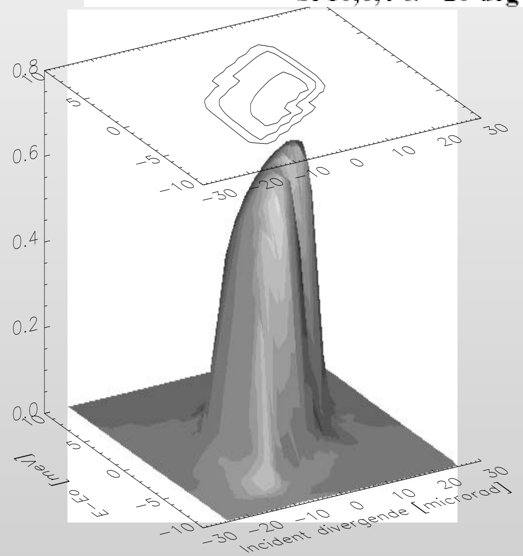


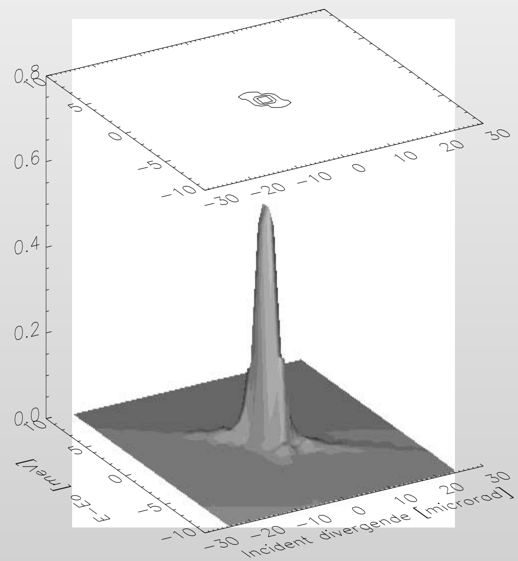
47(H) X 31(V) μm FWHM



Energy resolution







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X-Ray Bragg Diffraction in Asymmetric Backscattering Geometry

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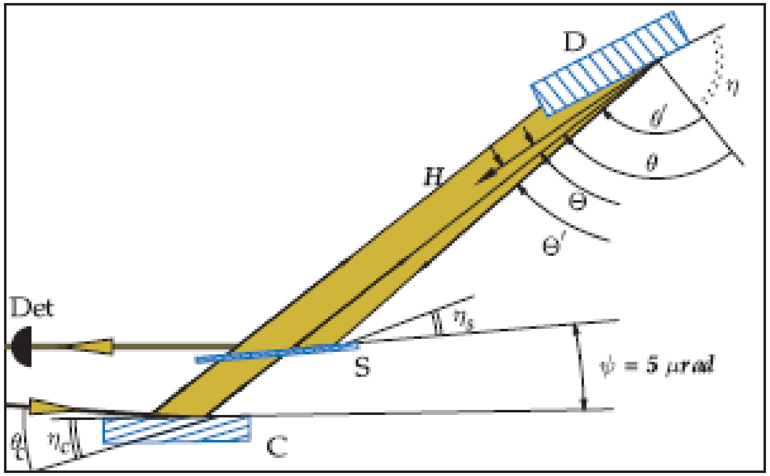
(Received 9 May 2006; published 8 December 2006)

We observe three effects in the Bragg diffraction of x rays in backscattering geometry from asymmetrically cut crystals. First, exact Bragg backscattering takes place not at normal incidence to the reflecting atomic planes. Second, a well-collimated ($\simeq 1$ μrad) beam is transformed after the Bragg reflection into a strongly divergent beam (230 μrad) with reflection angle dependent on x-ray wavelength—an effect of angular dispersion. The asymmetrically cut crystal thus behaves like an optical prism, dispersing an incident collimated polychromatic beam. The dispersion rate is $\simeq$8.5 mrad/eV. Third, parasitic Bragg reflections accompanying Bragg backreflection are suppressed. These effects offer a radically new means for monochromatization of x rays not limited by the intrinsic width of the Bragg reflection.

