A Light for Science

RAY TRACING SIMULATIONS FOR OPTICAL CONFIGURATIONS

or

The geometrical limits for focusing ESRF beams

M. Sánchez del Río

srio@esrf.eu

MENU

- ***Geometrical*** limitations for nanofocusing ESRF beams with ideal mirrors
- Focusing with ID24UP setup:
  - Elliptical Horizontal Mirror
  - Bragg Polychromator
  - **Laue Polychromator**
    - **Problems**
    - **Crystal surface shape**
- Conclusions

Introduction: How to obtain nanospots

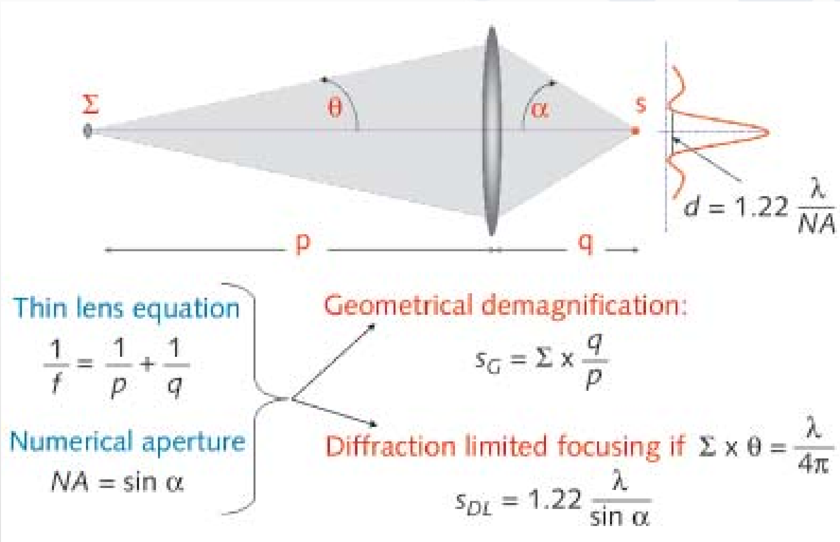


Figure 1.1.1: Optical demagnification: Assuming perfect imaging, the size of the focal spot, s, is given by the size of the source, Σ, multiplied by the distance from the focusing element to the focal spot, q, and divided by the distance from the source to the focusing element, p. The minimum spot size is limited by the geometrical demagnification, $s_G = \Sigma \times q/p$ and the diffraction limit, $s_{DL} = 1.22\ \lambda/\sin \alpha$.

Some choices/boundaries:

- N=1
- p>> to increase demagnification
- Sorce size ~10 microns

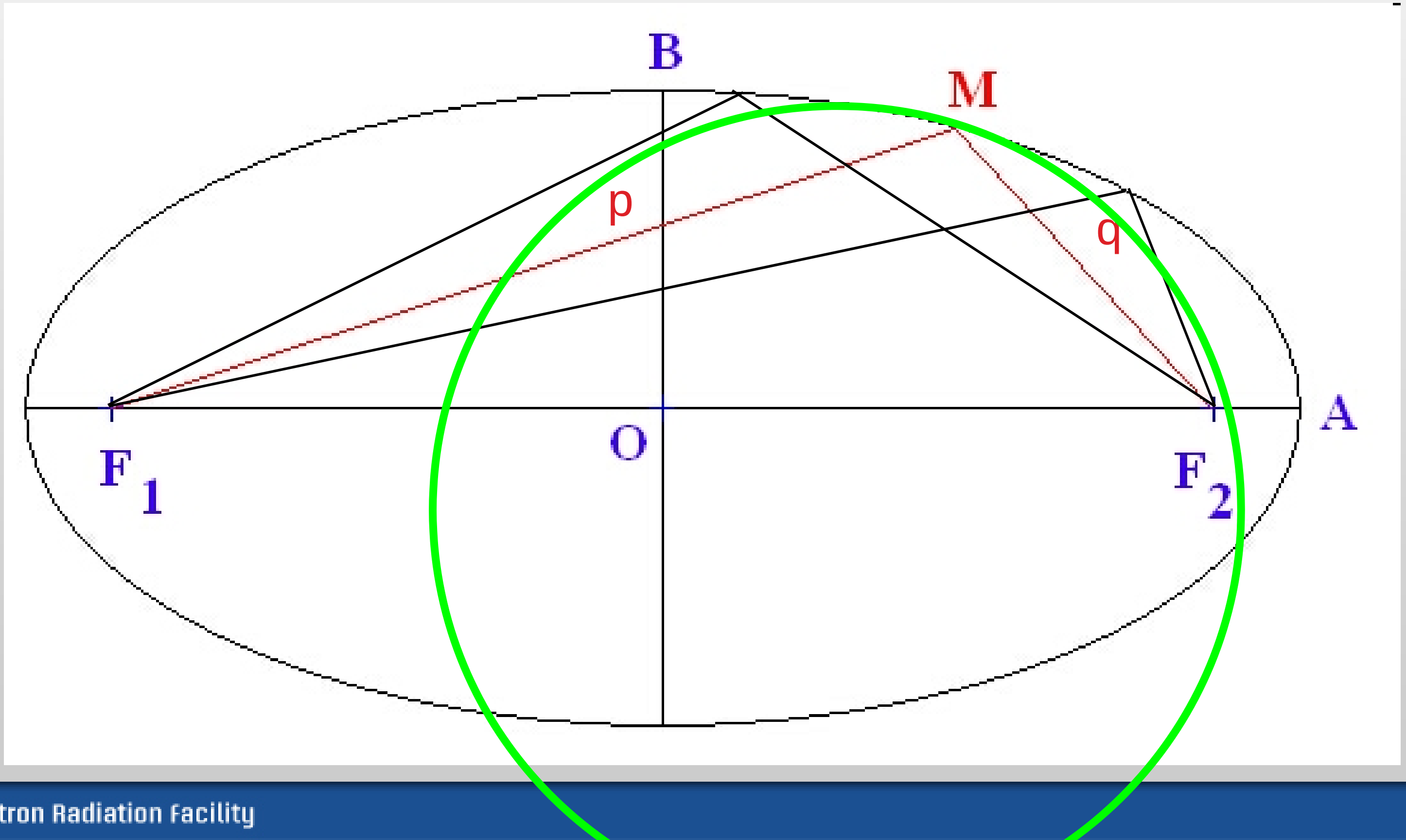
Some implications:

- No perfect imaging is possible for N=1 (The Abbé sine condition cannot be fulfilled for a single reflector)
- 10 microns -> 1 nm => Demagnification 10^4.

Q: Is still possible? What are the geometrical limits?

Perfect point to point reflector

- If we impose specular reflection, the surface that produces a point-to-point focus is called Cartesian surface.
- A Cartesian surface must satisfy the equations representing a conic of revolution
- "Circular" approximations of these surfaces relax some properties: Toroid (not point-to-point focus), sphere (astigmatic), etc. Surface errors (figure, slope, roughness) must be taken into account.



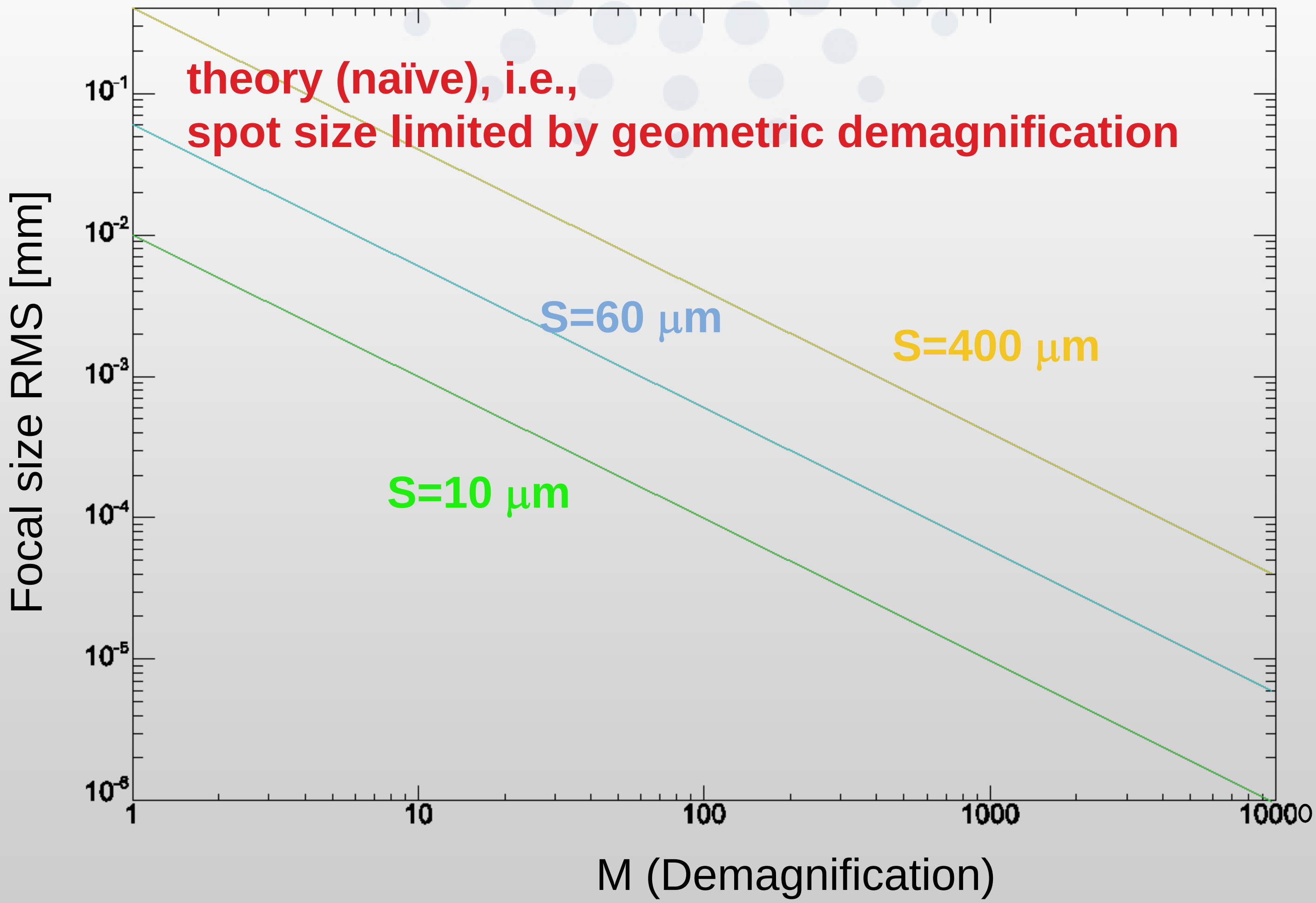
ESRF source sizes

- Synchrotron sources are simple
  - They can be calculated exactly
  - Very good Gaussian approximation (Size distribution is Gaussian)
- ESRF beam sizes do not improve significatively with the Upgrade

