Experience of synchrotron sources and optics modelling at Diamond Light Source

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Outline

- Microfocus MX beamline optics design
  (Principal Beamline Scientist G. Evans)

- Surface and interface structural analysis SISA
  (Principal Beamline Scientist Tien-Lin Lee)

- Simulation of parabolic CRL’s

- Towards design of nanofocusing lenses

Design of Phase II beamlines at Diamond Light Source

Non crystalline diffraction interdisciplinary beamline (I22) for studying large, complex structures including living organisms, polymers and colloids.
Joint engineering, environmental and processing (JEEP) beamline (I12) providing a multi-purpose facility for high energy diffraction and imaging of engineering components and materials under real conditions.

RAY (K Sawhney)

Test beamline on a bending magnet (B16) for testing new developments in optics, detectors and research techniques.

SHADOW + some ad-hoc in-house developed macros (L. Alianelli, U. Wagner and J. Sutter)

Small molecule single crystal diffraction high-intensity beamline (I19) for determining the structure of small molecule crystalline materials, such as new catalysts and 'smart' electronic materials.
High resolution powder diffraction beamline (I11) specialising in investigating the structure of complex materials including high temperature semiconductors and fullerenes.
Microfocus macromolecular crystallography beamline (I24) for studying the relationship between the structure of large macromolecules and their function within living organisms.
Circular dichroism beamline (B23) for the life sciences and chemistry, able to observe structural, functional and dynamic interactions in materials such as proteins, nucleic acids and chiral molecules.
Monochromatic macromolecular crystallography side station (I04-1) on one of the year one macromolecular crystallography beamlines, that will use monochromatic light to investigate the structures of protein complexes.
X-ray spectroscopy (XAS-3) beamline (I20) including a versatile X-ray spectrometer for studying chemical reactions and determining physical and electronic structures to support fundamental science.
Surface and interface high resolution diffraction beamline (I07) for investigating the structure of surfaces and interfaces under different environmental conditions, including semiconductors and biological films.
Core EXAFS (B18)
Infrared Microspectroscopy (B22) as a powerful and versatile method of determining chemical structure bringing new levels of sensitivity and spatial resolution, with subsequent impact across a wide range of life and physical sciences.
Beamline for Advanced Dichroism Experiments (BLADE) (I10) for the study of magnetic dichroism and magnetic structure using soft x-ray resonant scattering (reflection and diffraction) and x-ray absorption.
X-ray imaging and coherence (I13) for studying the structure of micro-and nano-objects. The information is either acquired in direct space or by inverting (diffraction) data recorded in reciprocal space.

Surface and Interface Structural Analysis (SISA) (I09) will combine low energy and high energy beams focused on the same sample area, and will achieve advances in structural determination of surfaces and interfaces, as well as in nano-structures,

Packages in use at Diamond for sources & optics calculations

Sources

• SRW (O. Chubar and P. Elleaume)

• Spectra (T. Tanaka et al, Spring8)

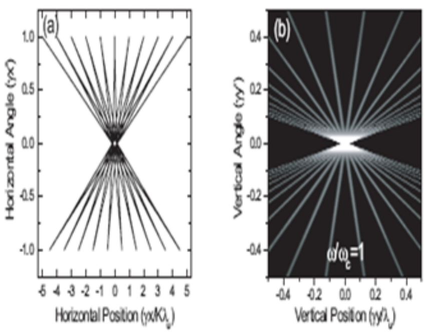


FIGURE 1. The photon distribution in the (a)horizontal and (b)vertical phase spaces, respectively, when the number of wiggler periods N is equal to 10. In (b), the photon energy ω is assumed to be equal to the critical energy ω_c. It should be noted that the photons lie on the lines in the horizontal phase space, but are not evenly distributed.

Optics & beamline layout

• Ray (F. Schafers et al, Bessy)

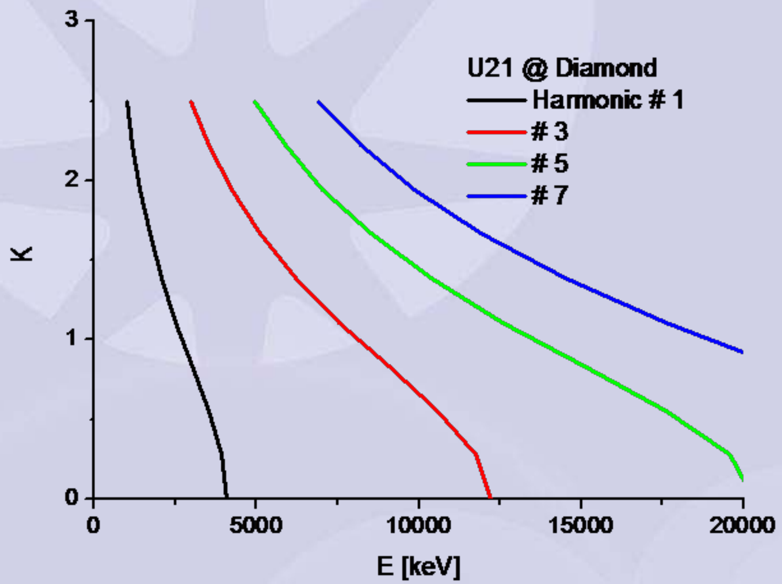
• Shadow (F. Cerrina, M. Sanchez del Rio et al)

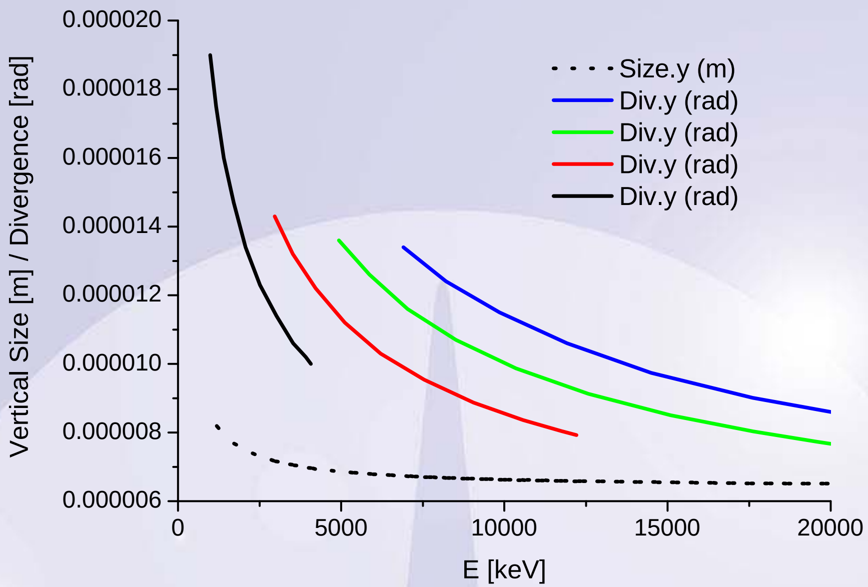
Optical constants database

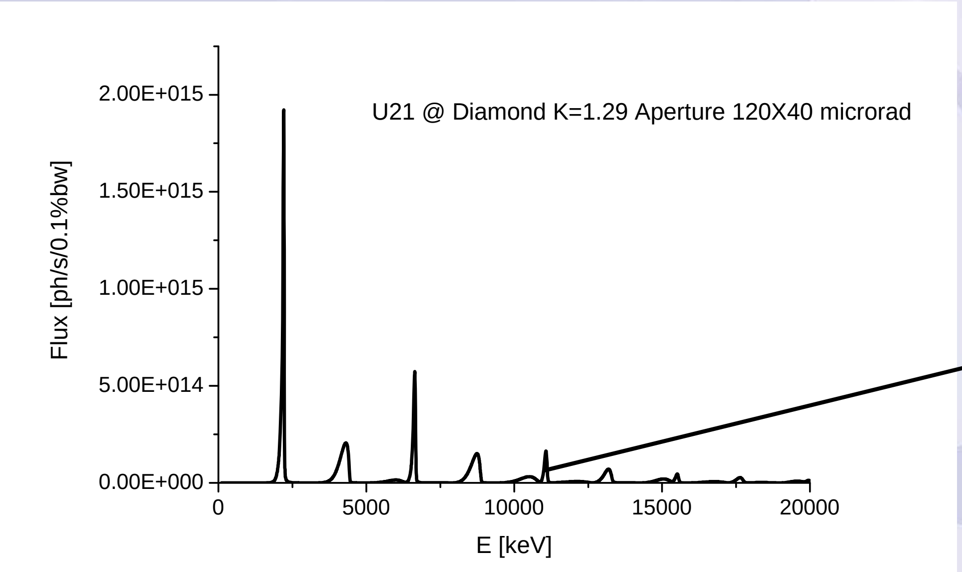
• XOP (M. Sanchez del Rio)