New devices…



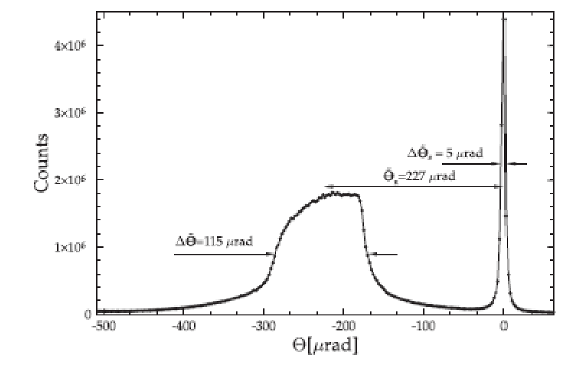
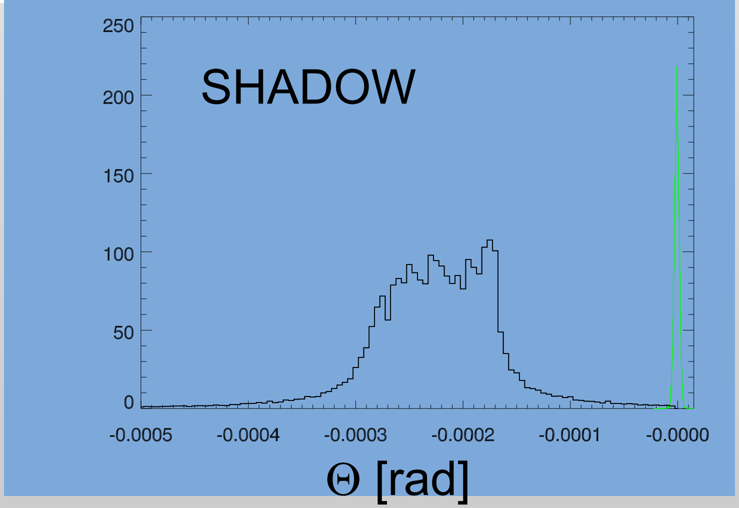


FIG. 4. Bragg reflectivity from crystal D of 9.1315 keV x rays, exactly backwards, as a function of the angle of incidence $\Theta = \pi/2 - \theta$ to the reflecting atomic planes.