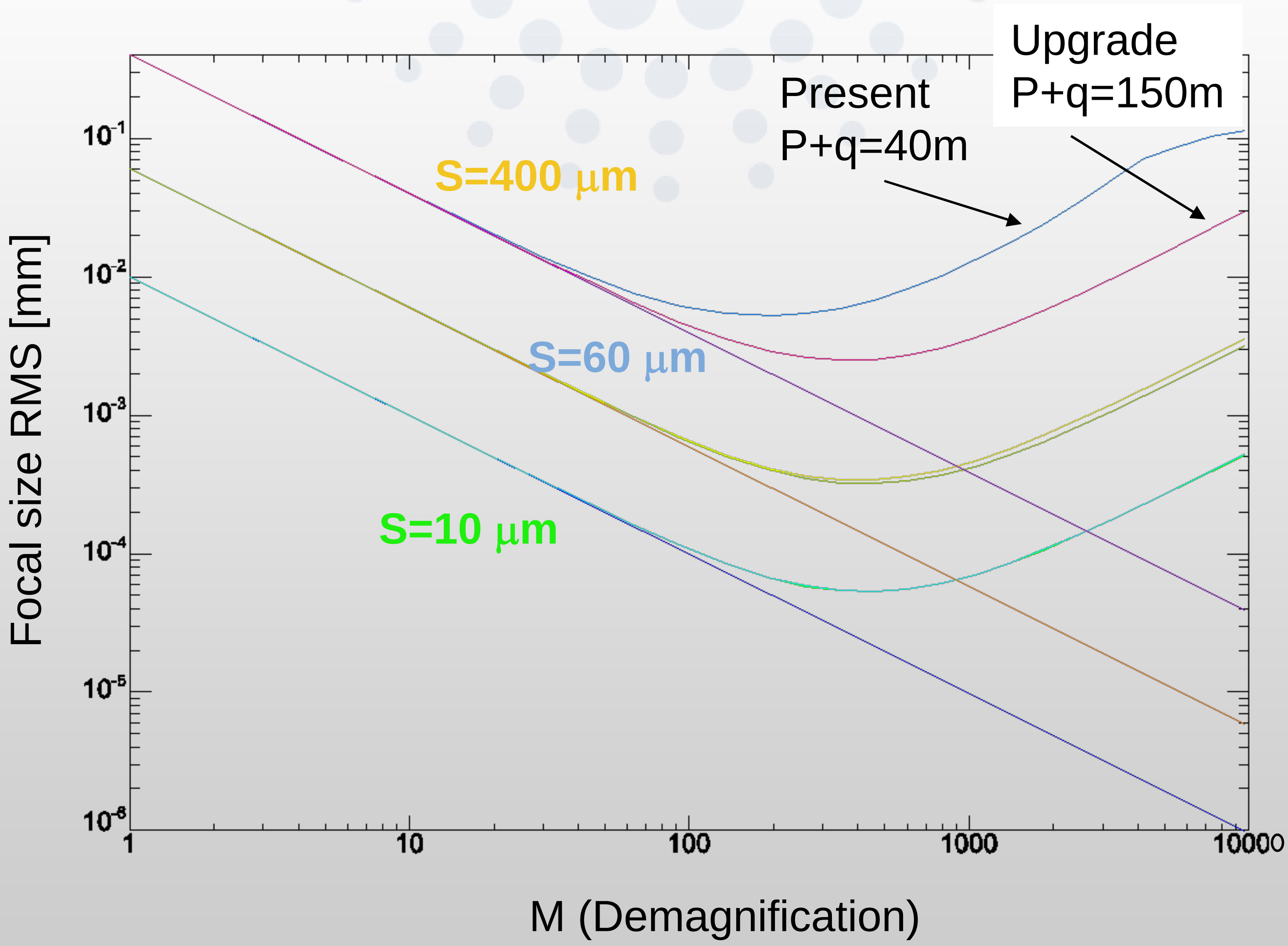
RMS Photon Beam Sizes and Divergences

Source	Plane	Electron Beam	Undulator Radiation					
Photon Energy [keV]			3	10	30	3	10	30
Undulator Length [m]			1.65	1.65	1.65	3.3	3.3	3.3
RMS Divergence [micro-rad]								
High Beta ID	Horizontal	10.5	15.3	12.1	11	13.1	11.3	10.8
	Vertical	3.9	11.9	7.3	5.3	8.8	5.9	4.7
Low Beta ID	Horizontal	88.3	89	88.5	88.4	88.7	88.4	88.4
	Vertical	3.8	11.8	7.2	5.2	8.8	5.8	4.5
Bending Magnet	Horizontal	108						
	Vertical	1.1						
RMS Source Size [microns]								
High Beta ID	Horizontal	395						
	Vertical	9.9						
Low Beta ID	Horizontal	57						
	Vertical	10.3						
Bending Magnet	Horizontal	126						
	Vertical	36.9						

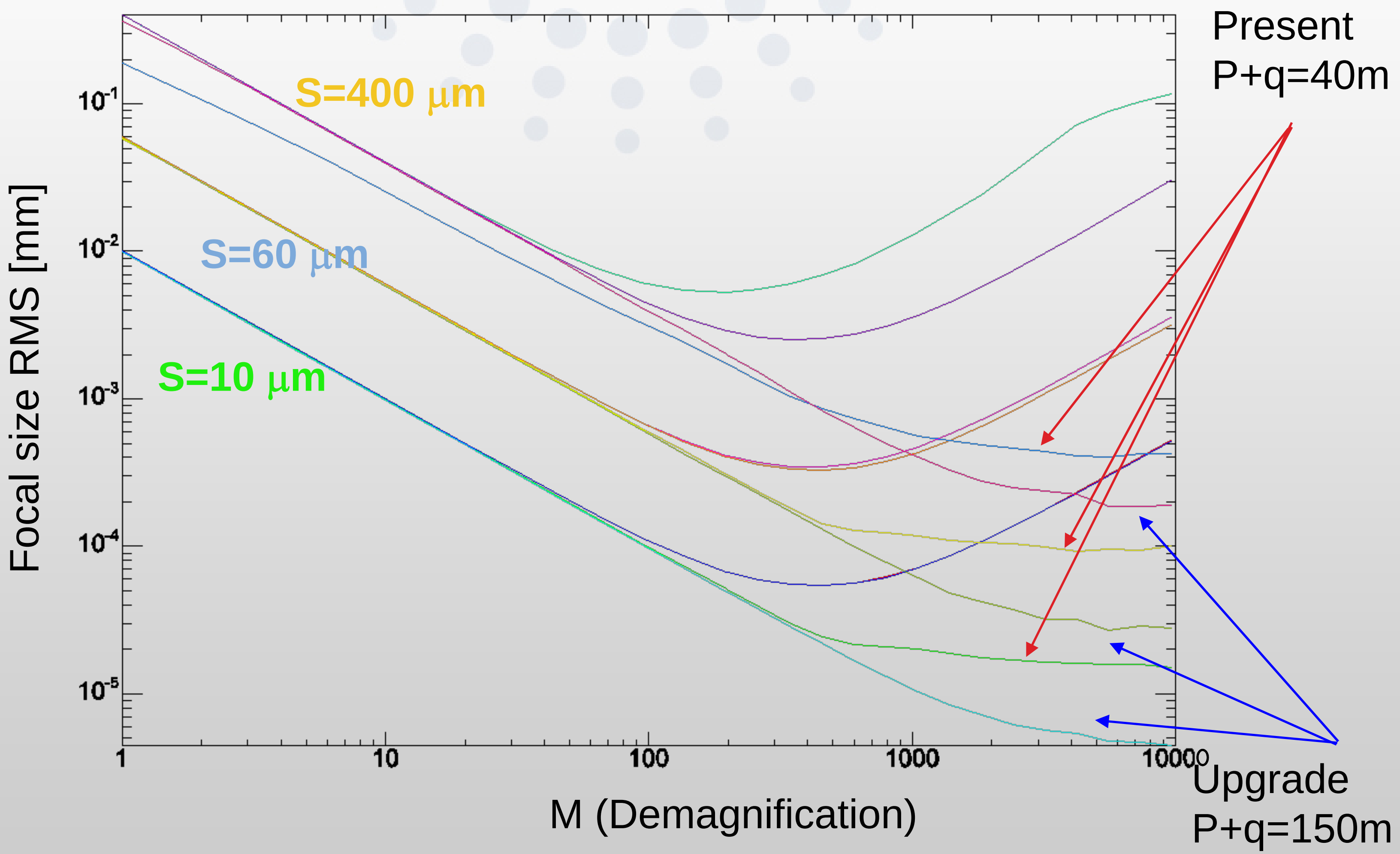
Evolution of the beam RMS THEORY p+q: Present:40m, Upgrade:150



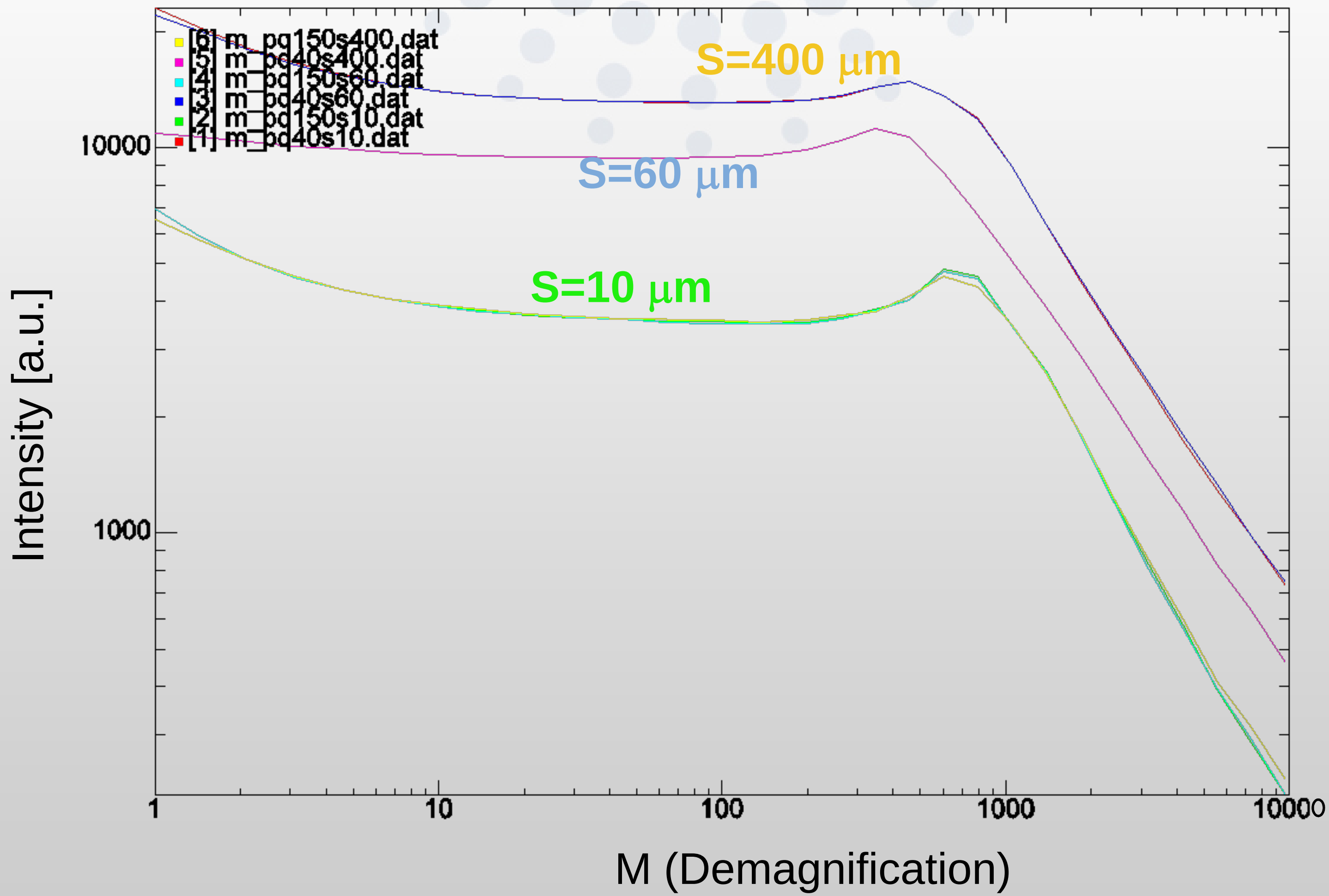
Evolution of the FULL beam (30μrad)



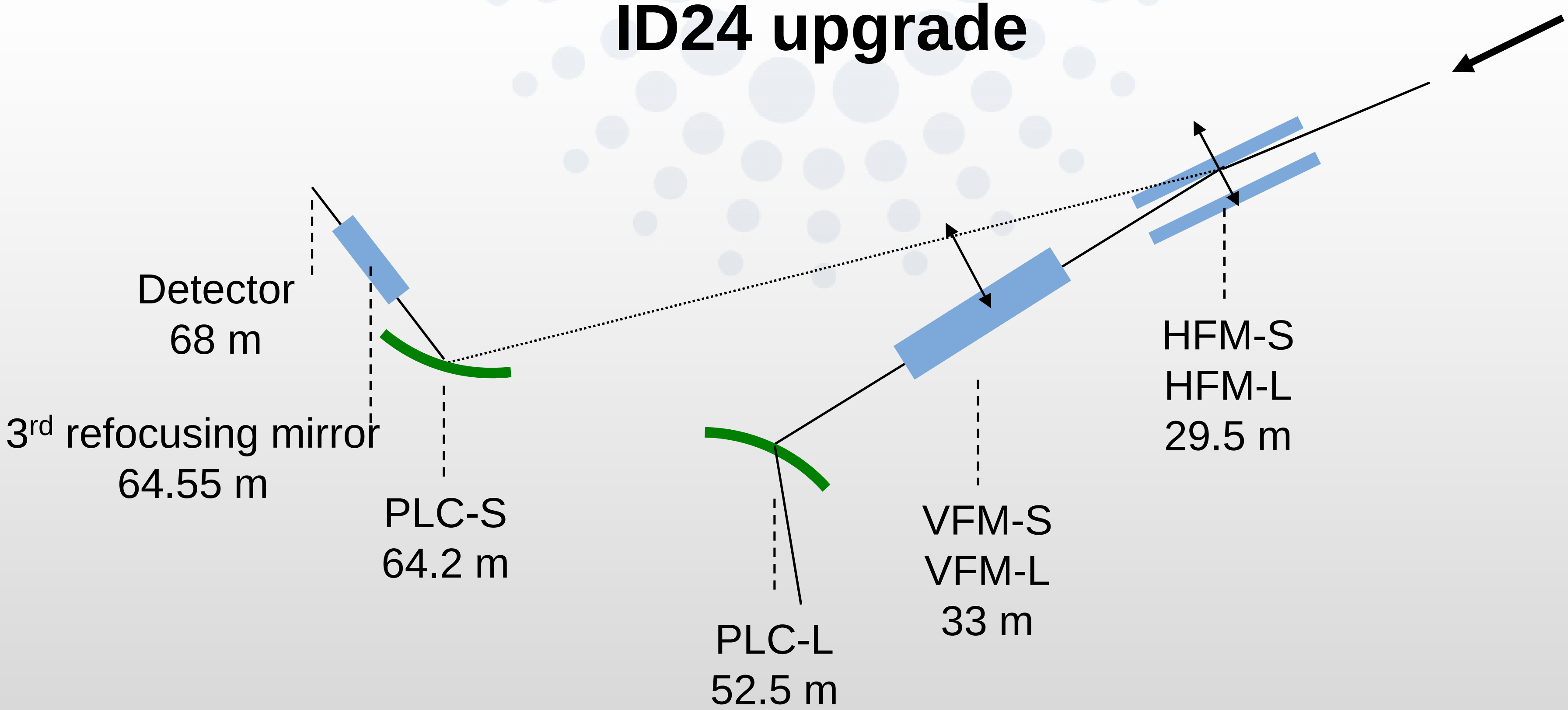
Evolution of the beam RMS
ACCEPTED by L=20cm



