ADAPTIVE OPTICS
and
WAVEFRONT CONTROL
in the
HARD X-RAY DOMAIN

PAST, PRESENT AND … FUTURE

Dr. Riccardo SIGNORATO
ACCEL Instruments

Where it all started…

Published on SPIE 1997 proceedings

Structured slope errors on real x-ray mirrors: Ray-tracing versus Experiment

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Data collected in 1996

Mirrors polished in 1995

ABSTRACT

Ray-tracing plays an essential role for the design of a synchrotron radiation beamline optics. Nevertheless, it can also be extremely useful during the commissioning phase of a beamline. At that moment, it is possible to include real surface figure errors in the computer simulation of the optical devices. The resulting focal spot size and photon flux values are the final targets for the experimental optimization and alignment of the optics setup. We report on extensive ray-tracing of the mirror systems of the two beamlines placed at the ESRF insertion device 12. Slope errors measured after mirror delivery are included in the calculations. It is demonstrated how slope errors with characteristic periodicity between 1 and ca. 1/20 of the mirror length can affect the focal spot shape, size and position. In particular, they can create structures or satellites in the focal spot. The distortions from the ideal shape are generated by the polishing process itself and are intrinsic to each single mirror. Comparison between the effects of slope errors in ray-tracing using either real (measured) surfaces or numerically generated ones are also reported.

Keywords: ray-tracing, slope error, x-ray mirror, synchrotron radiation beamline, PSD, mirror metrology

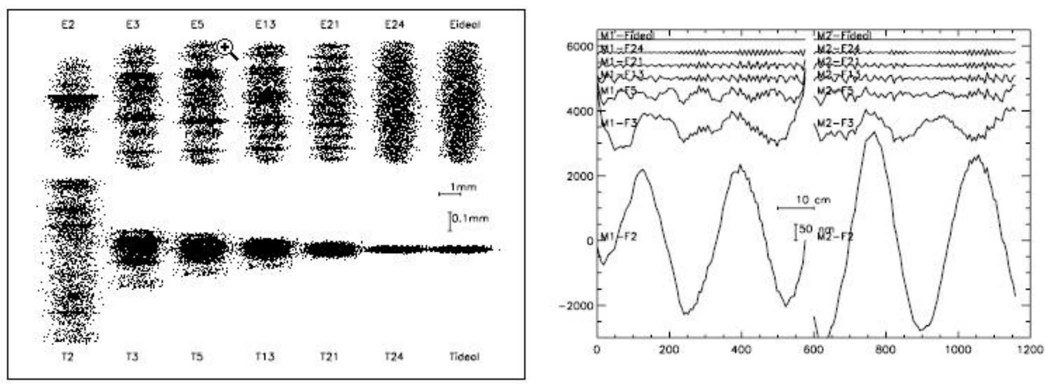


Figure 7. Left: Calculated spot shapes with Fourier filtered profiles for M1 and M2. The spot size is shown in two position: at the experimental location 7.62 m from M2 (labeled En) and at the theoretical focus location at 17.14 m from M2 (labelled Tn). The n value means that the applied cutoff frequency is n/L. Right: the corresponding filtered profiles for M1 and M2. Filtered values are labelled with Fn, with the described meaning for n. E/T/F$ideal$ stands for ideally spherical mirrors.

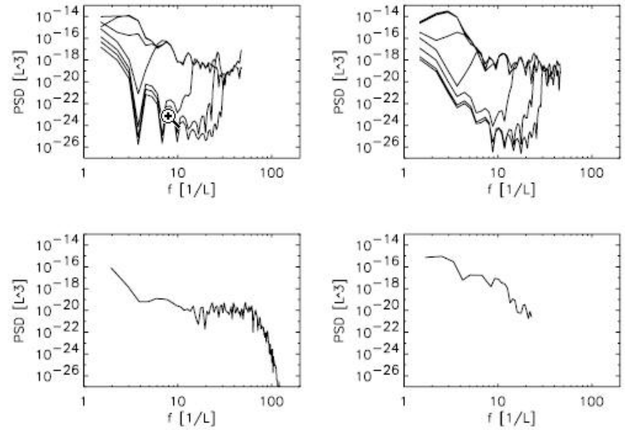


Figure 8. Top: Effect of progressive Fourier filtering on the PSD functions for ID12A mirrors M1 (left) and M2(right). The higher curve corresponds to the PSD of the non-filtered profile. The other six curves refer to the filtered profiles shown in Fig. 7 (cutoff frequencies: 2/L, 3/L, 5/L, 13/L, 21/L and 24/L, respectively). Bottom: PSD for ID12B VFM (left) and PFM (right). Note that the low frequencies are enhanced in the non-filtered ID12A mirrors respect to the ID12B ones. These peaks in the low frequency range are responsible for the focal spot structures (see text).