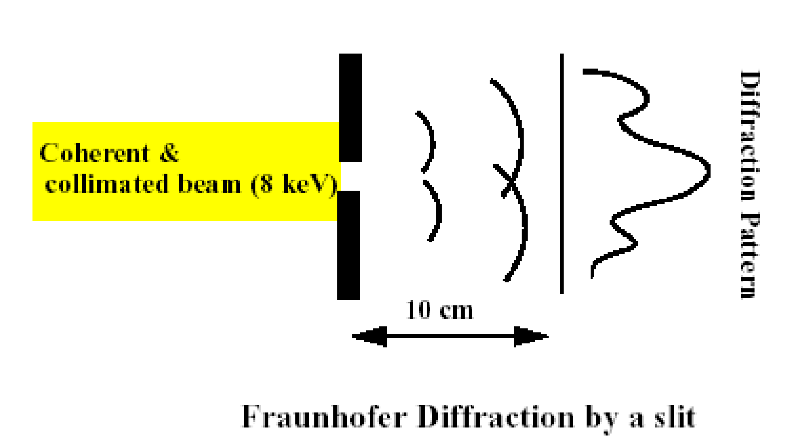


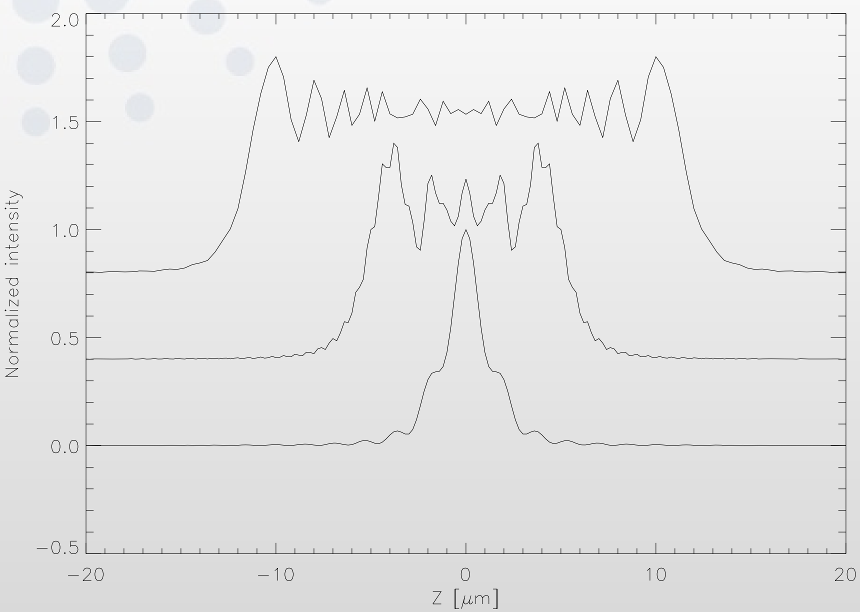
New Challenges

- Interference / Phase contrast
- Switch Ray optics <-> Wave optics
- Compound Refractive Lenses
- Variance Reduction
- Optical surfaces defined by Non-uniform Rational B-Splines (NURBS)
- Global optimization

Interference and diffraction by x-rays

1) Diffraction Fraunhofer 1-D : 5, 12.5 et 25 μm slits

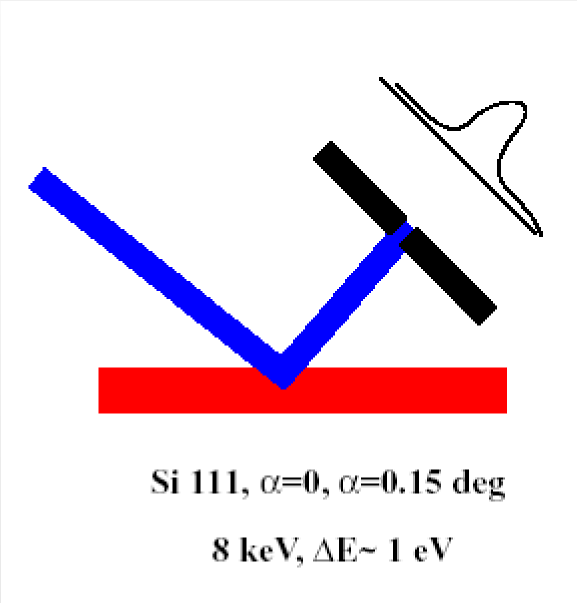


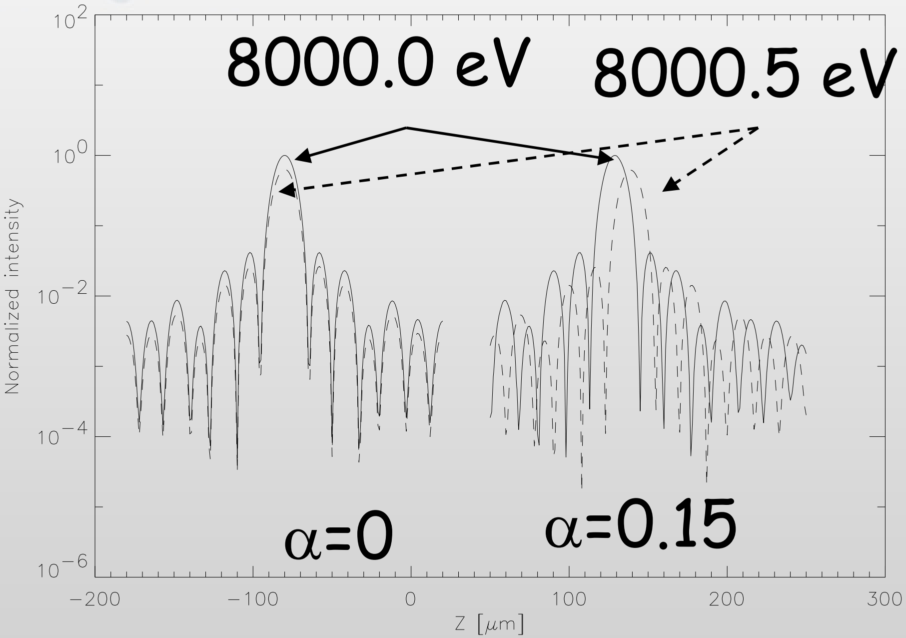


Fresnel-Kirchhoff Integral:

$$A'(\vec{r}') = \frac{i\bar{u}}{\lambda} \int_S A(\vec{r}) \frac{e^{ikR}}{R} d\vec{r}$$