• Zemax

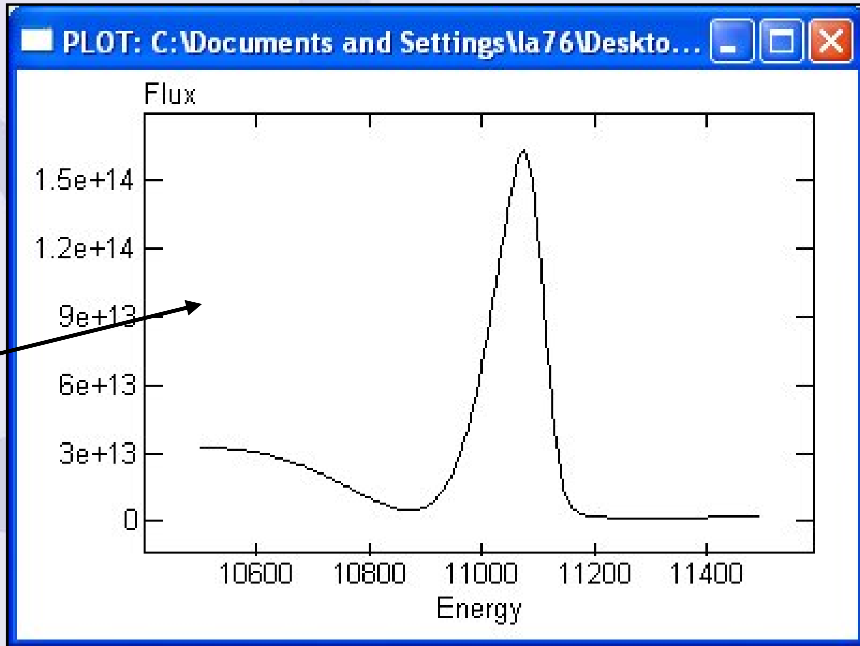
Undulator K-characteristics, photon beam size, divergence & flux





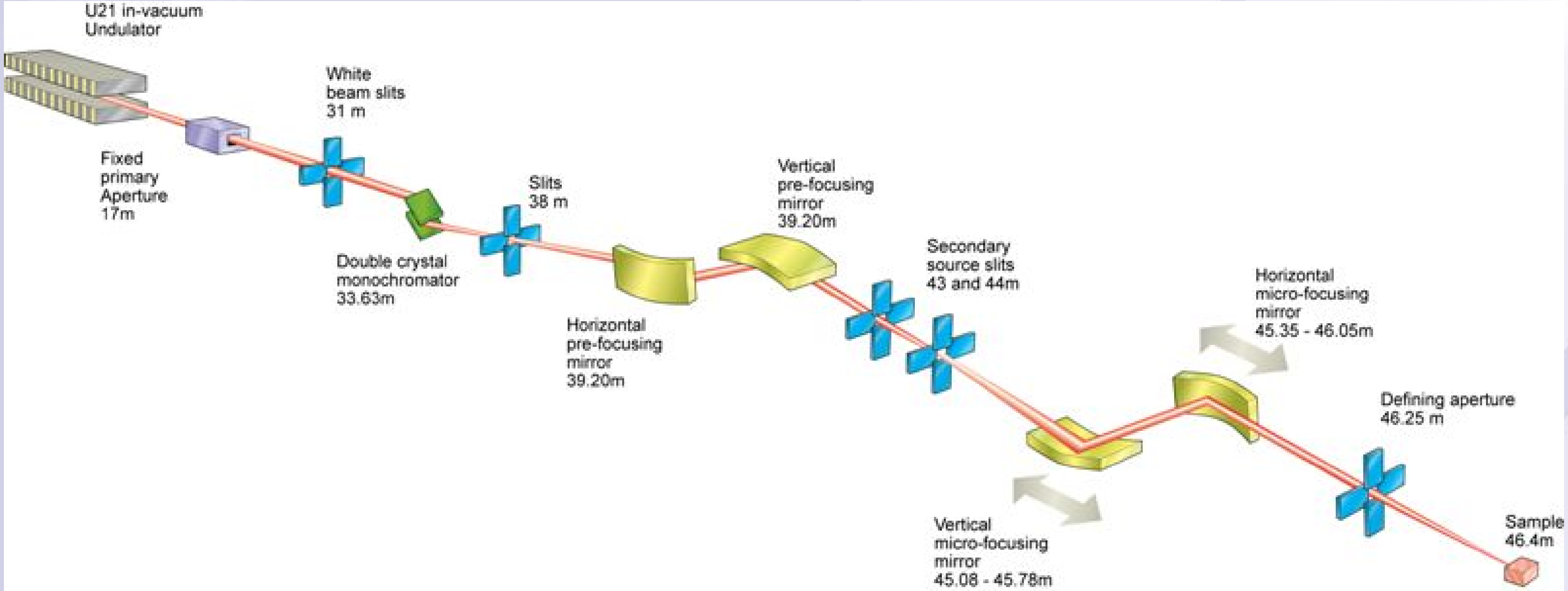


Spectra, T. Tanaka and H. Kitamura



Double KB mirror system for the µMX beamline I24

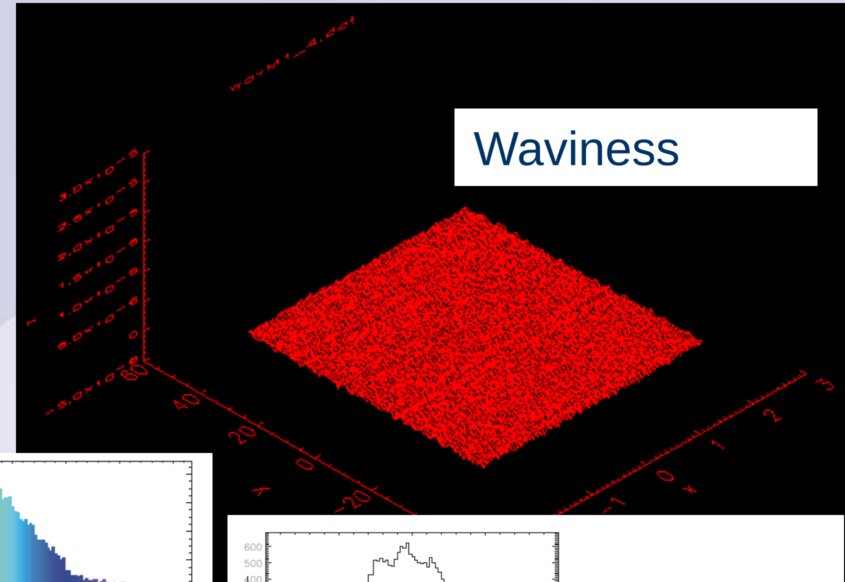
The microfocus beamline will have a beam size at the sample of 5-30 microns, and will be a major asset for the UK structural biology programme. It will enable measurements on small crystals that are not possible on conventional beamlines due to their small size or mosaicity, and will improve the screening of crystals for optimisation of crystallisation conditions.

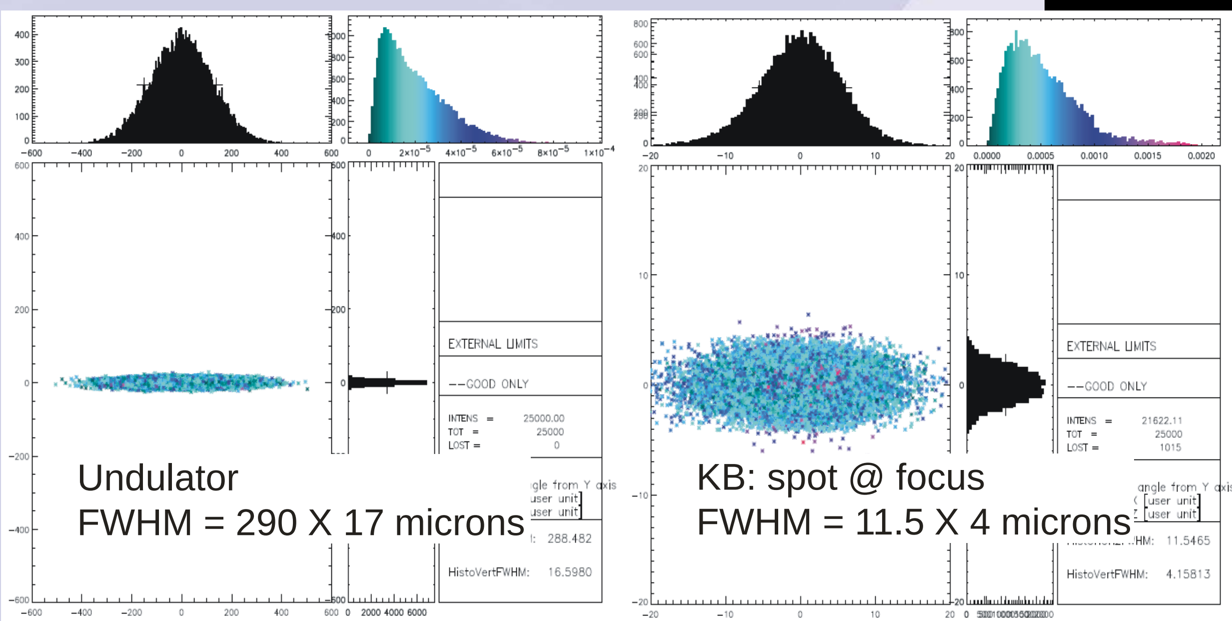


Principal Beamline Scientist G. Evans

Simulation of mirror imperfections

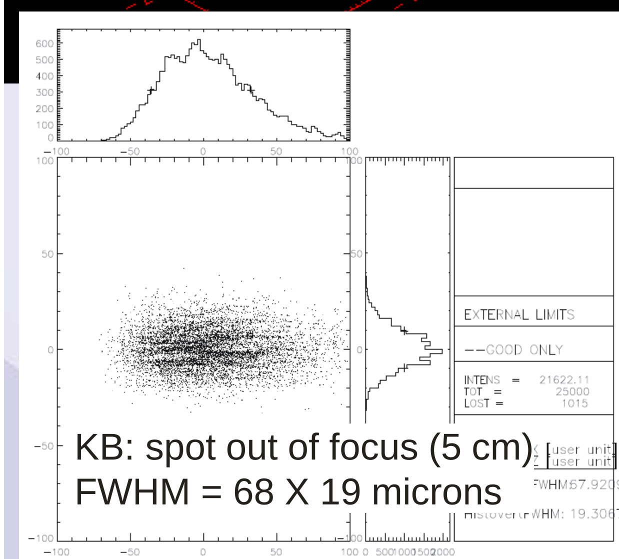
Shadow simulation of beamline with Kirkpatrick-Baez mirrors with elliptical bending. Rh coating reflectivity is included. Slope errors are simulated using a general description of waviness