Evolution of the beam INTENSITY

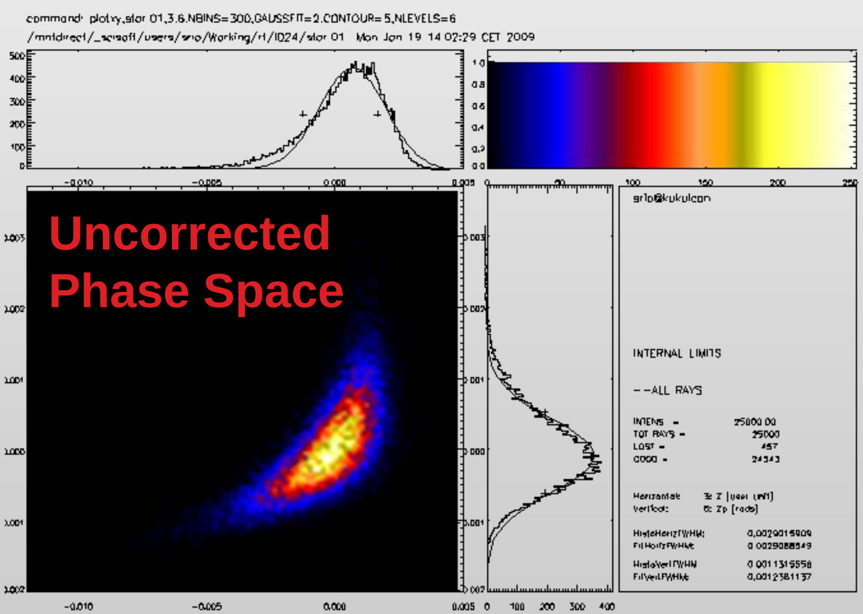


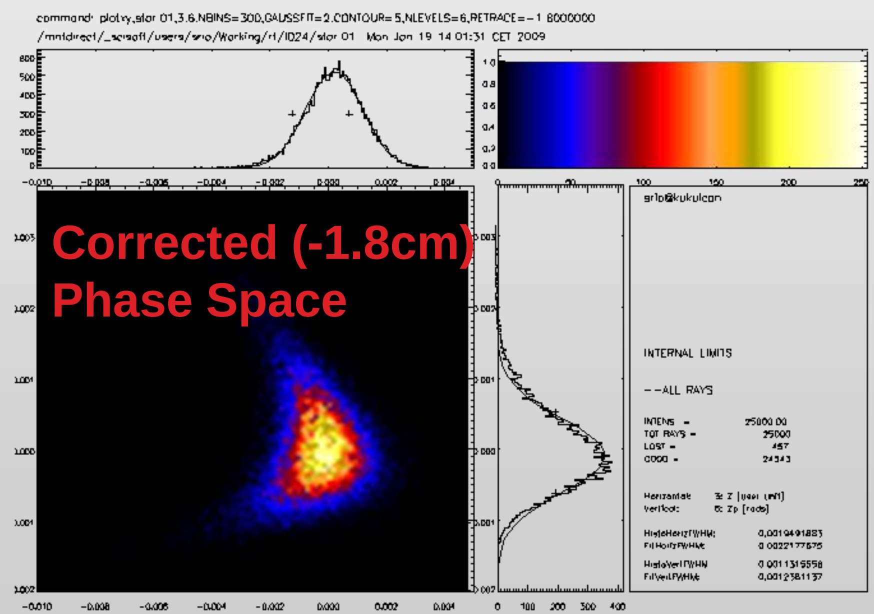
ID24 upgrade



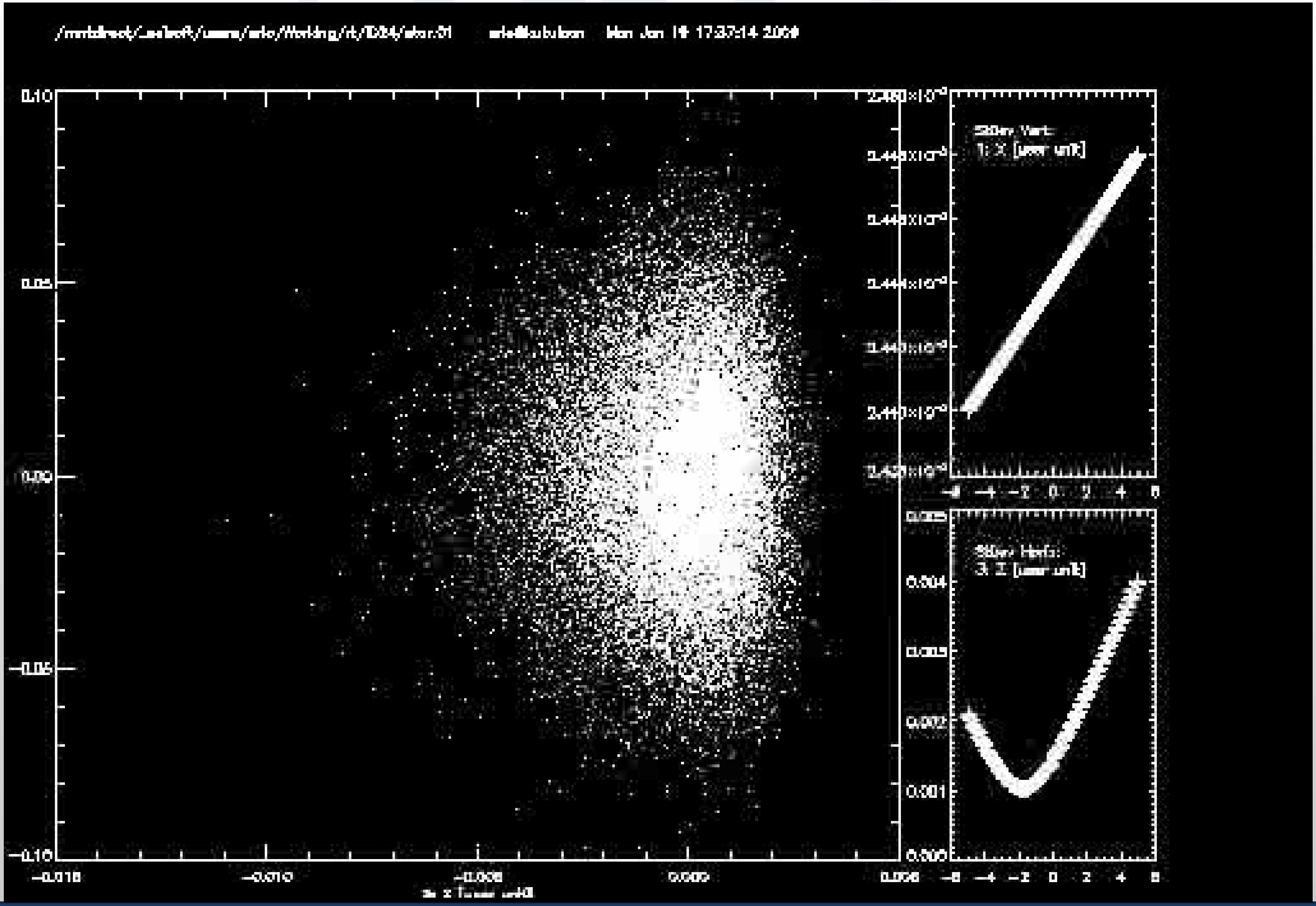
ELLIPTICAL HFM M=2950/100~30

- Theory 13.6 µm RMS 31.9 µm FWHM
- Ray tracing (uncorrected) 13.4 µm RMS 28±3 µm FWHM
- Ray tracing (corrected) 10.3 µm RMS 21±2 µm FWHM
- Divergence: 1.2±0.1 mrad FWHM (Theory 0.83 mrad)