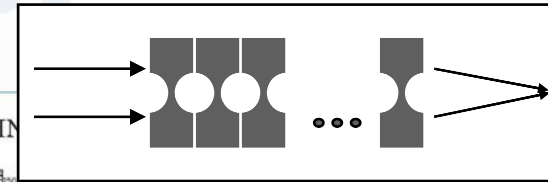
Asymmetric crystal





M. Sanchez del Rio
"Ray tracing simulations for crystal optics"
SPIE proceedings, vol. 3448, 230-245, 1998.

CRL



$$F = \frac{N}{2R\delta}$$

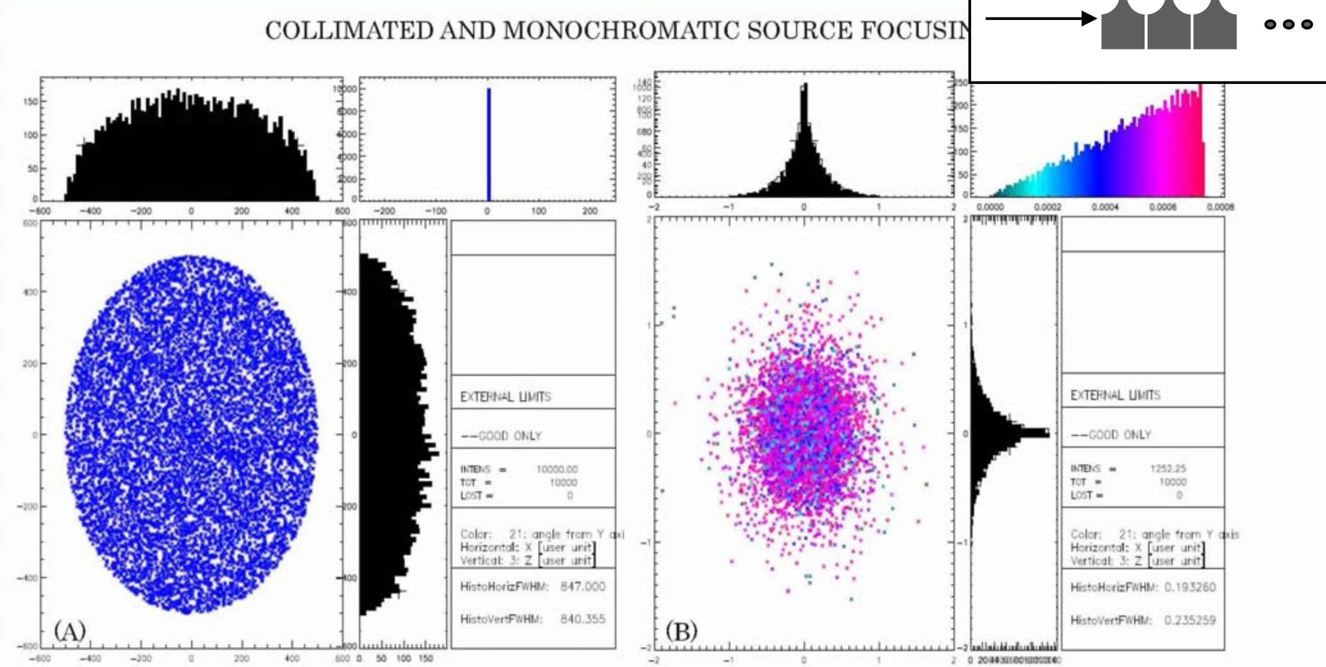
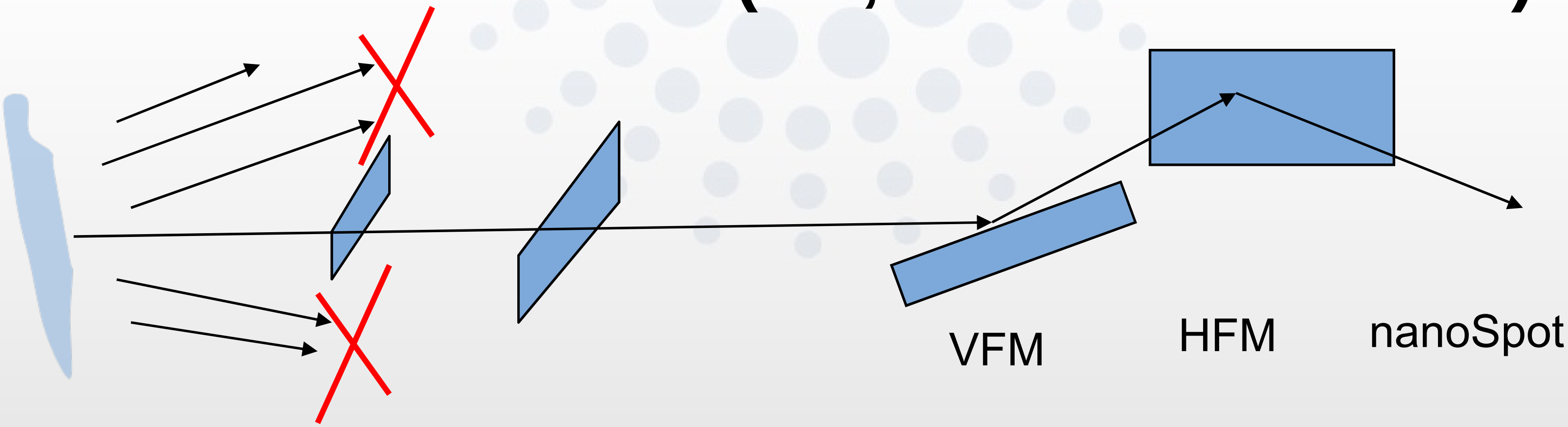