Undulator
FWHM = 290 X 17 microns

KB: spot @ focus
FWHM = 11.5 X 4 microns



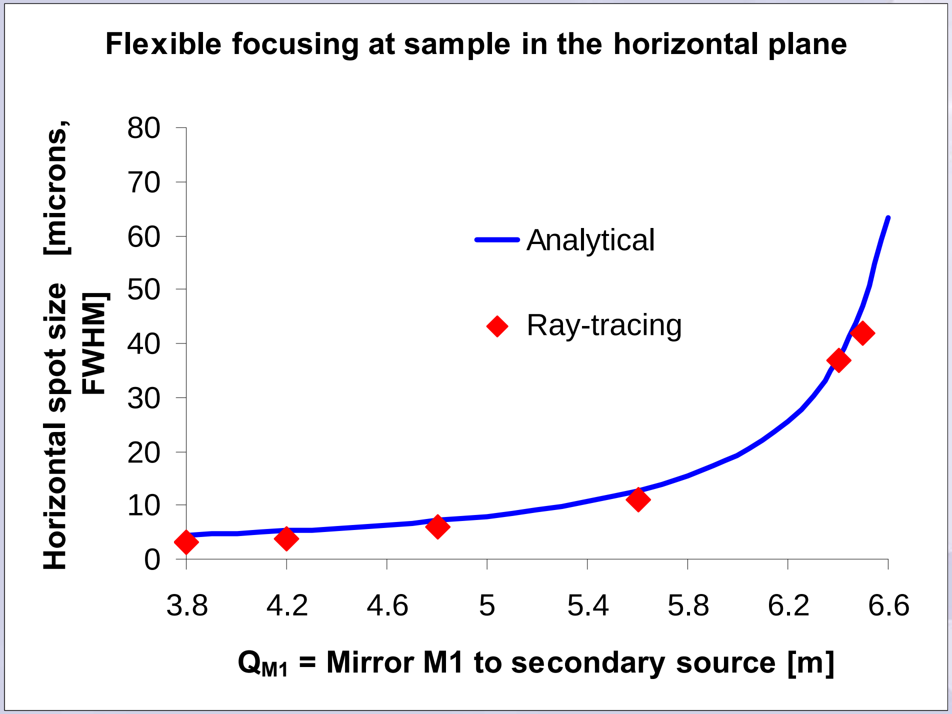
KB: spot out of focus (5 cm)
FWHM = 68 X 19 microns

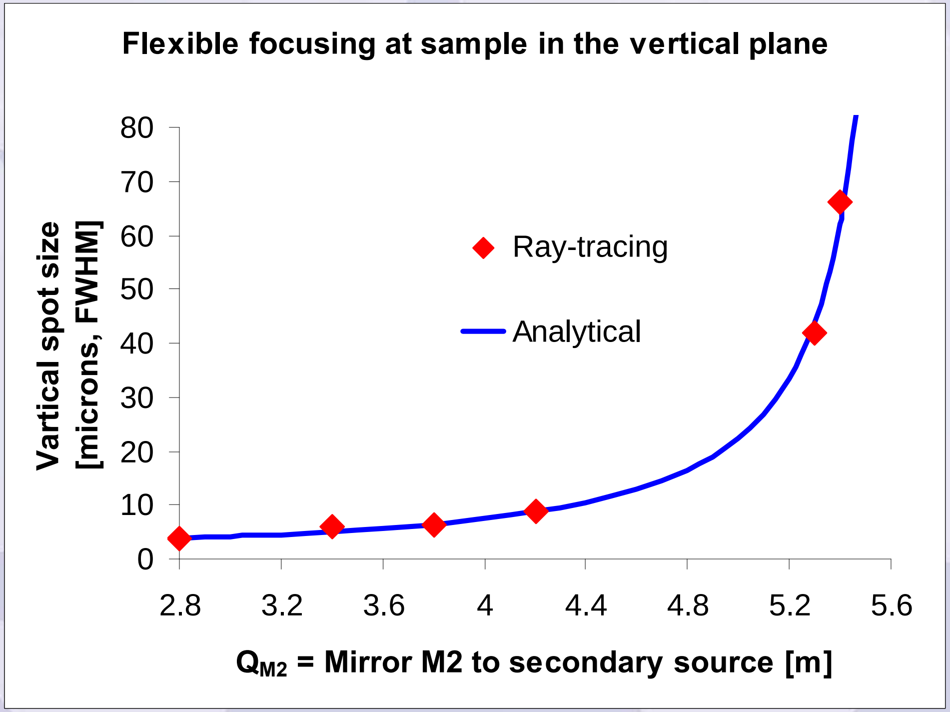
B. Lai et al, Nucl. Instr. and Meth. A 246 (1986) 337.
M. Sanchez del Rio et al, Nucl. Instr. and Meth. A 319 (1992) 170.

Double KB mirror system on I24: variable demagnification at sample & detector

$$\sigma_{virtual\ source} = \sqrt{\left(\sigma_{source} M_{1stKB}\right)^2 + \left(2\sigma_{1stKB}^{SLOPE} Q_{1stKB}\right)^2}$$

$$\sigma_{focus} = \sqrt{\left(\sigma_{virtual\ source} M_{2ndKB}\right)^2 + \left(2\sigma_{2ndKB}^{SLOPE} Q_{2ndKB}\right)^2}$$





Microfocus MX beamline I24

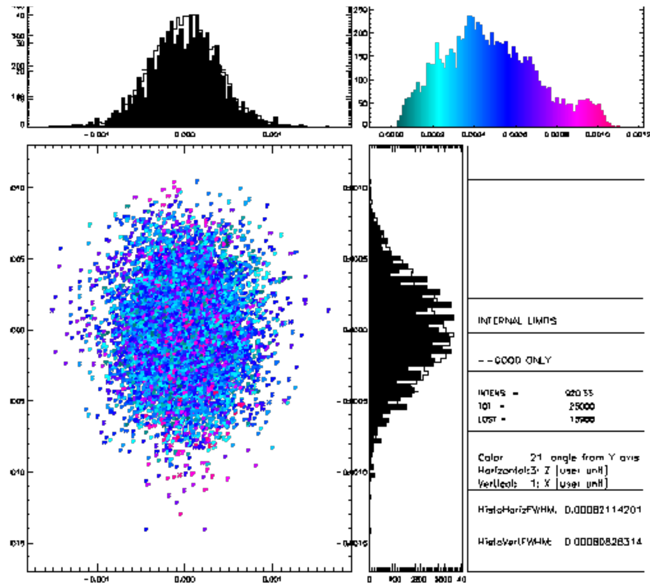
Mirror setting # 1:

Secondary source at 44 m

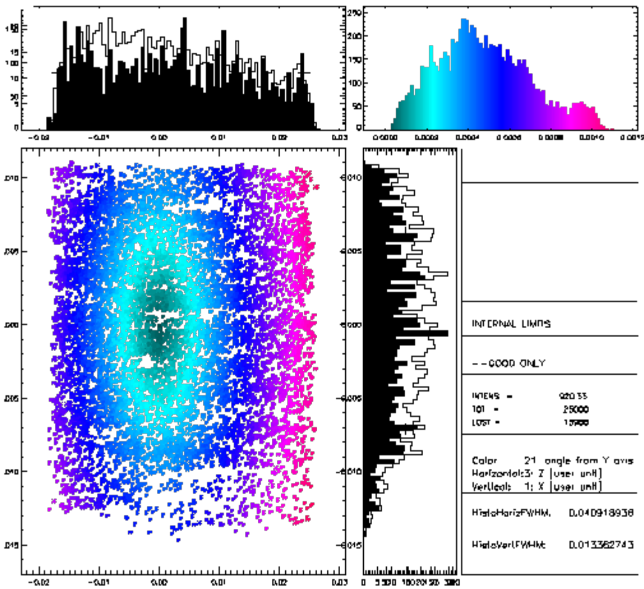
Sample at 46.4 m

Detector position is variable

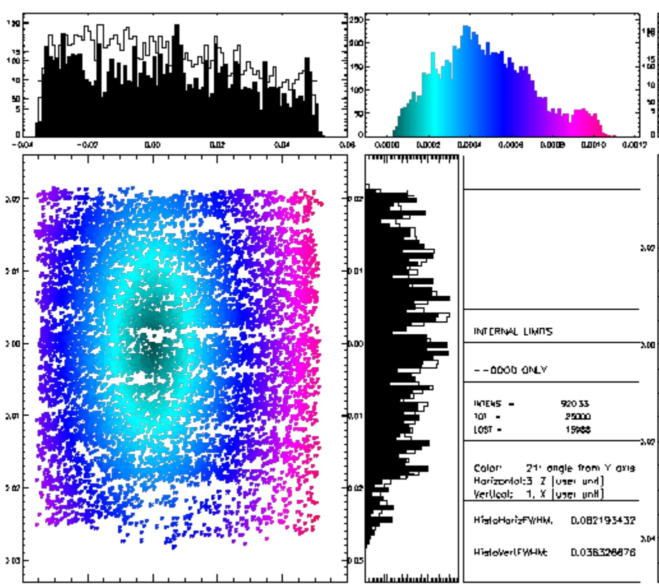
Beam at sample 8 X 8 μm (focused)