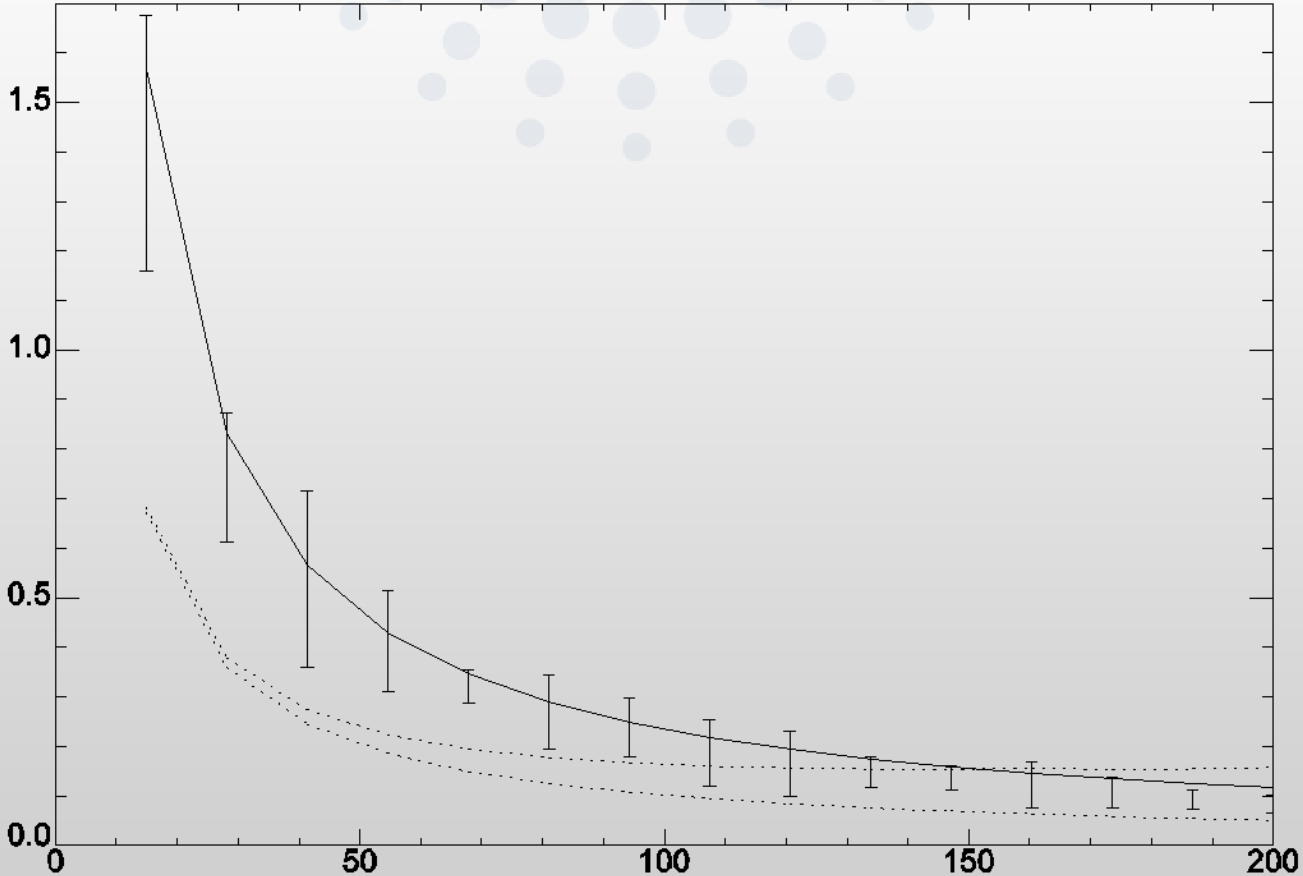




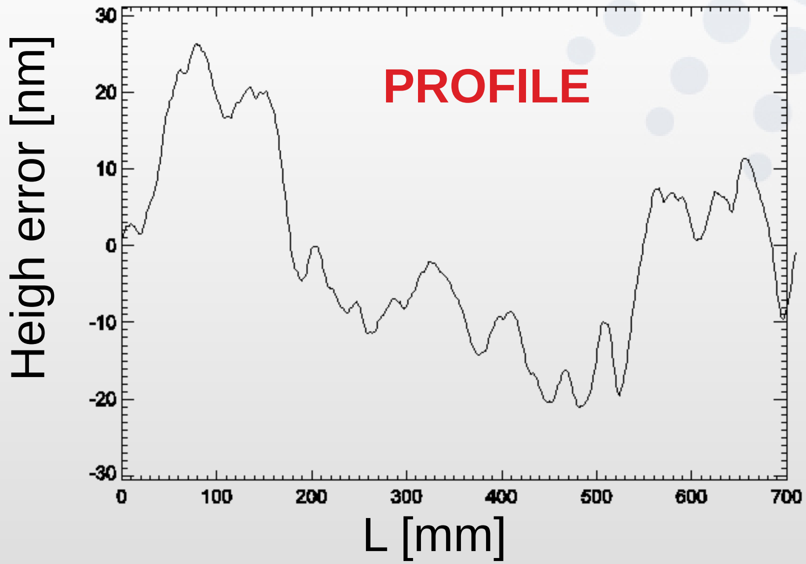
Beam evolution [-5,5] cm

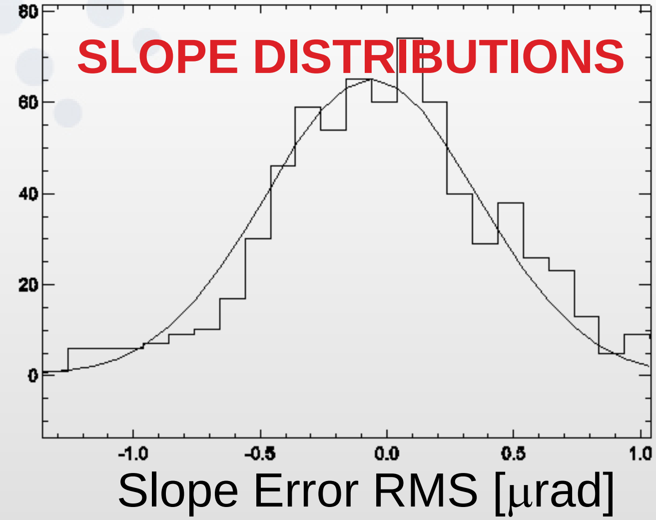


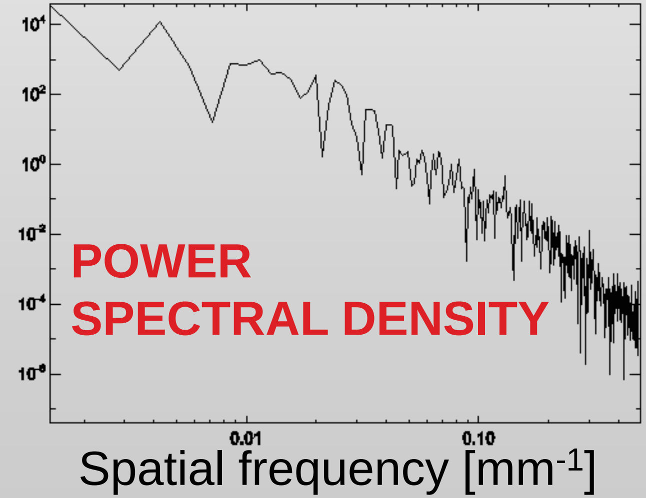
Correction



Slope errors (0.45 μrad RMS as for VFM-SESO-2004)



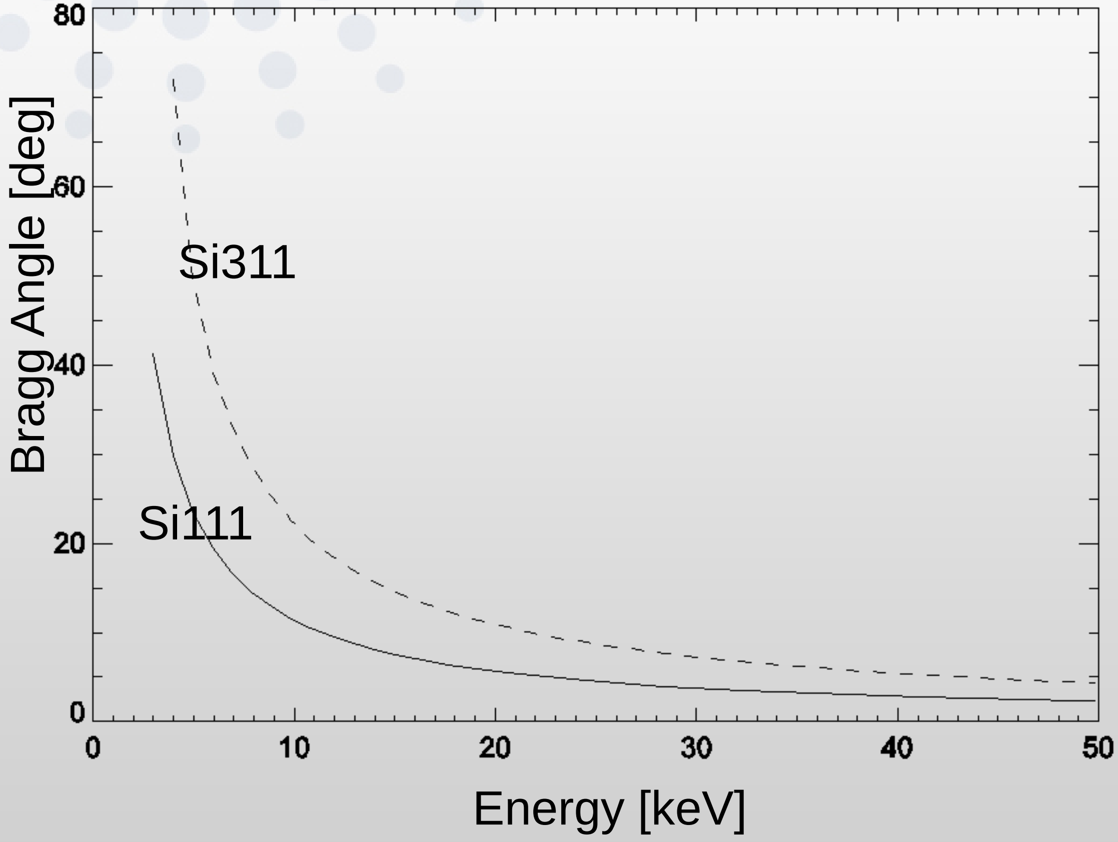




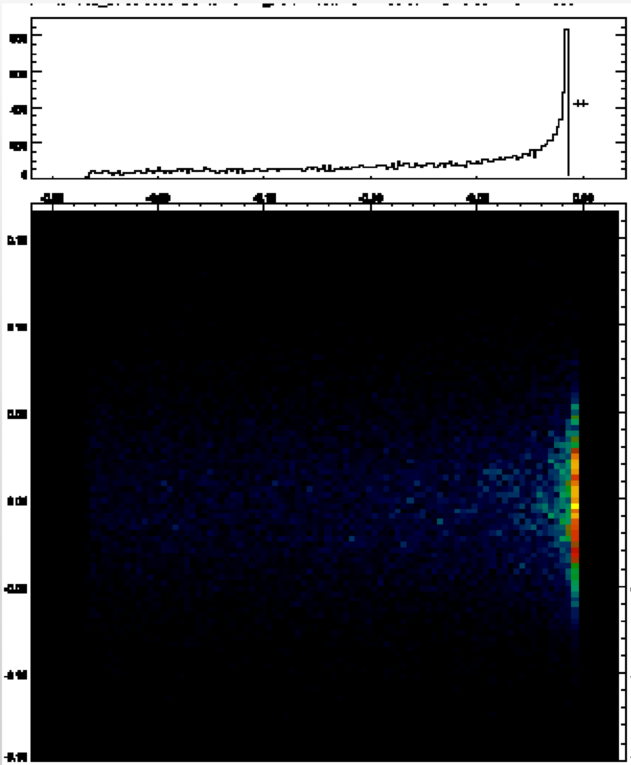
- NO MAIN EFFECT WITH VERY GOOD MIRRORS
- 10.3 μm RMS; 21±2 μm FWHM
- 1.2±0.1 mrad FWHM

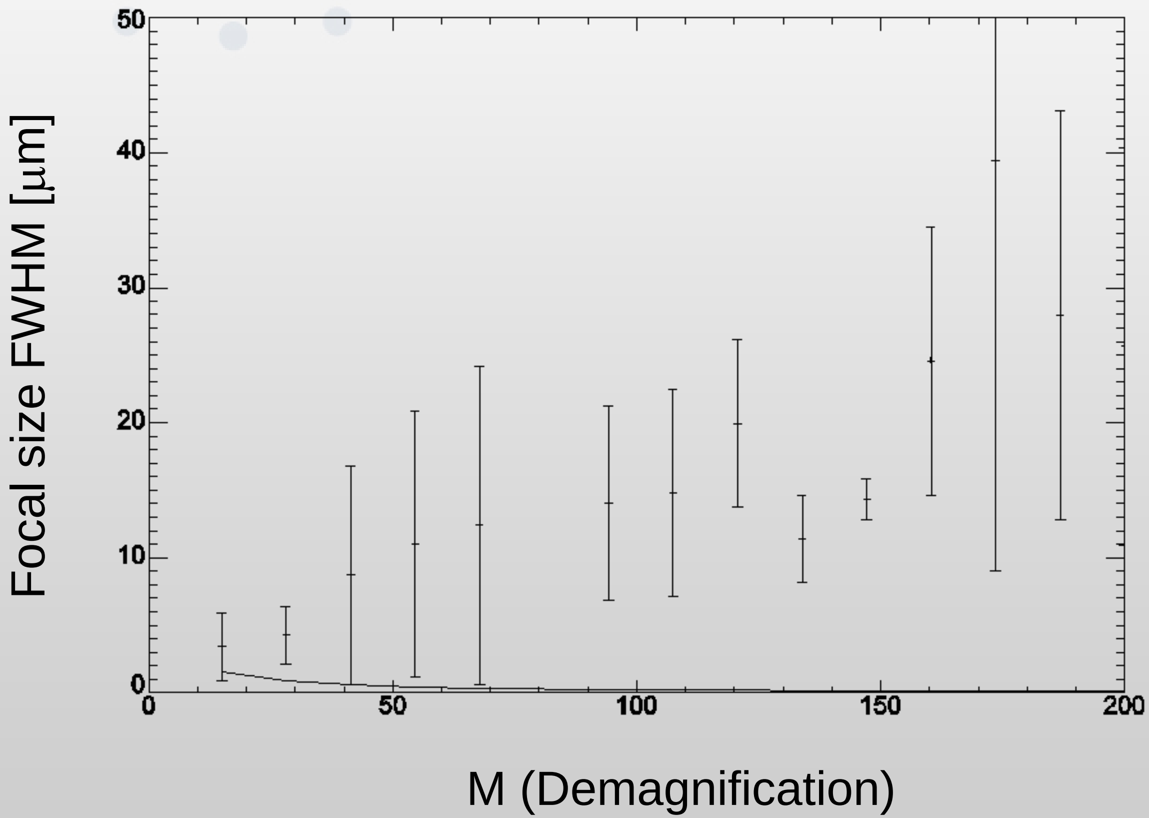
polychromator

- BRAGG
  - P=33.7 m q=0.2-2 m => M=168.5-16.5
  - E=5-27 keV
- LAUE
  - P=22 m q=0.2-2 m => M=110-11
  - E=5-50 keV

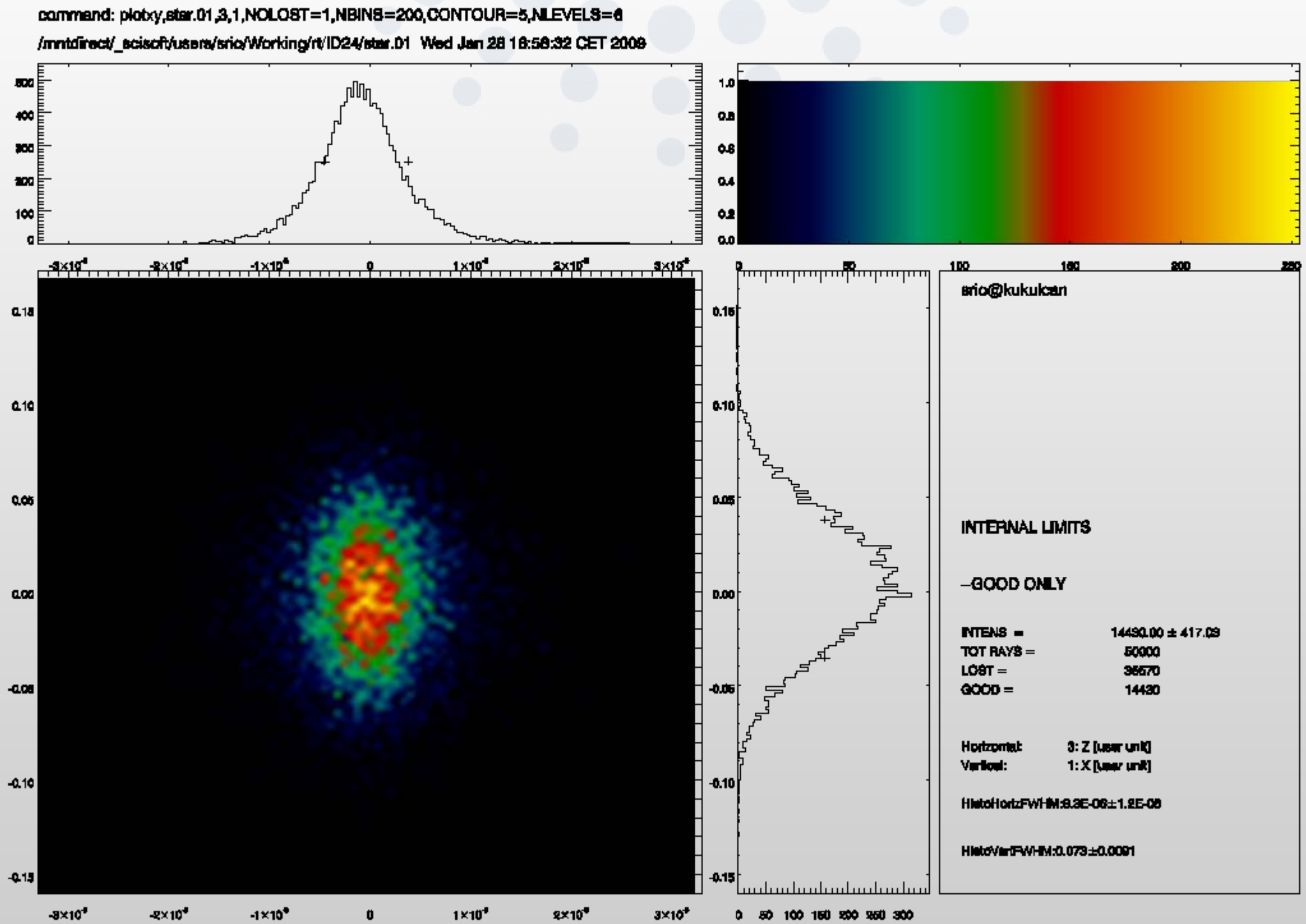


BRAGG CYLINDRICAL POLYCHROMATOR θ_B=3 deg; M=200 Spot size (microns) vs M (Errors=3sigma)