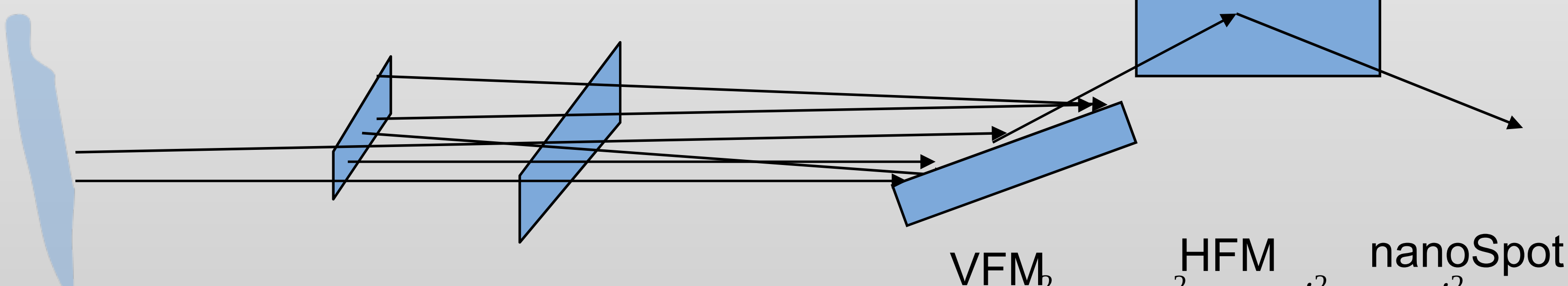
Fig. 1
(A) Collimated and monochromatic source with uniform filling over the entire lens aperture. E = 12 keV.
(B) Focus obtained with a parabolic beryllium CRL. The transmission is 12.5%. The focus FWHM is of order 0.2 μm. The ray spatial distribution is not the usual gaussian or lorentzian, but rather the combination of a narrow peak with a slowly decreasing background. Longer tails would probably be observed, if the scattering due to surface imperfections and to the Compton effect could be simulated (here Compton is present only as a cause of absorption). Ray-tracing does not include diffraction effects, and care has to be used when simulating geometries leading to point-like focusing, i.e. focusing down to approximately 10 nm. Units are μm. The colour scale represents the angular deviation from the optical axis (radians). The CRL program is used in combination with Shadow [1].

L. Alianelli, M. Sanchez del Rio, K.J.S. Sawhney
Ray-tracing simulation of parabolic compound refractive lenses
Spectrochimica Acta Part B: Atomic Spectroscopy 62 (2007) 593-597.