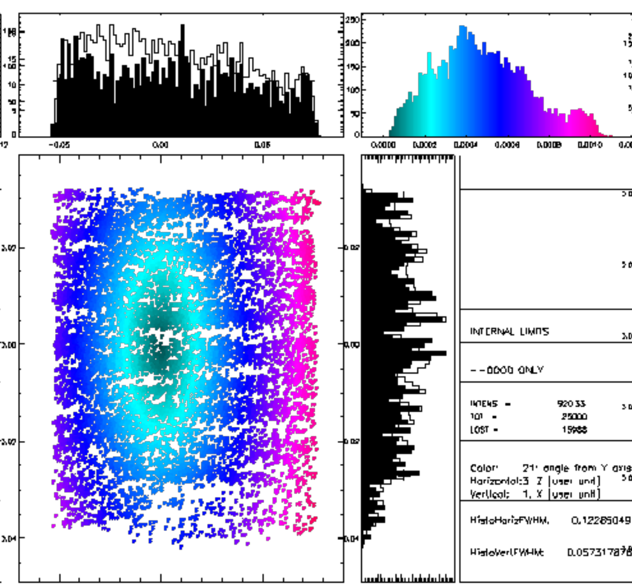
250 mm



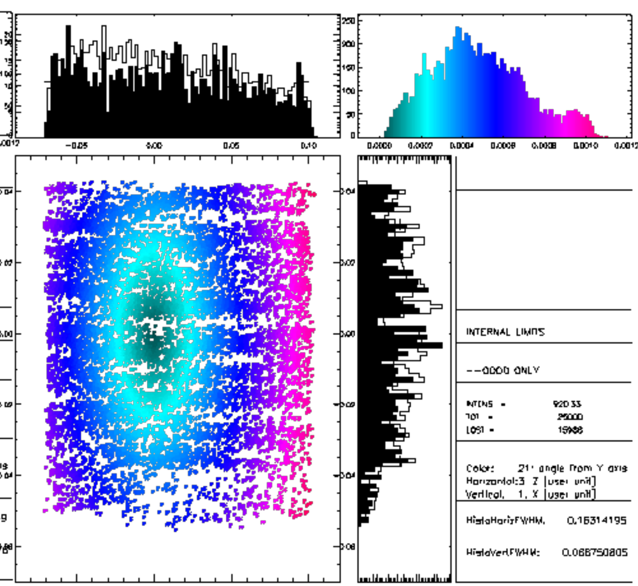
500 mm



750 mm

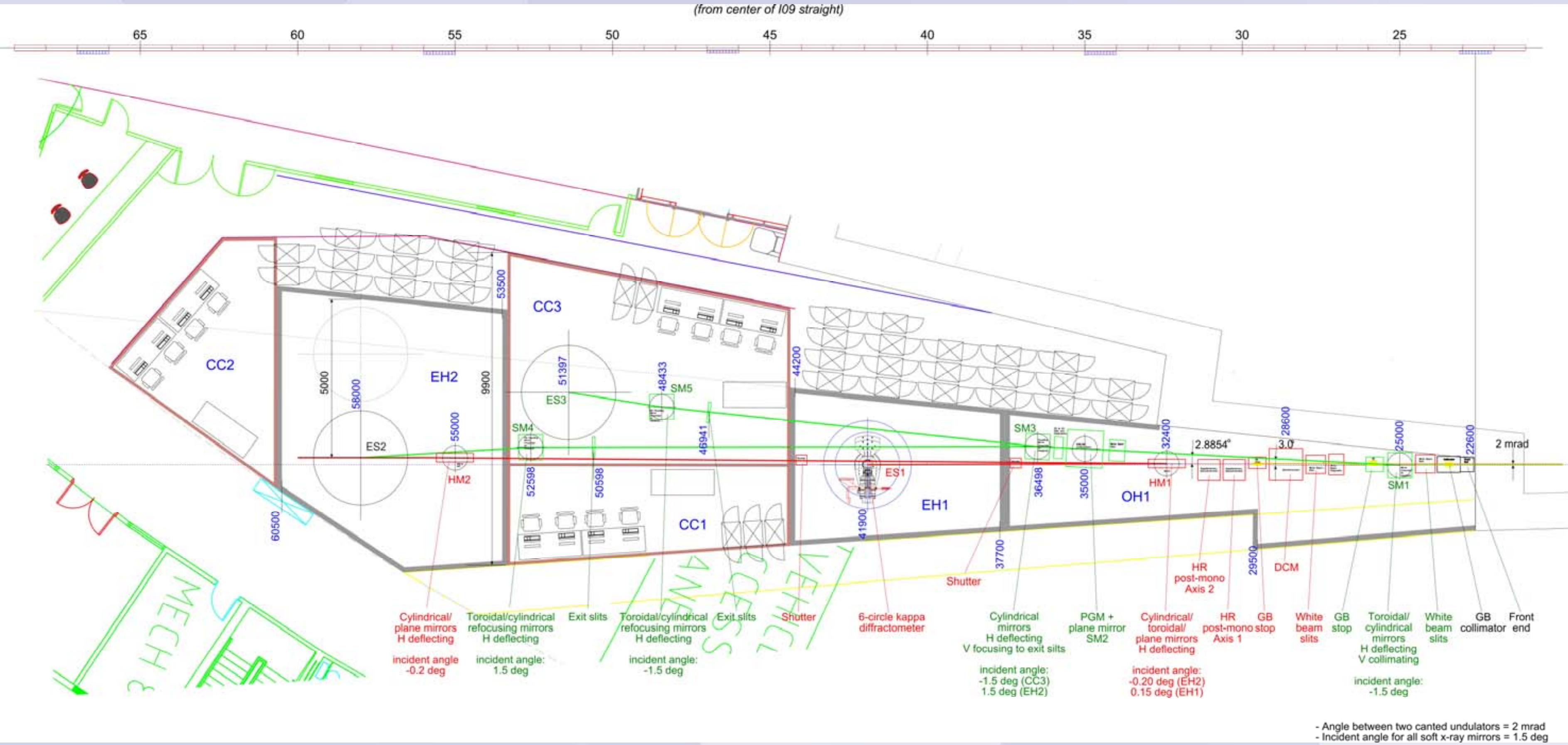


1000 mm



Surface and Interface Structural Analysis beamline SISA

An x-ray facility for studying atomic structures and properties of surface and interfaces of wide varieties. A unique feature of this beamline is that it will allow sample characterization with both hard and soft x-rays.