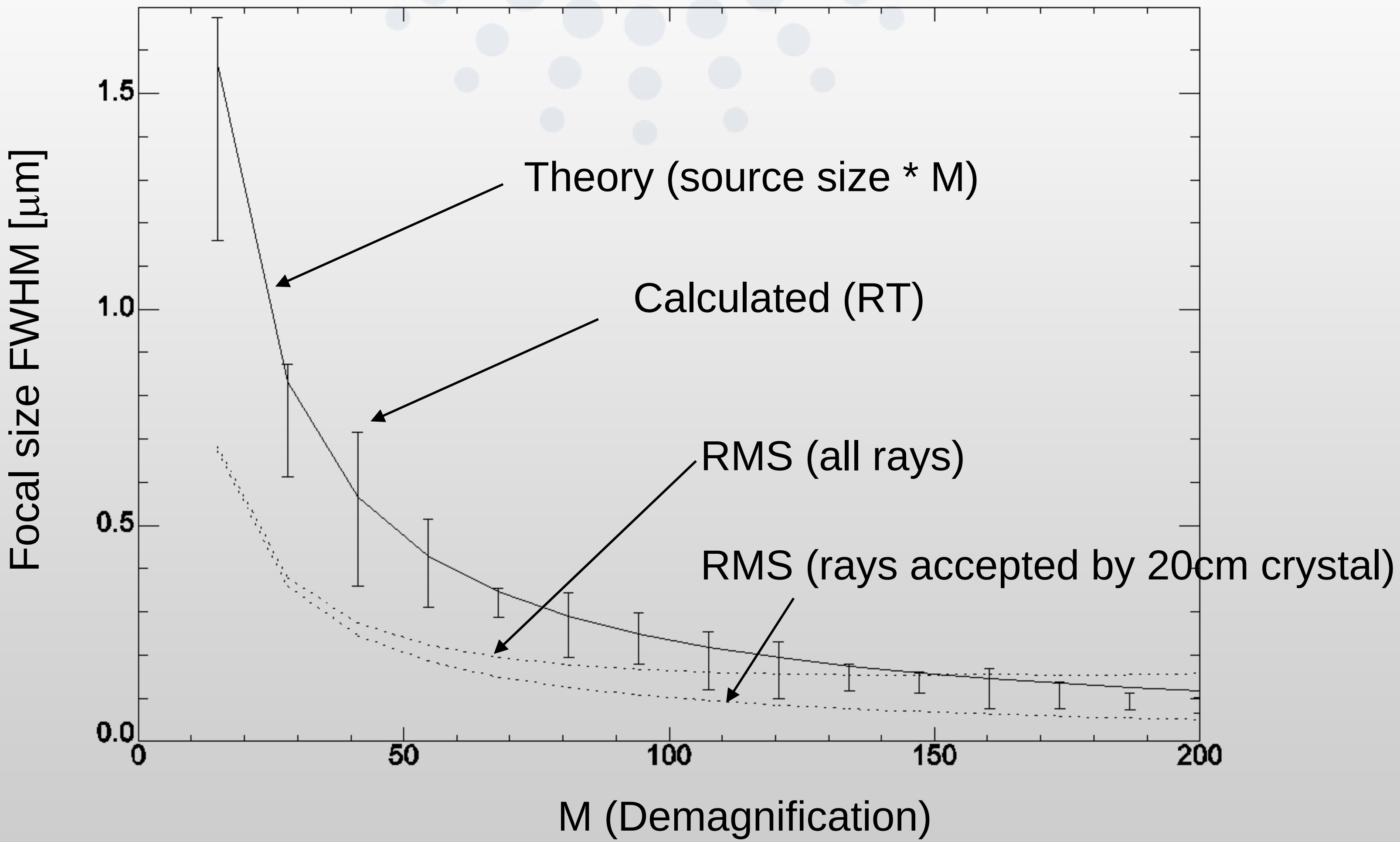




Ellipse

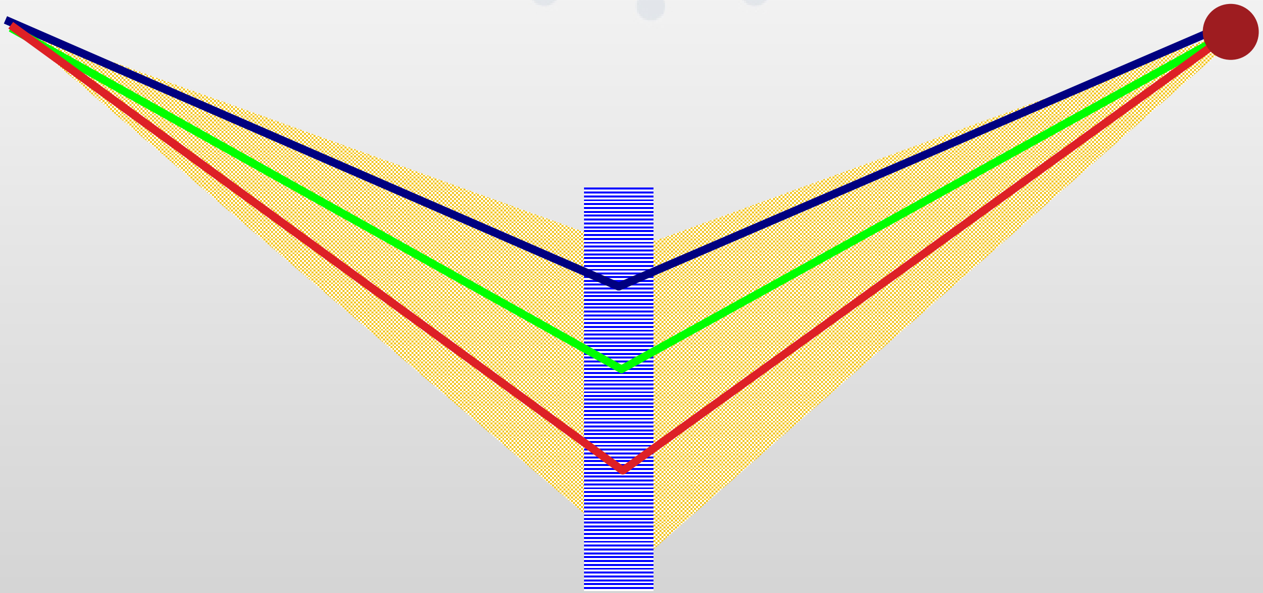

command: plotxy,star.01,3,1,NOLOST=1,NBINS=200,CONTOUR=5,NLEVELS=6
/mntdirect/_sciscft/users/srio/Working/rt/ID24/star.01 Wed Jan 28 16:58:32 CET 2009
srio@kukulcan
INTERNAL LIMITS
--GOOD ONLY
INTENS = 14430.00 ± 417.09
TOT RAYS = 50000
LOST = 35570
GOOD = 14430
Horizontal: 3: Z [user unit]
Vertical: 1: X [user unit]
HistoHorizFWHM:9.3E-06±1.2E-06
HistoVertFWHM:0.073±0.0091

Elliptical crystal

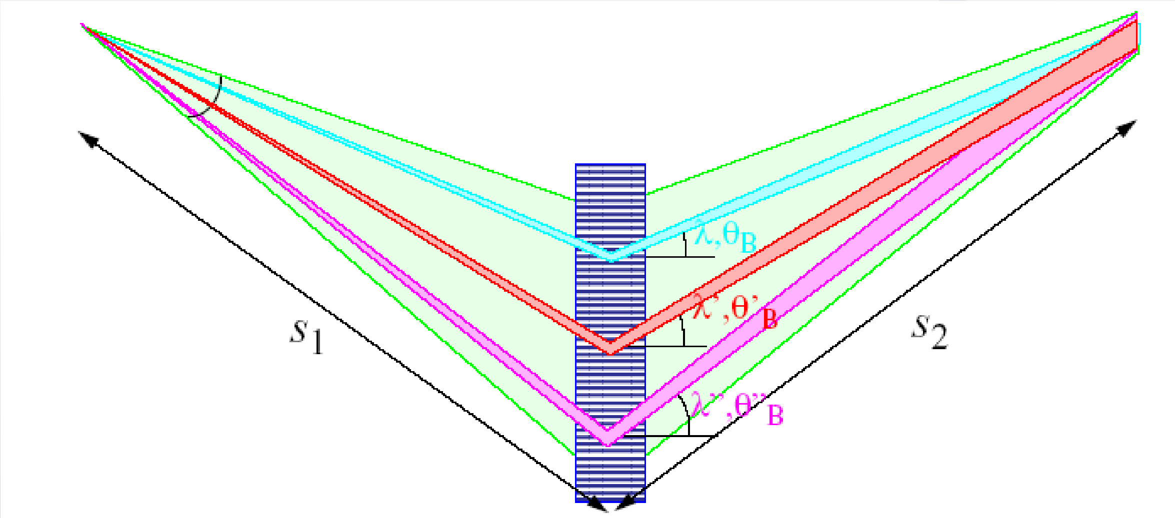


Transmission Crystal Polychromator
Laue FLAT POLYCHROMATOR
(Matsushita)

Q: How big is this point?



Laue FLAT Polychromator
polychromatic PSEUDO-focusing
Monochromatic divergence (Classical Electrodynamics)



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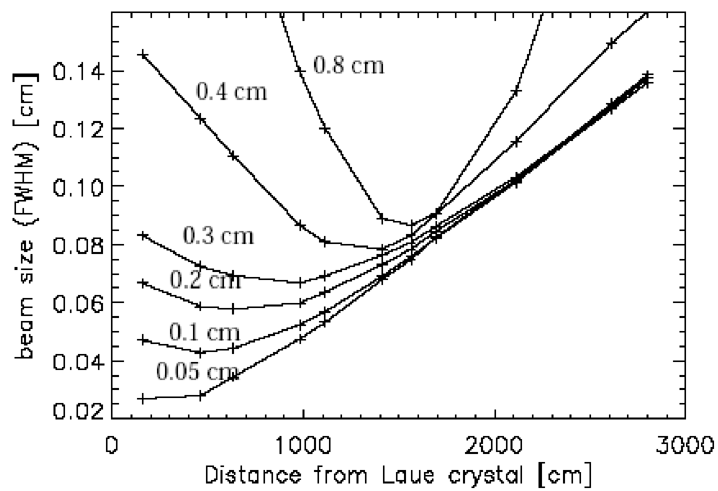
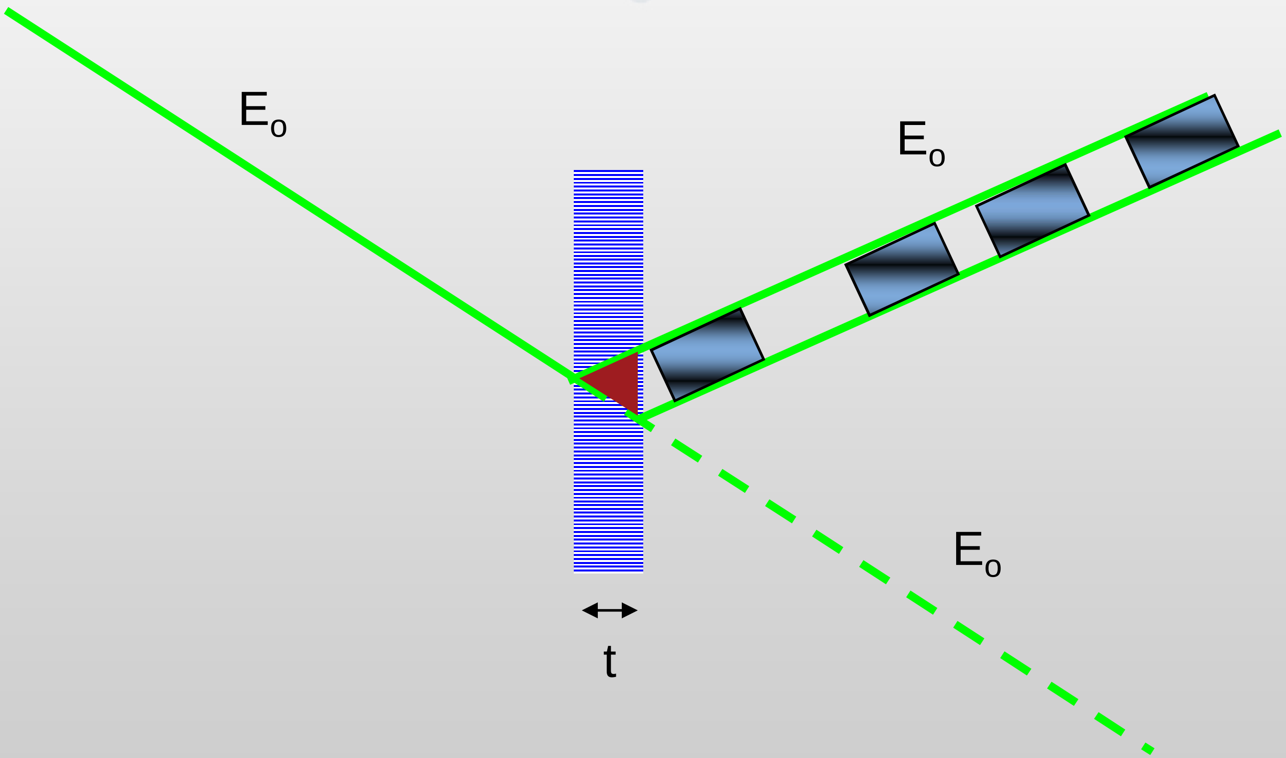
M. Sanchez del Rio et al, Rev Sci Instrum, 66 (11) 5148- 5152, Nov 1995