Variance reduction (KB, Gaussian sources)



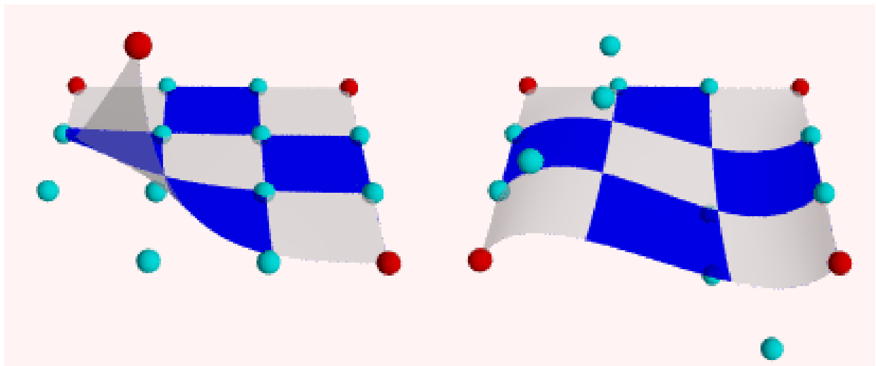
Very inefficient system



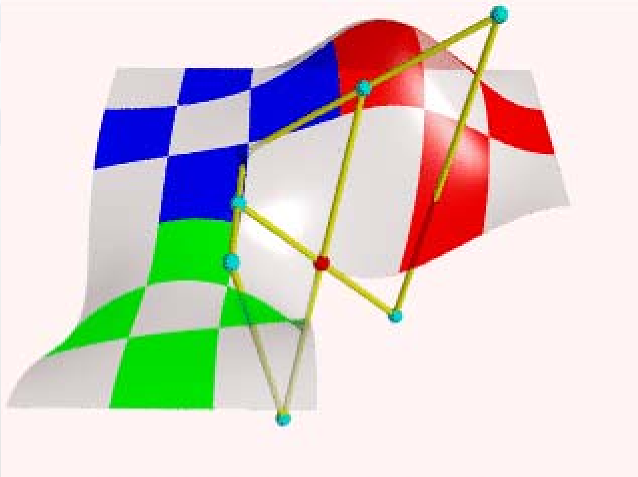
W=1 for central ray x=z=x'=z'=0

$$W = e^{-\frac{x^2}{2\sigma_x^2}} e^{-\frac{z^2}{2\sigma_z^2}} e^{-\frac{x'^2}{2\sigma_{x'}^2}} e^{-\frac{z'^2}{2\sigma_{z'}^2}}$$

Numerical representation of Optical Surfaces
NURBS (Non Uniform Rational B-Splines)



Bicubic_patch with control points



3 patches, some control points

- General definition of ANY optical surface
- Exact interpolation of quadrics (“rational”)
- Fast computing
- Problems: General and fast routine for intersection Surface-Ray
- SEE POSTER

The future

- Shadow 3.0
  - New SHADOW kernel
  - Interfaced with F2004, C, IDL, Python and perhaps Matlab that will allow to create user's main programs for large optimised calculations
  - ShadowVUI will be adapted
  - Prepare the frameworf for the "new challenges" already discussed.

Requirements

- Remove present limitations in:
  - Dimensions (number of rays, optical elements, mesh points, etc.)
  - Optical library (100 keV)
  - Old programming techniques (Common blocks, etc).
- Be flexible to easily modify and add new features
- Availability of a shadow library, where the user can easily modify the main code
- Maintain Shadow's flavour (i/o, file format, back compatibility). Users that know SHADOW must feel "confortable" with the new one.
- Alpha version targeted for the end of this year

Conclusions

- Shadow has been of great help in the development of SR beamlines
- Shadow has performed very well in more than 25 years of services
- Many of us have learn a lot of x-ray optics using Shadow, and took profit from its existence
- The reciprocal is also true: many of us have also contributed to make Shadow a unique tool in Synchrotron optics
- Shadow is open (both the algorithms and the source code)
- It is a patrimony of the SR community, thus it is fundamental to take care of it
- **We face an upgrade of Shadow, simultaneous to the ESRF upgrade, with mutual benefits**
- **Your help is not only welcomed, but IT IS NEEDED. SO PLEASE CONTRIBUTE!**