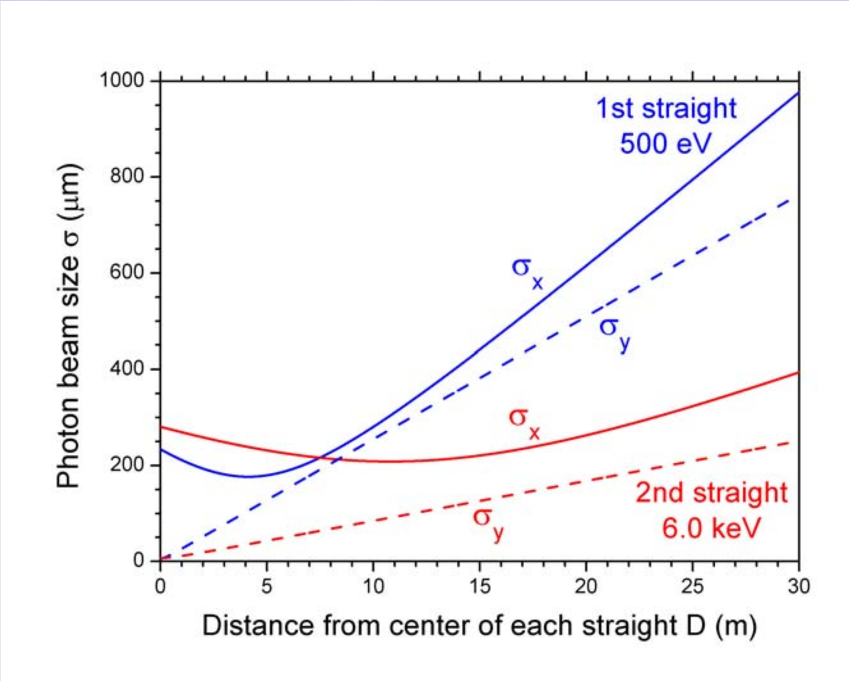


Soft X-Ray Branch

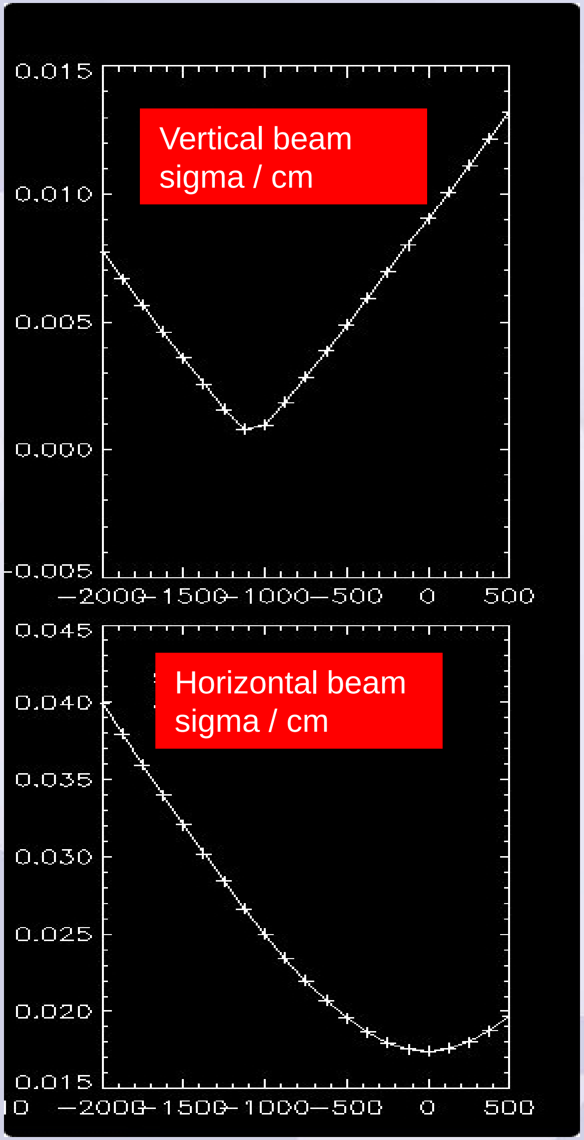
Hard X-Ray Branch

Principal Beamline Scientist Tien-Lin Lee

SISA canted undulators: ad-hoc Shadow simulation of mini-beta scheme (i.e. astigmatic electron beam source)



Courtesy B. Singh, TL Lee, DLS



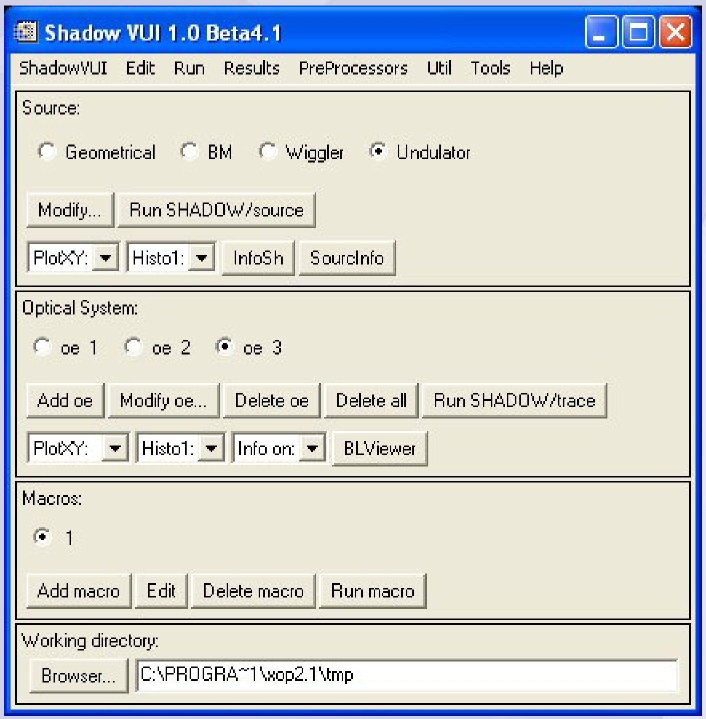
Distance / cm

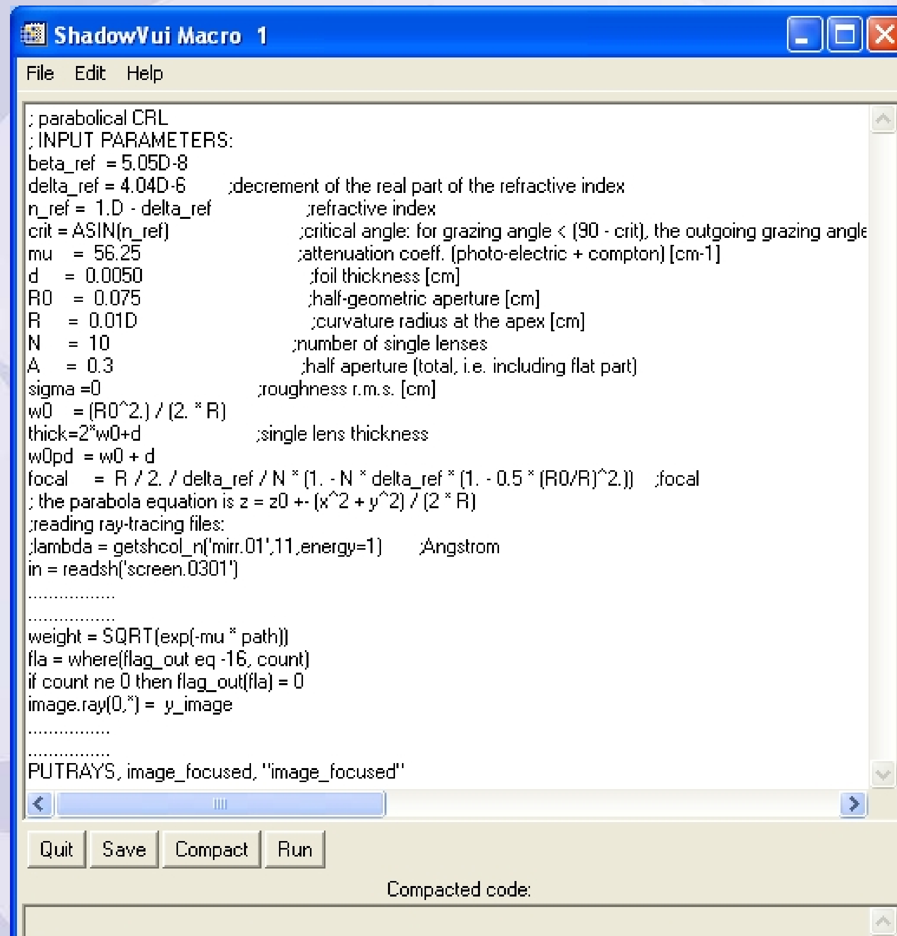
Simulation of parabolic CRL's

✓**Refractive lenses in use at Diamond**

✓ **Numerical methods useful for efficiency estimate i.e. comparison with other optics**

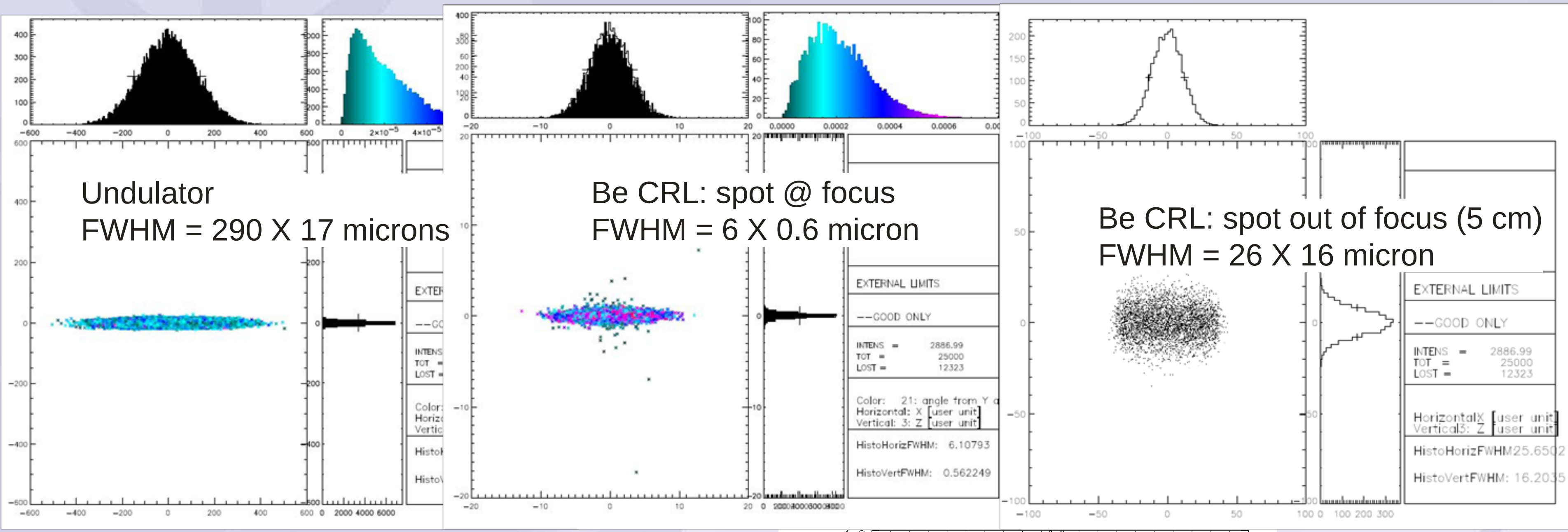
✓ **Analytical ray-tracing developed (phase calculation neglected)**