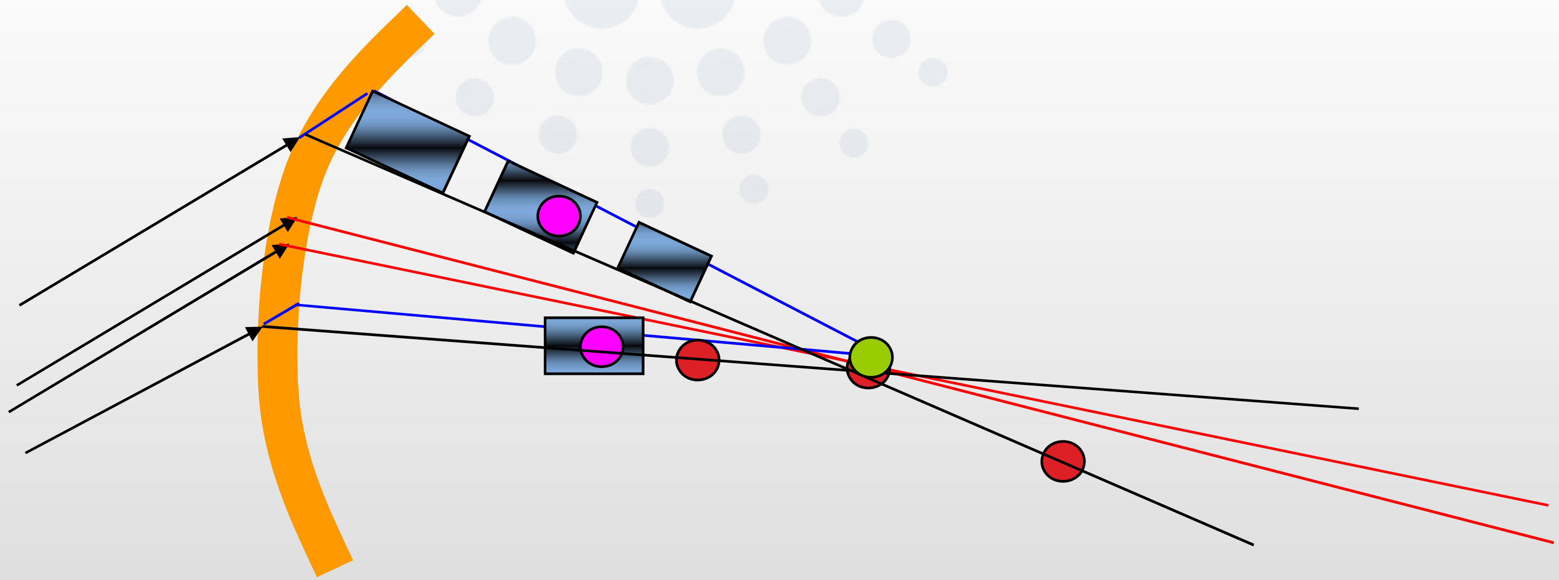


Laue FLAT MONOCHROMATOR (Dynamic Theory of Diffraction)

G. Borrmann, Beitr. Phys. Chem. 20. Jahrhunderts, Vieweg & Sohn, Braunschweig, 262–282 (1959)



Bent crystals: multifocus problem



1) Monochromatic geometrical focusing 🔴

2) Polychromatic geometrical focusing 🟢

3) Monochromatic focusing of Borrmann triangle 🟣

4) Polychromatic focusing of Borrmann triangle

Where these focii are located?

How big they are?

How they combine?

How to optimize them?

Transmission Lenses

http://www.physics.umd.edu/lecdem/services/demos/demosl6/l6-03.htm

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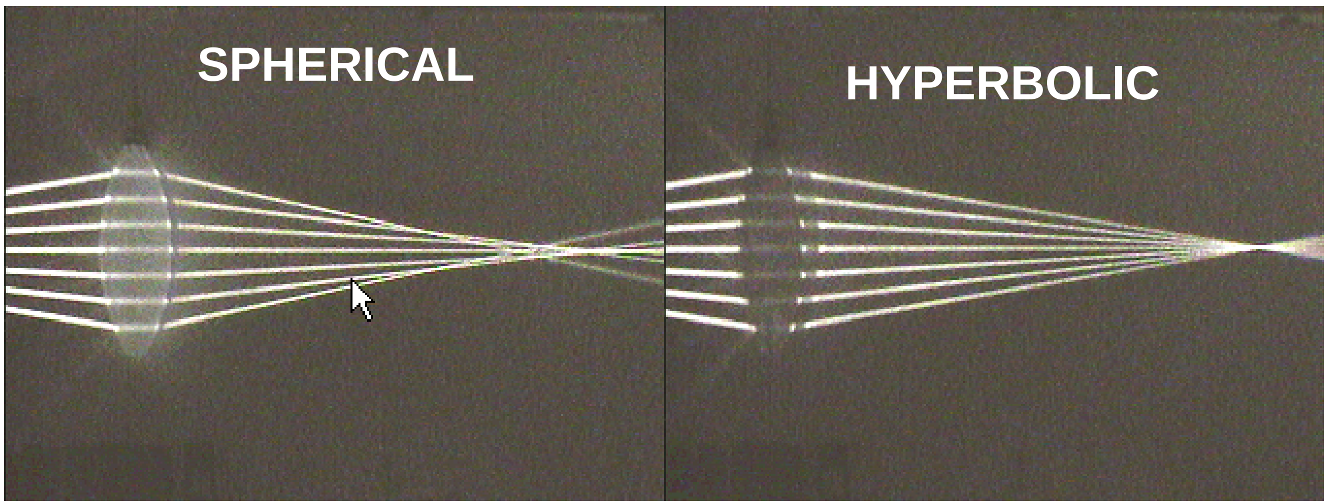


L6-03: OPTICAL BOARD - HYPERBOLIC LENS

PURPOSE: To show focusing of a hyperbolic lens.

DESCRIPTION: The shapes of the surfaces of a lens which exactly focuses a point object to a point image are hyperbolas. Parallel rays incident on an 18 inch long spherical lens converge at the focal point, but have lots of spherical aberration, as seen in the photograph at the left. A hyperbolic lens is virtually free from spherical aberration, as seen in the photograph at the right. Chromatic aberration is still present, as can be seen by blocking off part of one of the extreme rays. Number of slits and their spacing can be changed by choice of slit baffle and distance of baffle from source.

Hyperbolic crystals

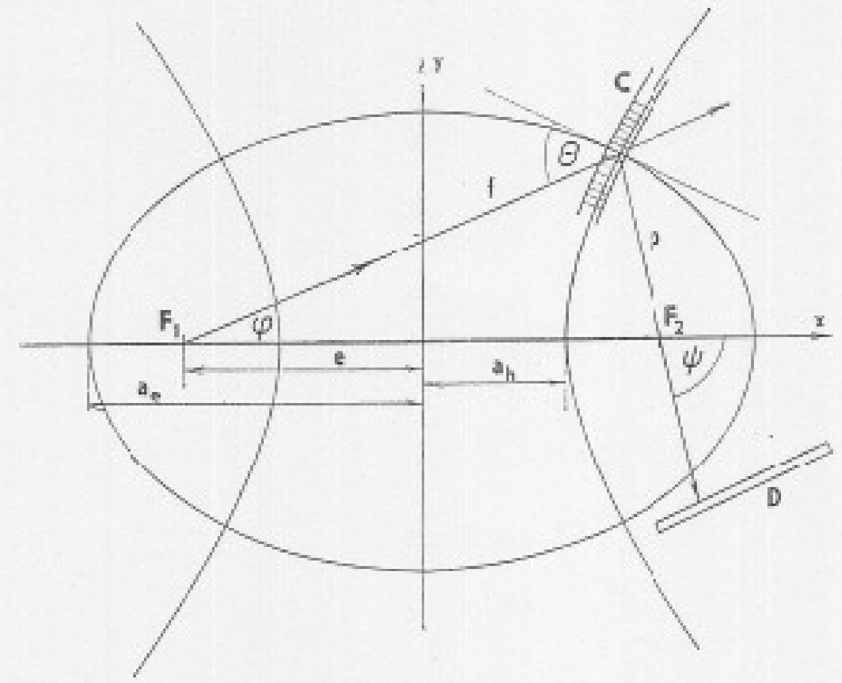


Fig. 1. A schematic drawing of the hyperbolical spectrograph. X-rays with the source in the focus F_1 are, after diffraction on the crystal *C*, focused into the focus F_2 and registered by the position sensitive detector *D*.

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.