Shadow 3.0 planning I

- Language: It is important to keep SHADOW open source and compiled with an open source compiler. Rewriting SHADOW in IDL, MatLab, etc could be fast, but all these are proprietary codes. Translate into C/C++ will be a great pain. So we propose to keep it in Fortran, using the g95 compiler (www.g95.org) and slowly migrate to fortran95 .
- Fortran95 can help in improving the code a lot because:
  - In principe (only) all f77 is f95, so a “soft” transition is expected
  - Common blocks must be encapsulated in “modules”
  - Is not limited to dimensioned arrays (free number of rays)
  - Has interfaces to other programming languages and in principle external tools
  - g95 is free. Opensource and works on Linux, Window and MacOS, the three main platforms we should support
- For backwards compatibility, we should keep the current file format, based on gFiles for parameters and star files for beam dumps.
  - All code for “namelist”compatibility should be removed
  - All star files will always have 18 columns (for simplicity)
  - In future, this could be changed, for instance gFiles can be substituted by XML, and star files by some binary compressed format.

Shadow 3.0 planning II (sources)

- At present gen_source deals with all kind of sources (geometrical, BM, wiggler and undulator). This is a real problem, and the intense use of preprocessor makes things very complicated. We propose to split gen_source, into three smaller programs:
  - Source_g: keep only the geometrical sources (perhaps re-splitted in random and grid sources)
  - Source_bm: bending magnet. Use always the "exact"calculation (it is as fast as the precalculated one), thus remove all dependencies of extra data files.
  - Source_cdf: reads a cdf created by preprocessors (like is done now for undulators). A preprocessor for undulator and another for wiggler could be provided. Right now, undulators are in very good approximation Gaussian sources, so they can be modeled accurately with the Source_g. Wigglers are not very much used today, and SHADOW has the drawback that it created the full emission. We should think in upgrading these later.

Shadow 3.0 planning III (trace)

- There are several fundamental points to solve:
  - Mirr.F is very long. It should be splitted in several parts. Separate well the geometrical reflection from the physical calculations (reflectivities).
  - Sort common blocks
  - “trace” should read input files with physical constants or cdf created with the library.
  - The optical library must be updated with recent data, and extend in photon range. Also Compton cross section should be implemented for absorption at high energies.
- Presently, the oe is “a single surface”. For the future, it will be defined an input and an output surface for each oe. That will permit to create “long” oe, like compound refractive lenses, wave guides that bend the beam, and to glue many mirror in a single oe, like for astronomical telescopes.

Shadow 3.0 planning IV (main)

- The "main" SHADOW program should be extremely simple, in the sense that the user could change it, make loops, customized scoring etc. It must run both source and system. An skeleton like:

```
ierror = read_gfile('start.00',g0) ! g0 is the ouput "glist"
ierror = read_systemfile('systemfile.dat',g) ! g is an array of glists

ierror = source_g(g0,rayOut)  ! make source
ierror = trace_align(g)  ! call setsour, imref, etc for all oes, read
input files
DO I=1,N_Elements(g)
      rayIn=rayOut
      ierror = trace_mirror(g[I],rayIn,rayOut)
      ierror = write_ray(rayOut,'star'//I)
ENDDO
END
```

- This structure garantizes that no file i/o is done during the loop, so we can make an external loop for creatig more rays at the source and run again the system. It can be seen that the "mirror alignment" that is done in the current version just before tracing the rays, should be done at the beginning for all oe's, thus creating "multiple instances" of the input variables.

The path to Shadow 3.0 beta

- Alpha1 version:
  - Compilation should be done with small script files. The present configuration and makefiles are extremely complex, and is not easy to find and correct problems.
  - Group the minimum input/output needed (gfiles, ray, string manipulation). The start and ray files should be compatible with alder versions.
  - The random number generator must be changed. There are now recent implementations in fortran (77_95) of the Mersenne Twister that seems to work very well.
  - Create a source program for only geometrical sources extracting the code from gen_source
  - Work with trace
    - Readjust common blocks
    - Split mirr.F and separate geometrical part (needed here) and physical part (for later)
    - Separate the trace procedure in the element/beamiline setup (alignment, prepare inputs) and ray-tracing
    - Make it working for mirrors, gratings
  - Create case tests for the
    - different geometrical sources
    - different systems (no reflectivity)
  - Compare tests with old versions.
- Alpha2 version
  - Create source for bending magnet
  - Update the optical database using xraylib
  - Implement mirror, multilayer and crystal reflectivities
  - Implement mirror imperfections: splines and others
- Alpha3 version
  - Source_cdf and undulator + wiggler
  - Postprocessors (without graphics)
  - Final tests
- At this point a first beta should be ready