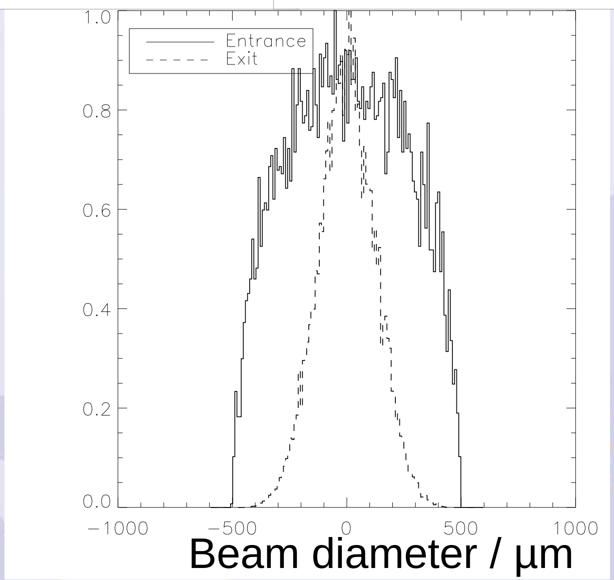


L. Alianelli, M. Sanchez del Rio and K.J.S. Sawhney *Spectrochimica Acta Part B* 62 (2007) 593–597

Examples of parabolic Be CRL simulation



- ✓ Exact trajectory through N lenses calculated
- ✓ Absorption included
- ✓ Gain, absorption aperture in agreement with **B. Lengeler et al *Imaging by parabolic refractive lenses in the hard X-ray range*, J. Synchr. Rad. 6 (1999) 1153-1167.**

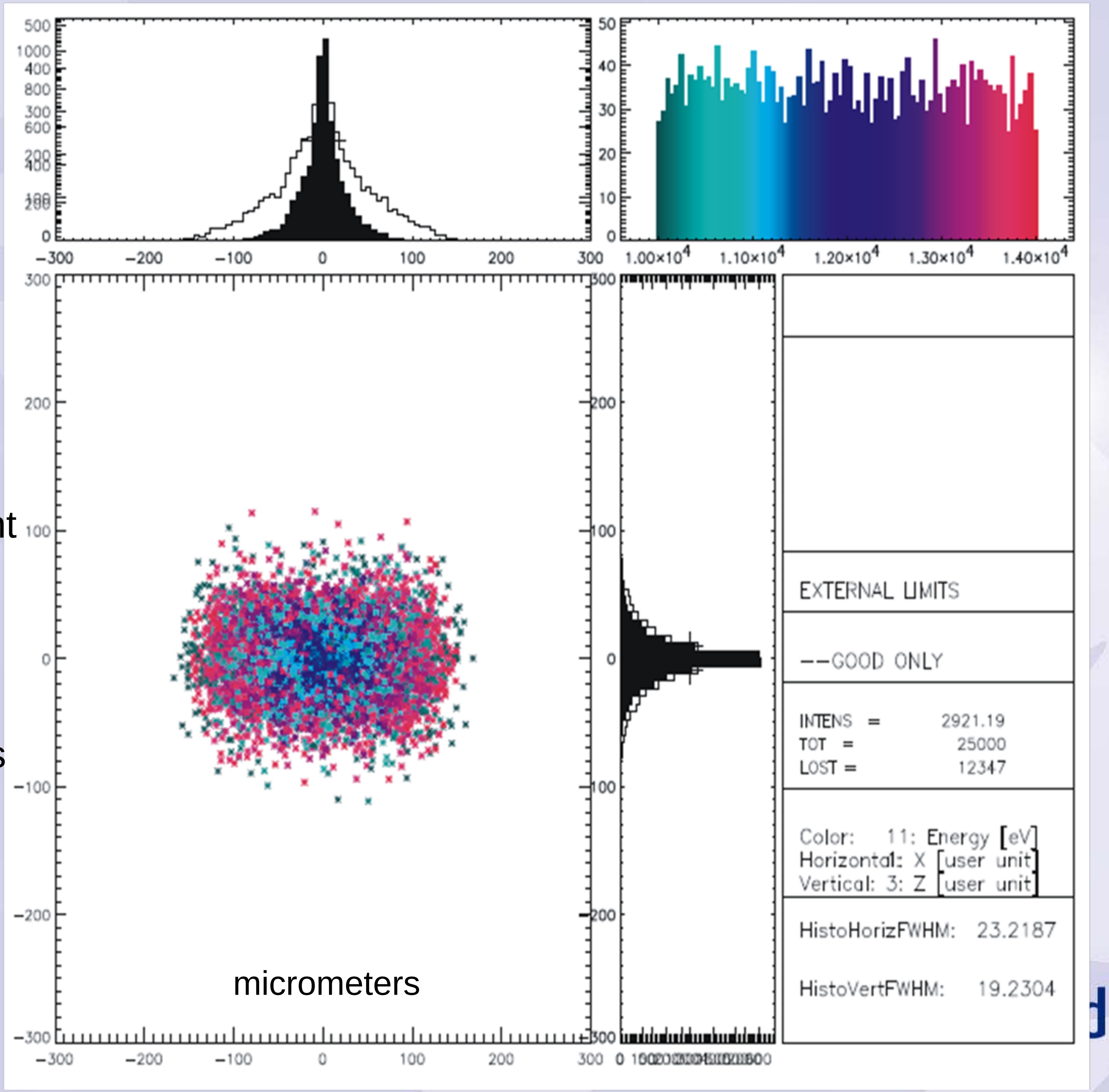


Polychromatic case.

Focal spot produced by the CRL with an almost perfectly collimated incident beam.

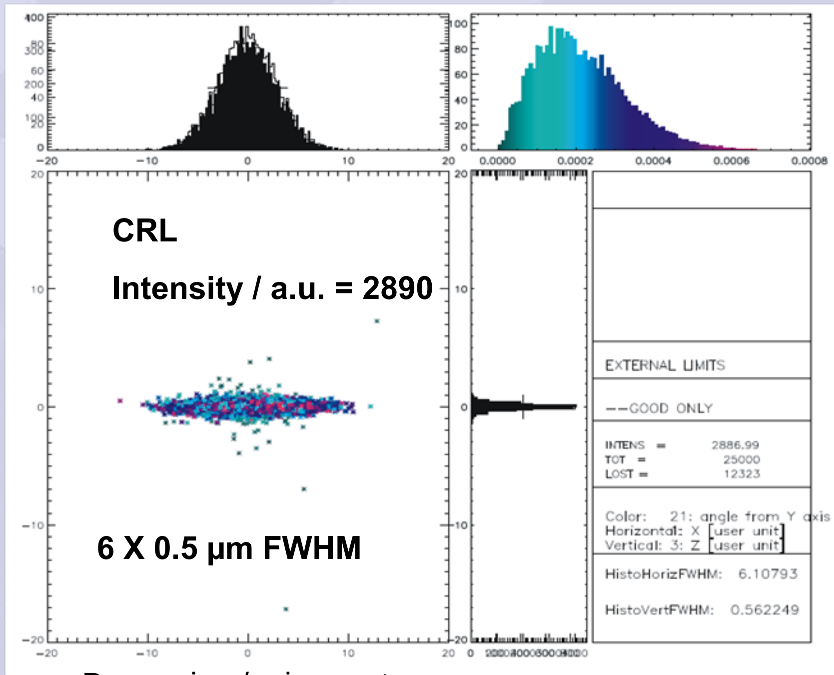
Units are micrometers.

Colour represents energy.