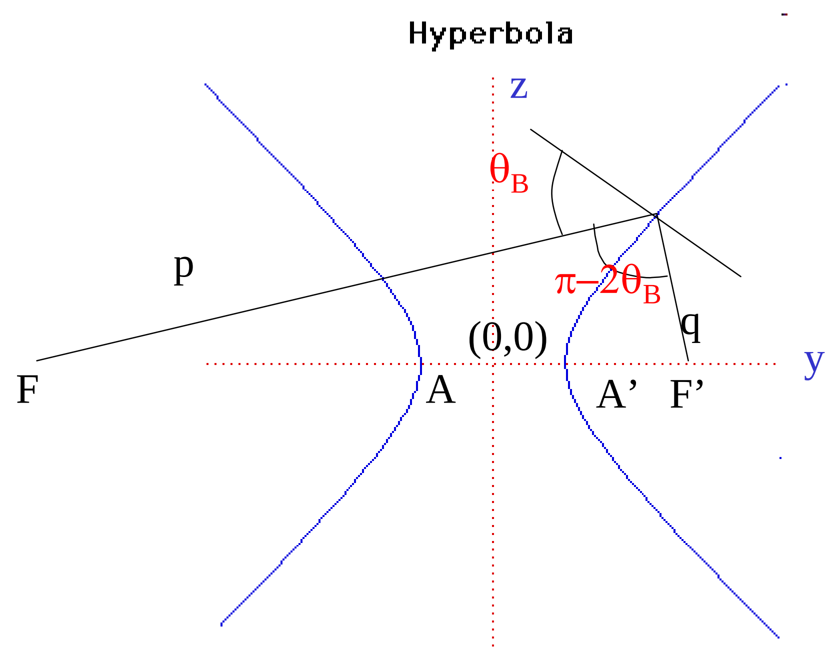
Ray tracing with hyperbolic crystals

$$\frac{y^2}{a^2} - \frac{z^2}{b^2} = 1$$

$$a = \pm \frac{p-q}{2}$$

$$b = \sqrt{pq}\cos\theta_B$$

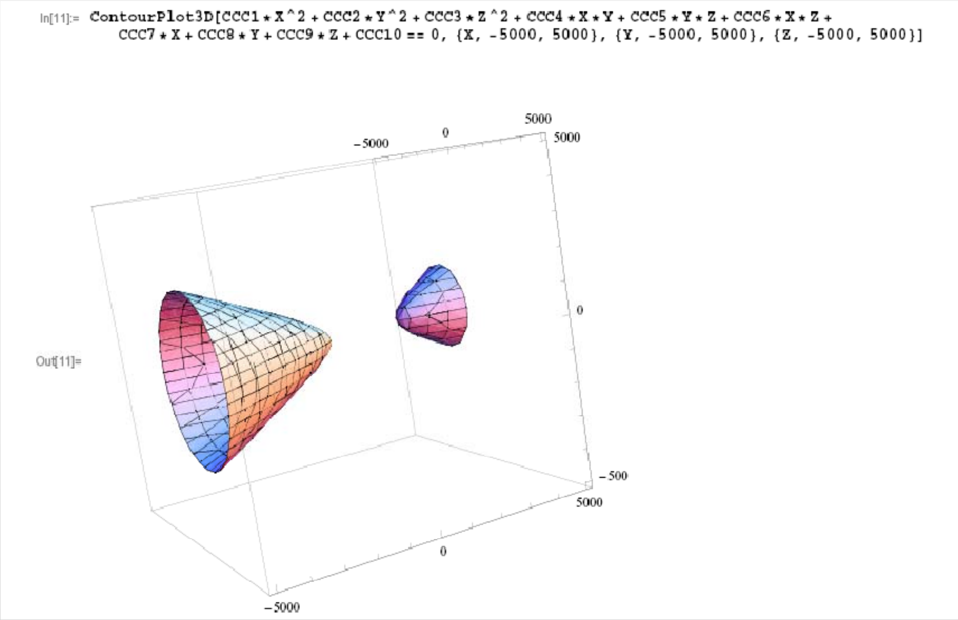
$$c = F = \sqrt{a^2 + b^2}$$



Conic equation

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

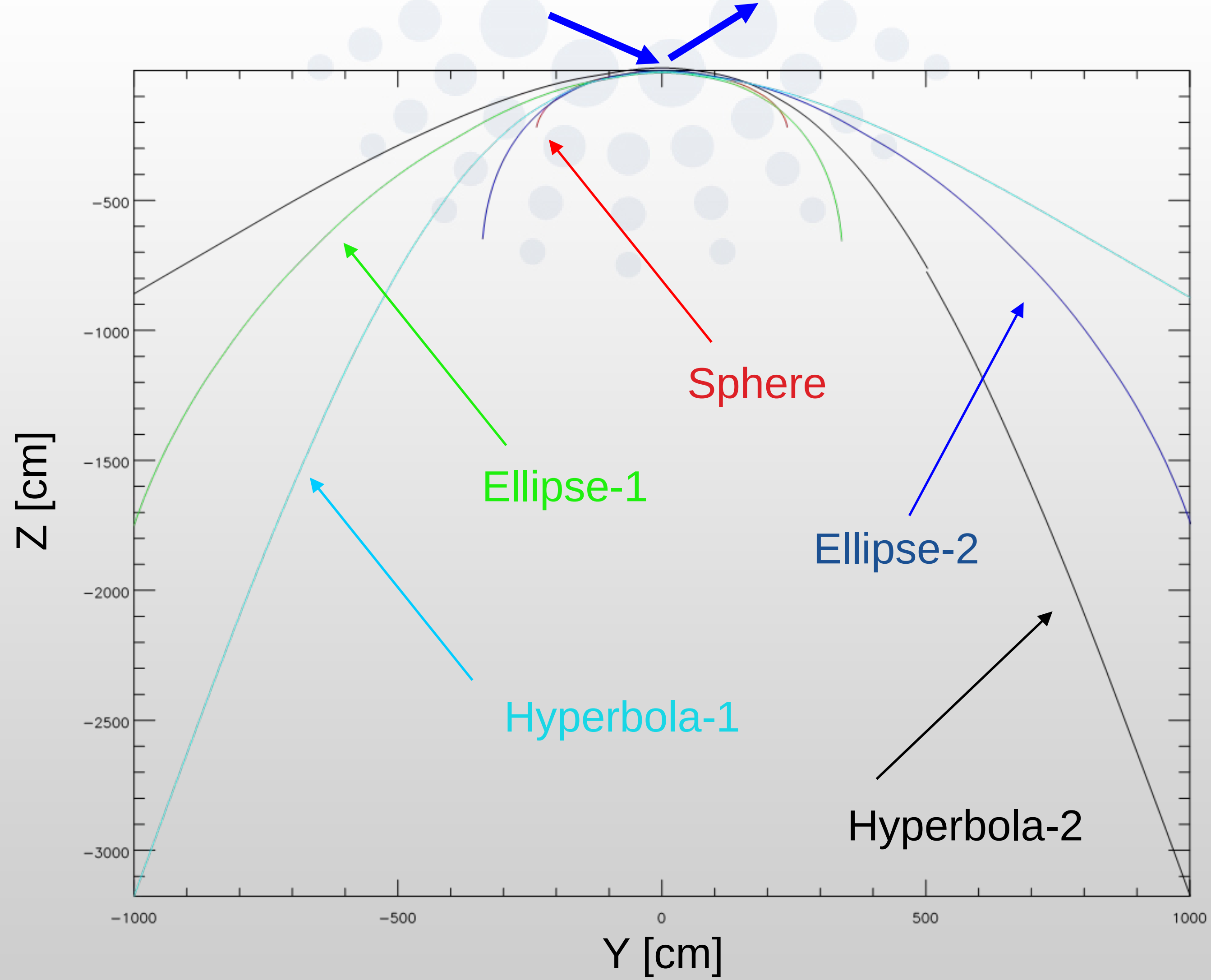
	plane	sphere	ellipse1	ellipse2	hyperbola1	hyperbola2
c0	0	1	2.99E-06	2.99E-06	-3E-06	-3E-06
c1	0	1	2.81E-06	2.81E-06	-2.8E-06	-2.8E-06
c2	0	1	6.01E-07	6.01E-07	3.1E-07	3.1E-07
c3	0	0	0	0	0	0
c4	0	0	-1.3E-06	1.32E-06	-1.6E-06	1.55E-06
c5	0	0	0	0	0	0
c6	0	0	0	0	0	0
c7	0	0	0	0	0	0
c8	-1	476.1324	0.001336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



p=2790, q=120 and θ_B=14.3deg.

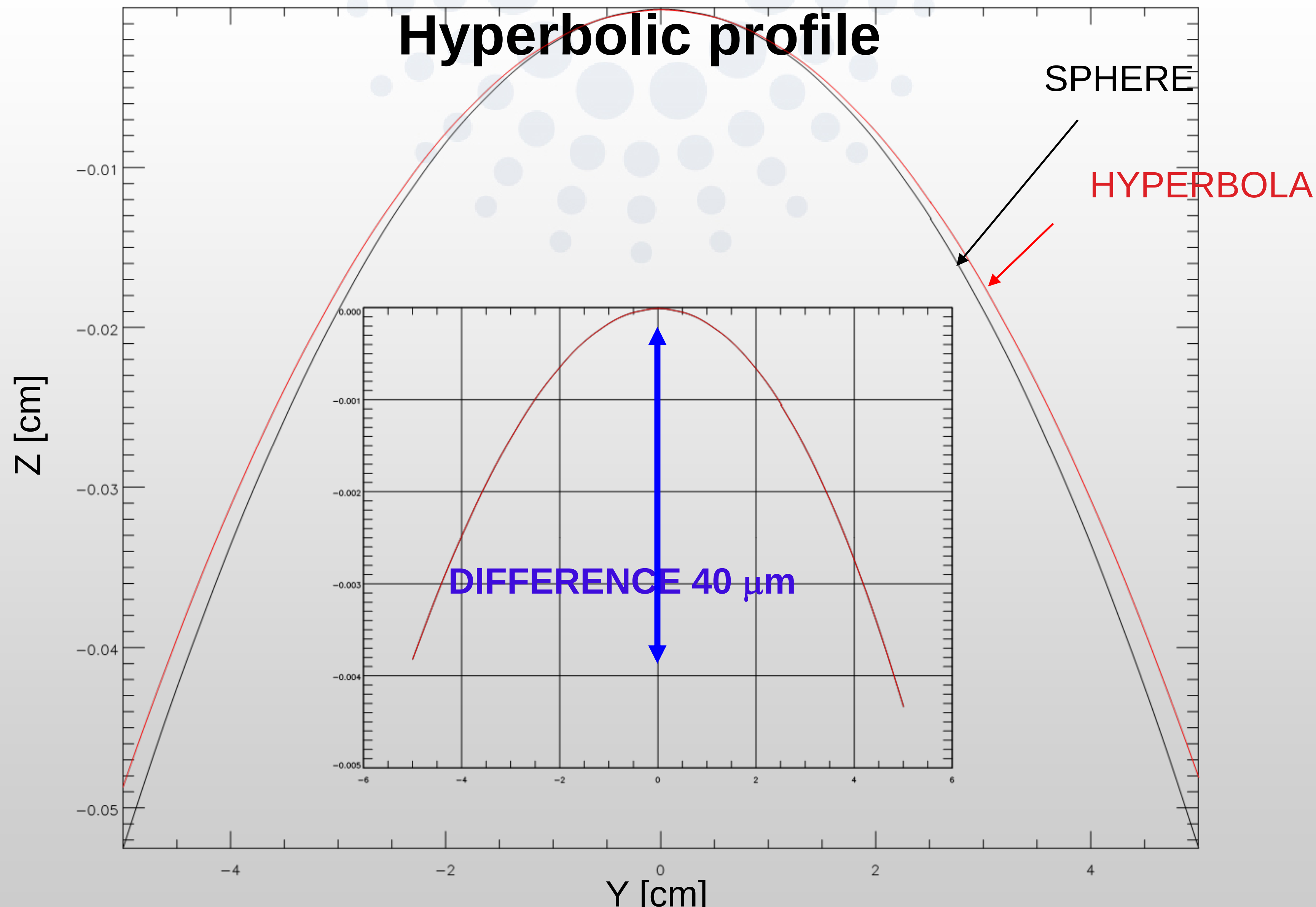
Ellipse2 (Hyperbola2) is obtained from ellipse1 (Ellipse1) by symmetry with respect to the (x,z) plane (i.e., y->-y).

Conic surfaces



The Y dimension has been exaggerated to recognize the conic.

Hyperbolic profile



Monochromatic focusing:
Elimination of aberrations using an hyperbolic crystal

- the hyperbolic crystal works better in terms of focusing an ideal beam:
  - monochromatic (E=8000eV) point source
  - with a Si111 100μm thick bent symmetrical-Laue crystal.

	z FWHM [cm] (weighted with rays)	z FWHM [cm] (weighted with intensity)	Intensity [a.u.]
plane	5.23	0.0496	1048
spherical	0.44	0.00027	70
ellipse1	0.43	0.00027	70
ellipse2	0.44	0.00027	70
hyperbola1	0.000187	2.24E-07	76
hyperbola2	0.0077	1.49E-07	76

•The rays ("weighted with rays") are not focused with the plane crystal, and are focused with all the other crystals. The best focalization is for hyperbola1, as expected, with profile with about 2 μm.

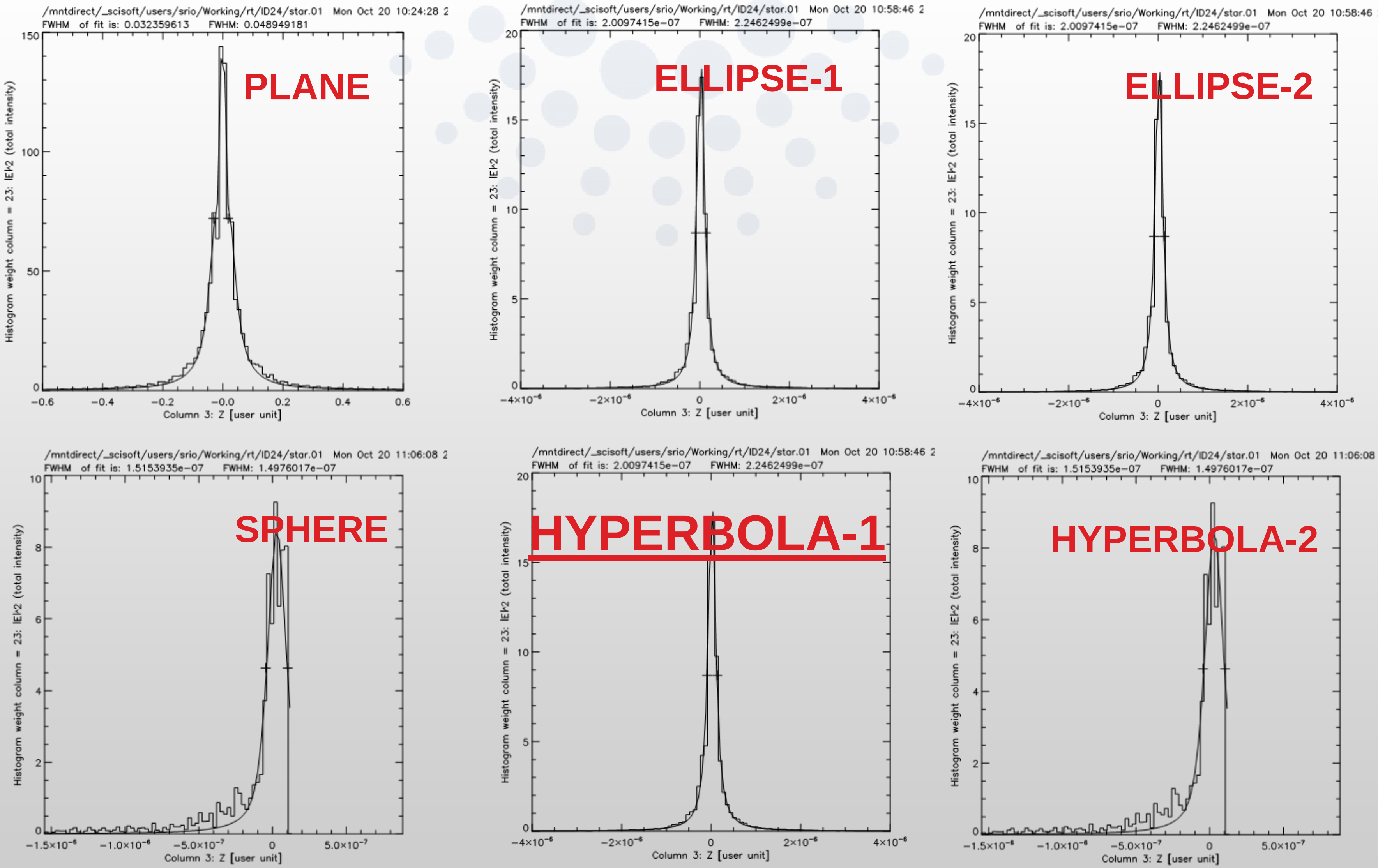
•The intensity is very small in all cases, due to the fact of the very small angular acceptance of the crystal (we use a monochromatic source)

•The intensity given by all bent crystals is much smaller than for the flat case. This can be understood because the convexity of the crystal increases the dispersion of the beam along the crystal surface, thus reducing the transmitivity.