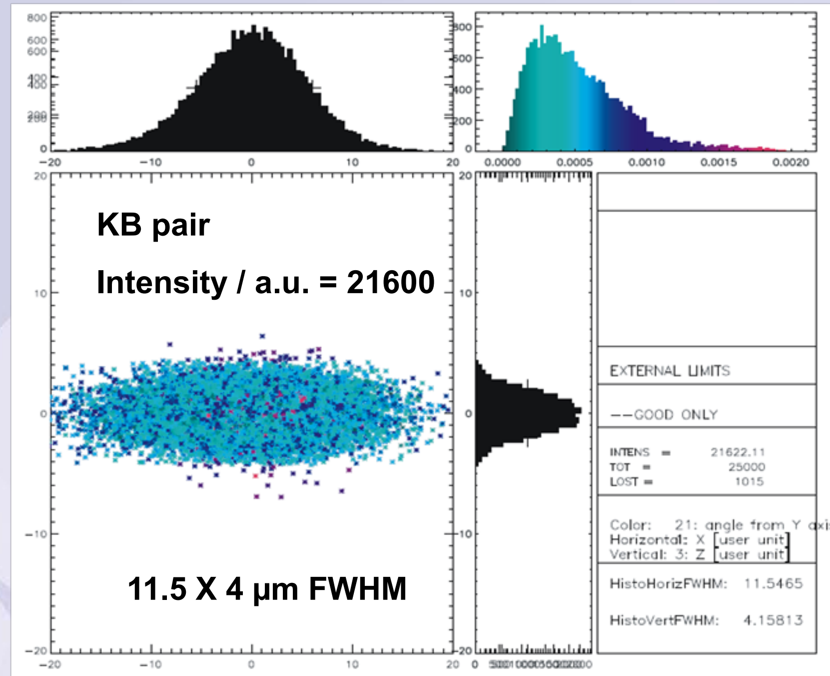


Undulator source

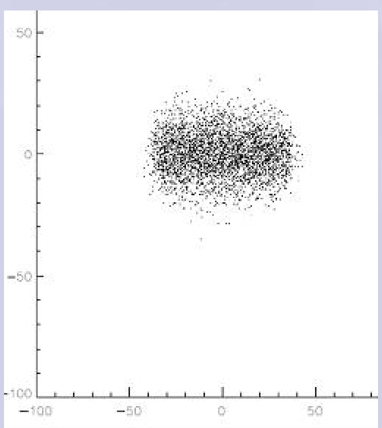
Focal spots produced by a Be CRL (left) and a KB pair (right) with similar focal lengths.



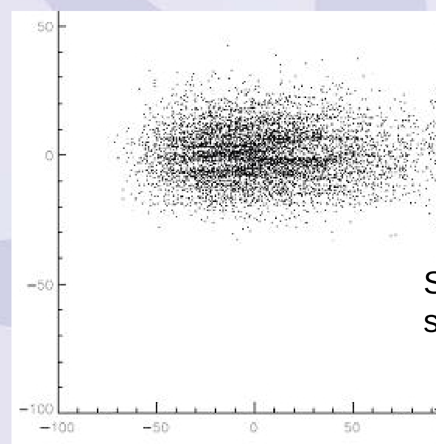
Beam size / micrometers



Beam size / micrometers



5 cm away from focal point



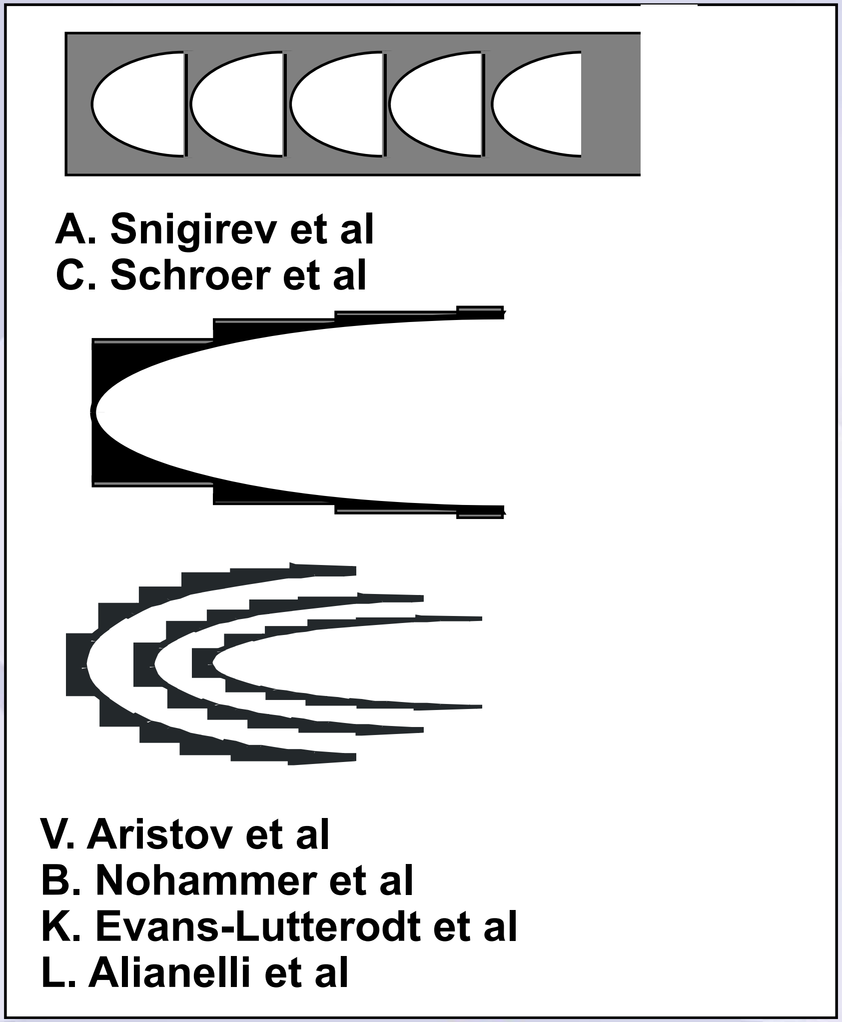
Striations due to slope errors

Design of Focusing Refractive Optics

$$\Delta = 1.22\frac{\lambda}{N.A.} = 1.22\frac{\lambda \cdot F}{D_{absorption}}$$

$$\Delta_{Single\,Kinoform} \sim \frac{\lambda}{\sqrt{2\delta}} \sim 50\,nm$$

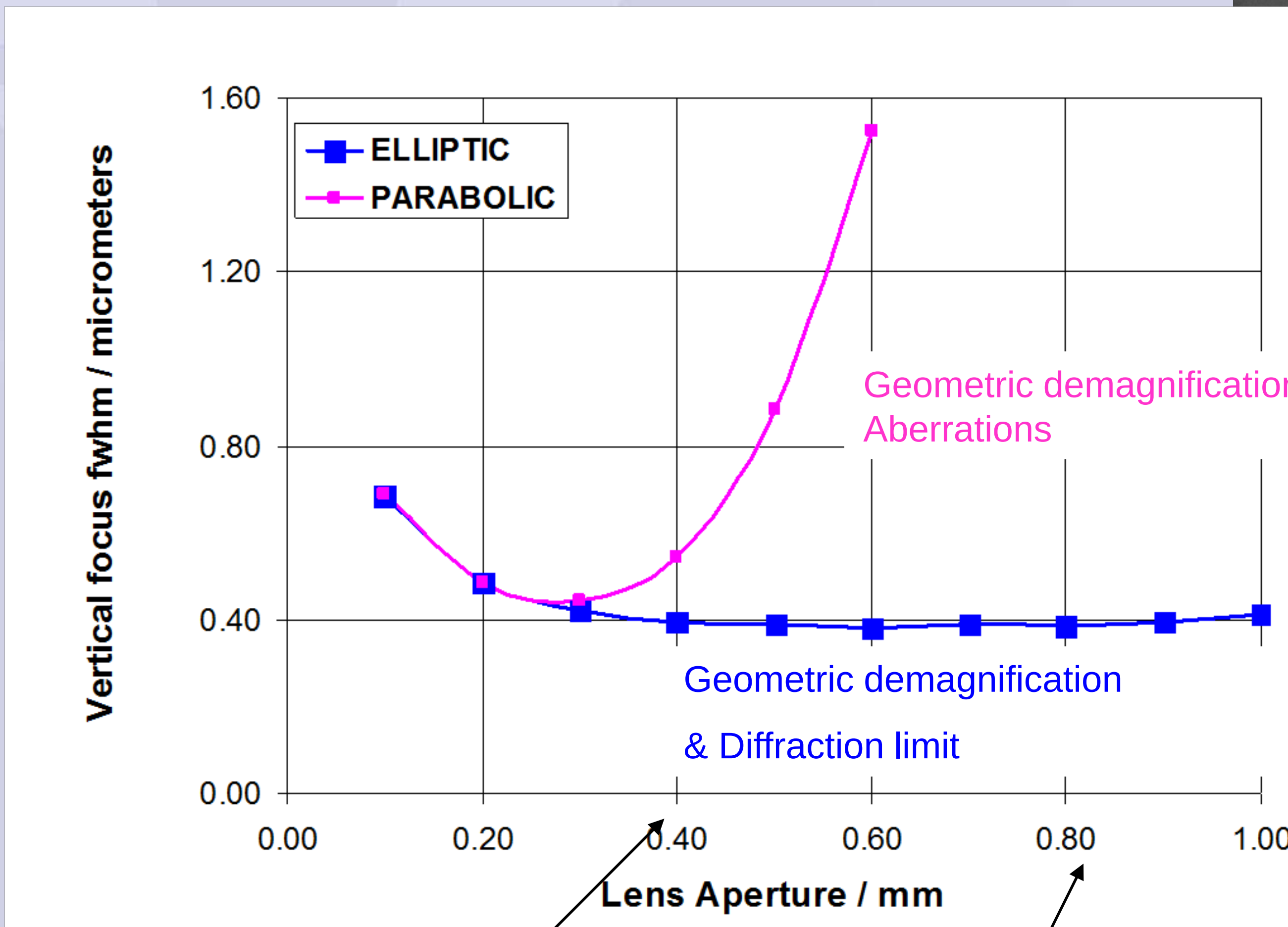
$$\Delta_{Kinoform\,Array} = \frac{\Delta_{Single\,Kinoform}}{N}$$

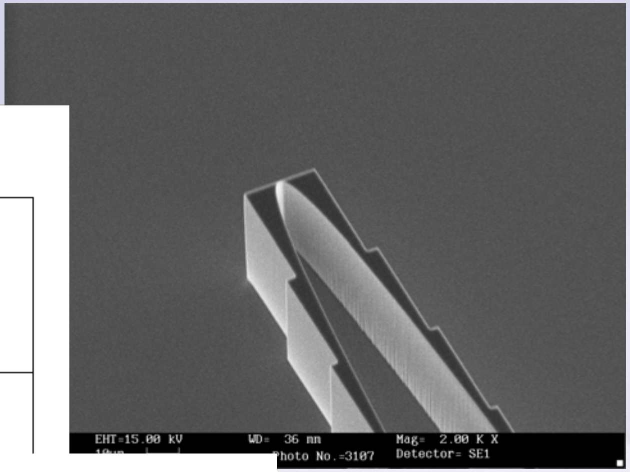


KINOFORM SINGLE ELEMENT LENS

- Ideal transmission > 90%
- Resolution no longer limited by absorption
- Resolution is limited by fabrication accuracy
- Refractive-diffractive behaviour => optimal efficiency reached at fixed energy

Design of single element kinoform lens with Shadow





Elliptic vs Parabolic
Single Element Lens

f = 1000 mm

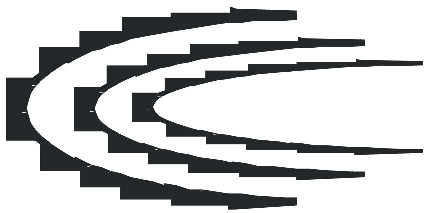
E = 8 keV

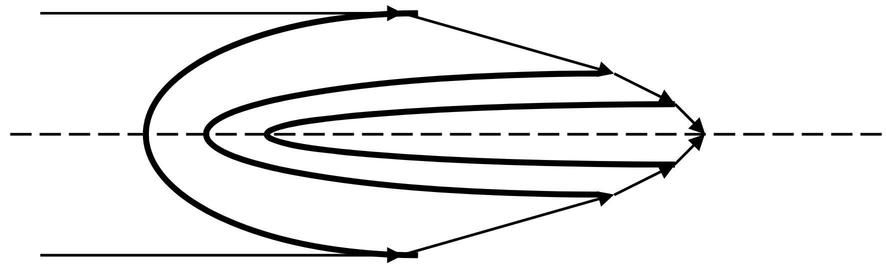
Diamond undulator
σ = 123 X 7 μm
σ' = 25 X 8 μrad

Lens length 2.6 mm

10 mm

Design of Arrays of nano-focusing lenses





PRL **99,** 134801 (2007)　　PHYSICAL REVIEW LETTERS　　week ending 28 SEPTEMBER 2007

Using Compound Kinoform Hard-X-Ray Lenses to Exceed the Critical Angle Limit

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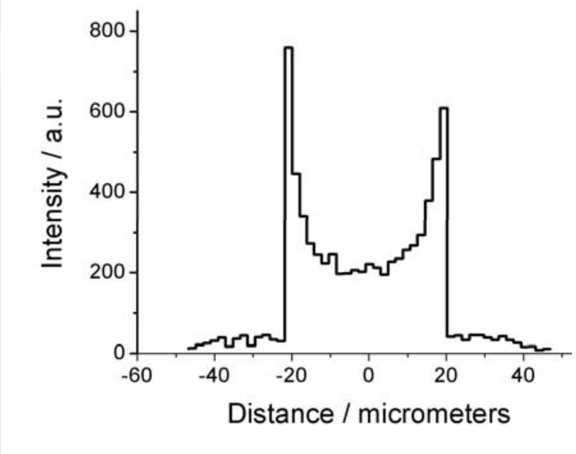
(Received 9 January 2007; published 28 September 2007)

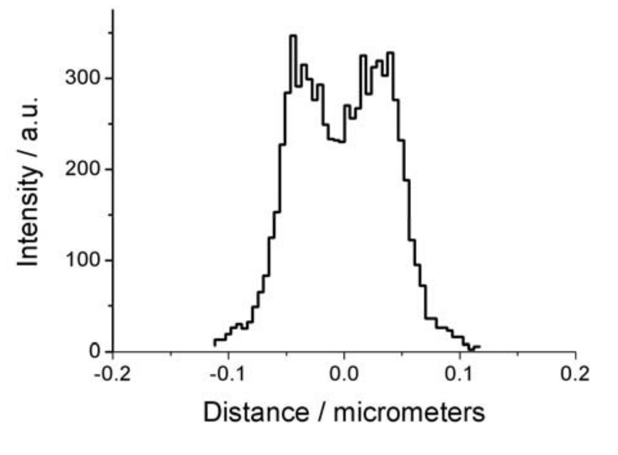
We have fabricated and tested a compound lens consisting of an array of four kinoform lenses for hard x-ray photons of 11.3 keV. Our data demonstrate that it is possible to exceed the critical angle limit by using multiple lenses, while retaining lens function, and this suggests a route to practical focusing optics for hard x-ray photons with nanometer scale resolution and below.

Design of Nano-Focusing refractive optics

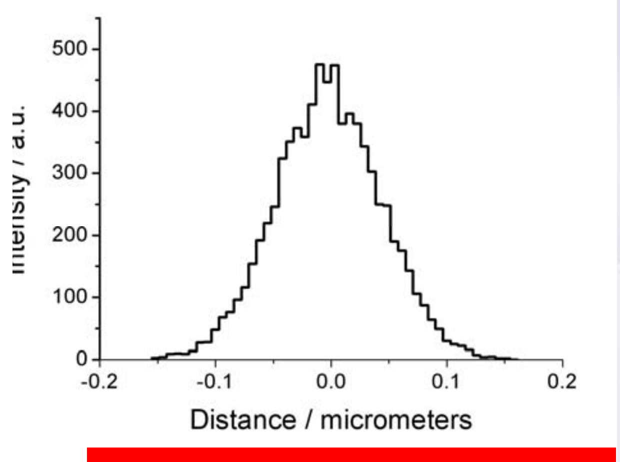
Parabolic lens f = 100 mm, aperture 300 µm



Elliptic lens f = 100 mm, aperture 300 µm **LENS LENGTH 18 mm**

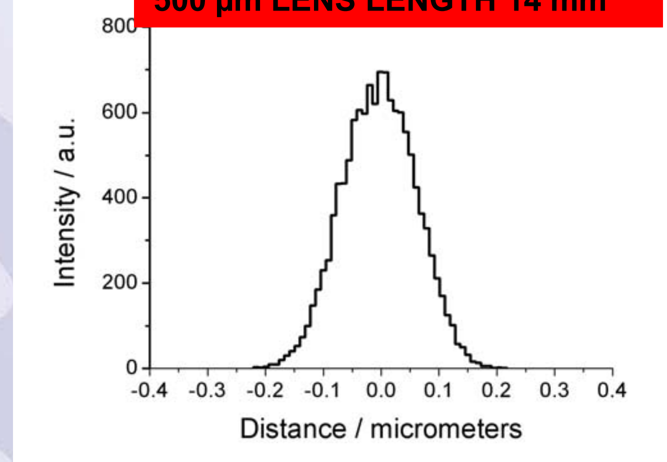


Elliptic lens **f = 300 mm**, aperture 300 µm **LENS LENGTH 5 mm**



Experiment.—Four kinoform lenses were designed in series with each other such that each lens was designed to focus the virtual source created by the prior lens in the array. The first lens was designed to approximate the synchrotron as a source infinitely far away, and had a focal length of 0.1 m. Lenses 2, 3, and 4 had focal lengths of 0.05, 0.033, and 0.025 m, respectively. The figure of each lens was deduced from Fermat's theorem and fabricated in silicon using fabrication techniques similar to those described previously [14]. A single kinoform lens was fab-

Elliptic lens **f = 300 mm, aperture 500 µm LENS LENGTH 14 mm**



Summary and Conclusion

•We need an optimisation software for the calculation of shape of nano-focusing optics - and for coherent, diffractive optics and interference.

•Availability of well-established ray-tracing codes -> extremely useful in a 3rd generation new synchrotron radiation lab. User friendliness important as many beamline scientists would not otherwise use the codes.

•Several Phase I beamlines simulated both with Ray and Shadow

•About 12 beamlines in Phase II simulated with Shadow

•Phase III started and the trend is continuing

diamond

Acknowledgments

- K. Sawhney & DLS Optics Group
- M. Sanchez del Rio (ESRF) for introducing me to X-Ray Optics