•Note that in all bent cases, the spot size (weighted with intensity) is smaller than 3 μm.

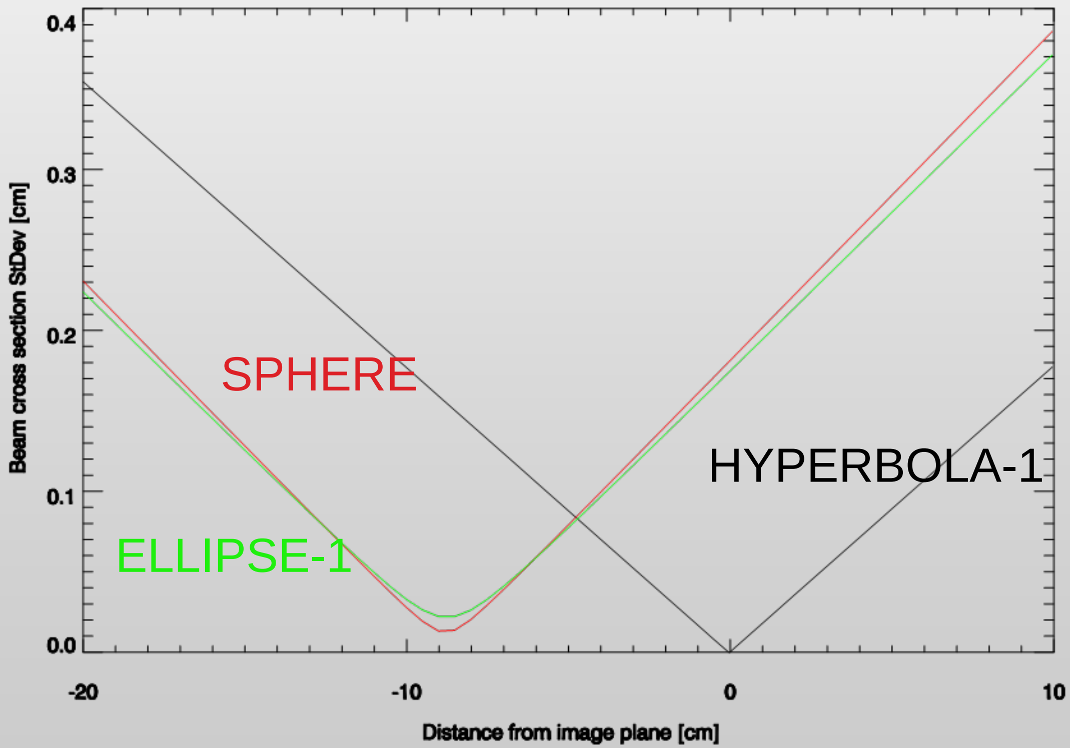
•Both hyperbola-1 and hyperbola2 give similar spot size, but the correct one is hyperbola1

Spot profiles



Polychromatic focusing

	Bandwidth FWHM eV	Intensity [a.u.]	FWHM [cm] at image plane	Best focus at [cm]	StDev at Best focus [cm]
plane	55	1280	5		
spherical	600	14	0.35	-9	0.013
ellipse1	751	14	0.31	-8.5	0.022
hyperbola1	770	13	0.0002	0	7.30E-05

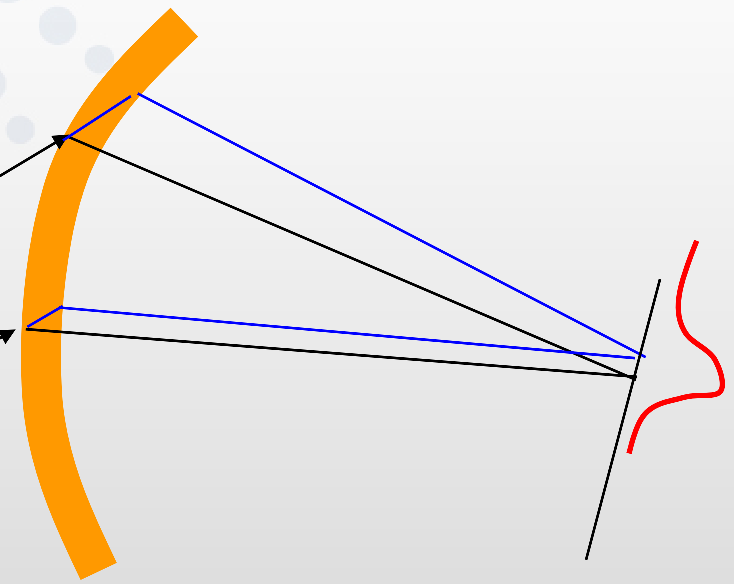


A polychromator with hyperbolic shape produces an ideal focus, point-to-point focusing and no defocus at all. It is a “perfect” system (remember that we use here a point source and the beam does not penetrate in the crystal).

If we approximate the hyperbola by a sphere (or ellipse) there is a defocus of about -10 cm and the best spot (remember we use a point source) is larger than 100 μm (RMS).

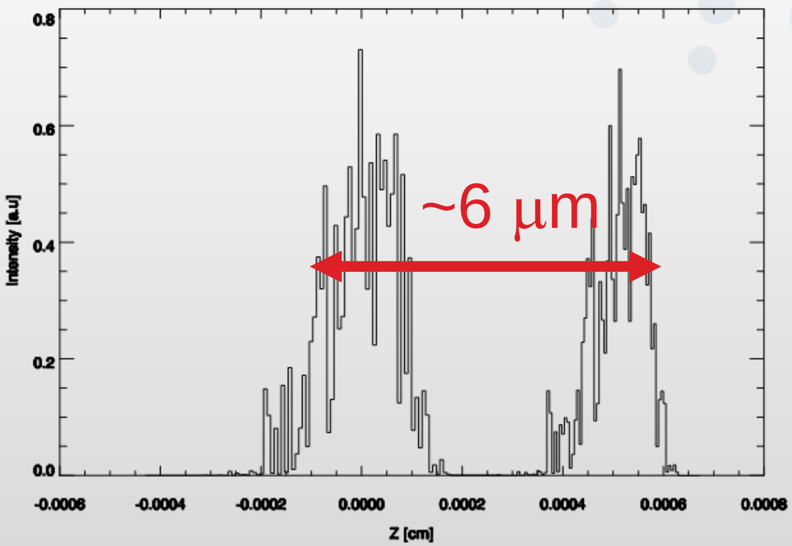
Spot broadening because of crystal thickness

- I assume here the hypothesis that *the maximum cross section of the diffracting beam cannot be larger than the incoherent sum of the beams diffracted by different crystal surfaces.*
- These surfaces are produced by translating the initial crystal surface (with pole at (0,0,0)) along the z (vertical) axis an amount , with *t* the crystal thickness.
- Therefore, for computing the spot size it will be enough to calculate the spot of the two limiting surfaces at **0** and *t*. The "real" spot will fill all the space between the spots produced by these two surfaces.

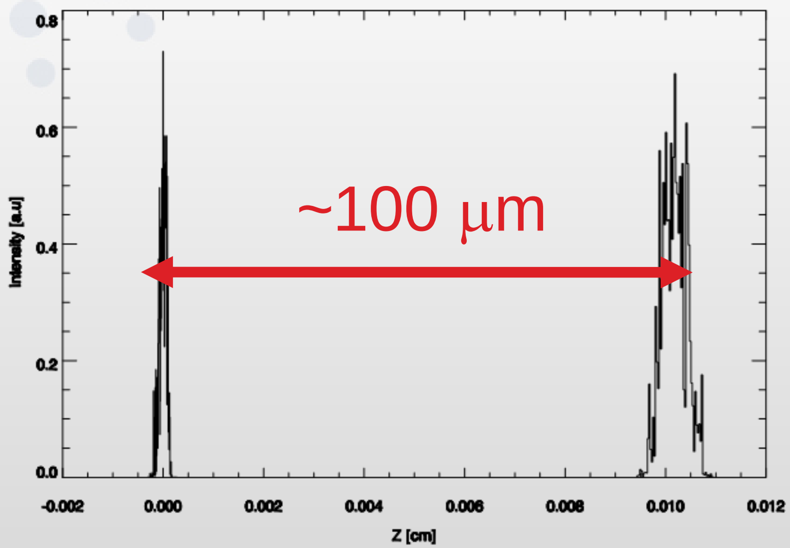


Spots produced by the two limiting surfaces

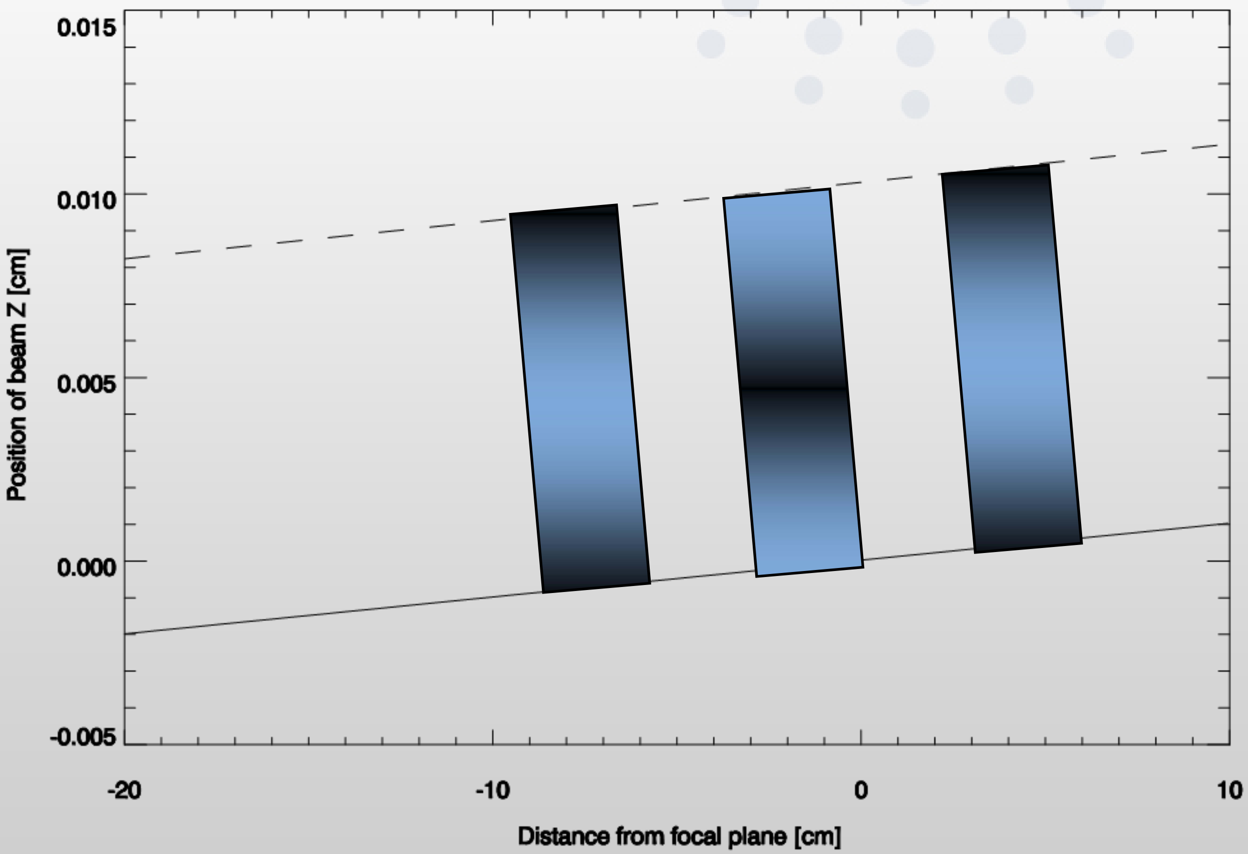
t=10 µm



t=200 µm



Evolution of the “extreme beams”



The fact that the diffraction takes place in a finite volume inside the crystal, implies that the crystal thickness is the limiting parameter when trying to focus x-ray beams even if all aberrations are corrected using hyperbolic crystal shape.

We neglected:

•effects of absorption inside the crystal

•possible focusing of the beam outgoing from the Borrmann triangle

Conclusions

- The ESRF source cannot be arbitrarily demagnified: problems will start with M>100
- The HFM, even if perfect, degrades the phase space. This may affect the polychromator performance. Slope errors should be kept less than 0.5 um RMS with care on the distribution of the low frequencies (figure errors). A small astigmatism may be present.
- For Bragg polychromators, use elliptical crystals (well known: Fontaine, San Miguel, Pascarelli, ID24)
- For Laue polychromatiors, one must use crystals with hyperbolic shape (spherical or ***elliptical*** approximations are not good)
- Spot size is influenced by geometry (shape), polychromatic and monochromatic focalization and crystal thickness. To reduce its effect, two solutions (of a combination of them)
  - Use very thin crystals
  - Focus the Bormann triangle. This is possible, but one should take into account that
    - i) the focusing of the Borrmann triangle must be at the same place of the geometric focusing
    - ii) all energies transmitted by the monochromator must be focused very close to the geometric focus (polychromatic analysis)
    - iii) the correct crystal curvature (hyperbolic) should be taken into account for correctly calculating the diffraction pattern

Evolution of the beam FWHM