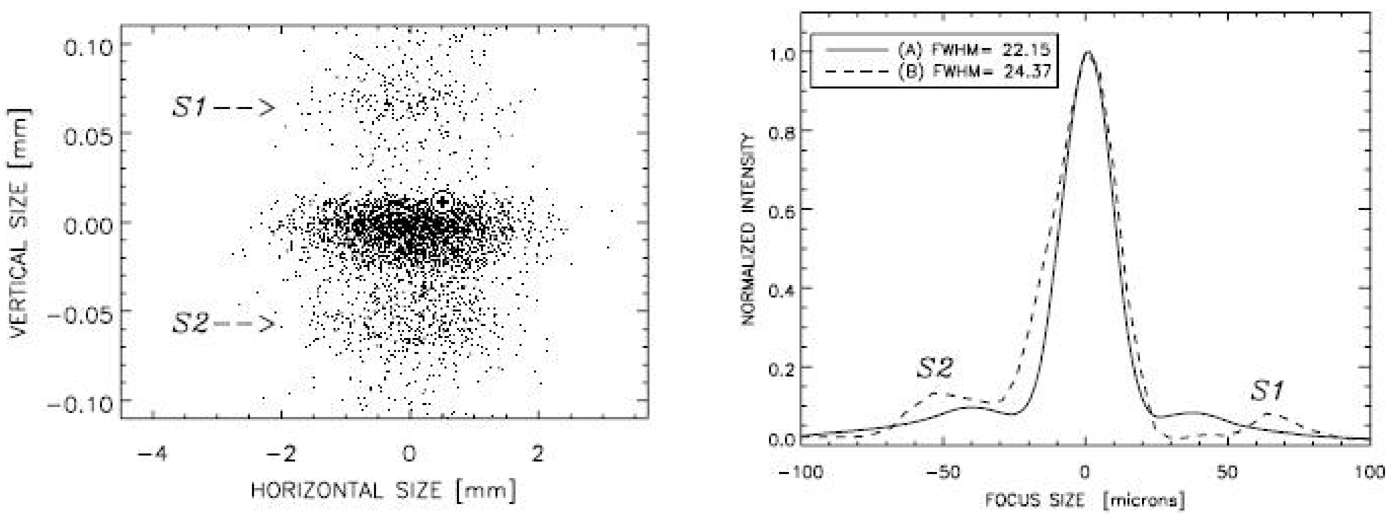
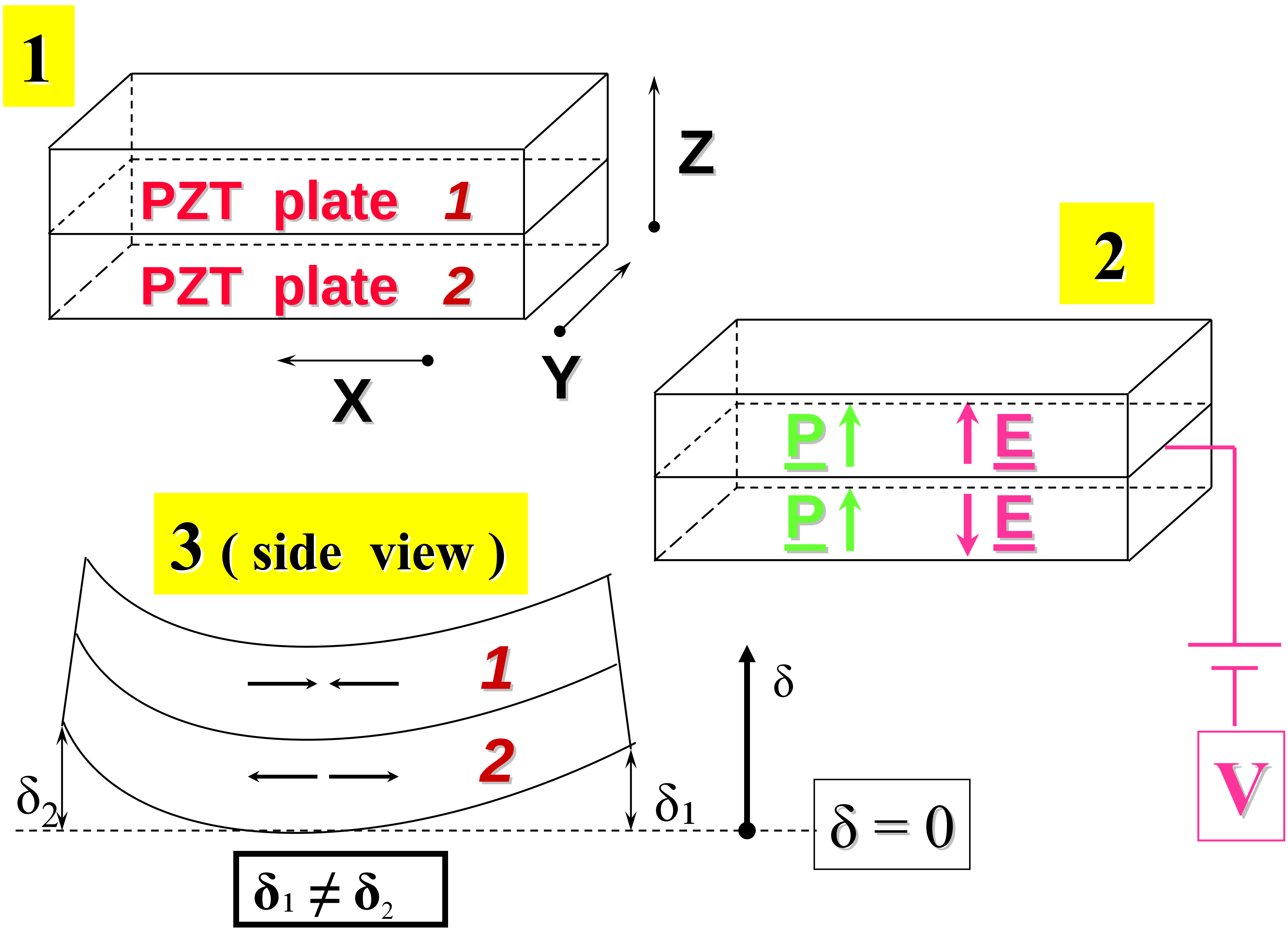
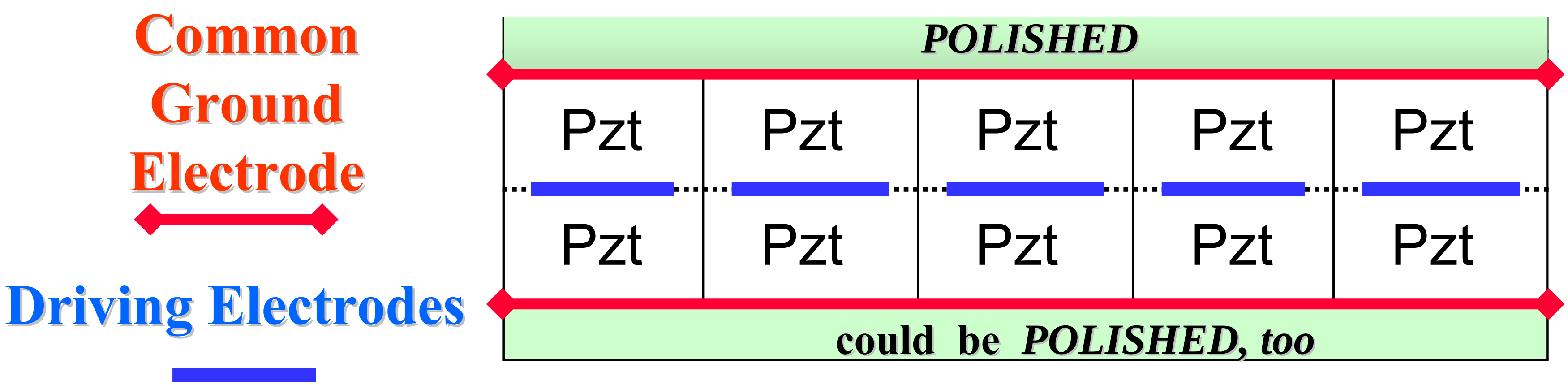


Figure 6. Left: SHADOW calculation for VF-2M focal spot (same as in Fig. 5 (center)). Right: Superposition of the experimental (A) and calculated (B) vertical intensity profile at the ID12A VF-2M focal position. The satellite structures $S1$ and $S2$, which are due to the mirror slope error are evident in both curves.


1
PZT plate 1
PZT plate 2
Z
X
Y
2
P
E
P
E
V
3 (side view)
1
2
δ
δ2
δ1
δ = 0
δ1 ≠ δ2

Bimorph Mirror Side View



Available bimorph mirrors lengths:

100/150/200/300/450/600/750/900/1050/1200/1350/1500 mm

Driving Electrodes length from 140 mm down to < 20 mm

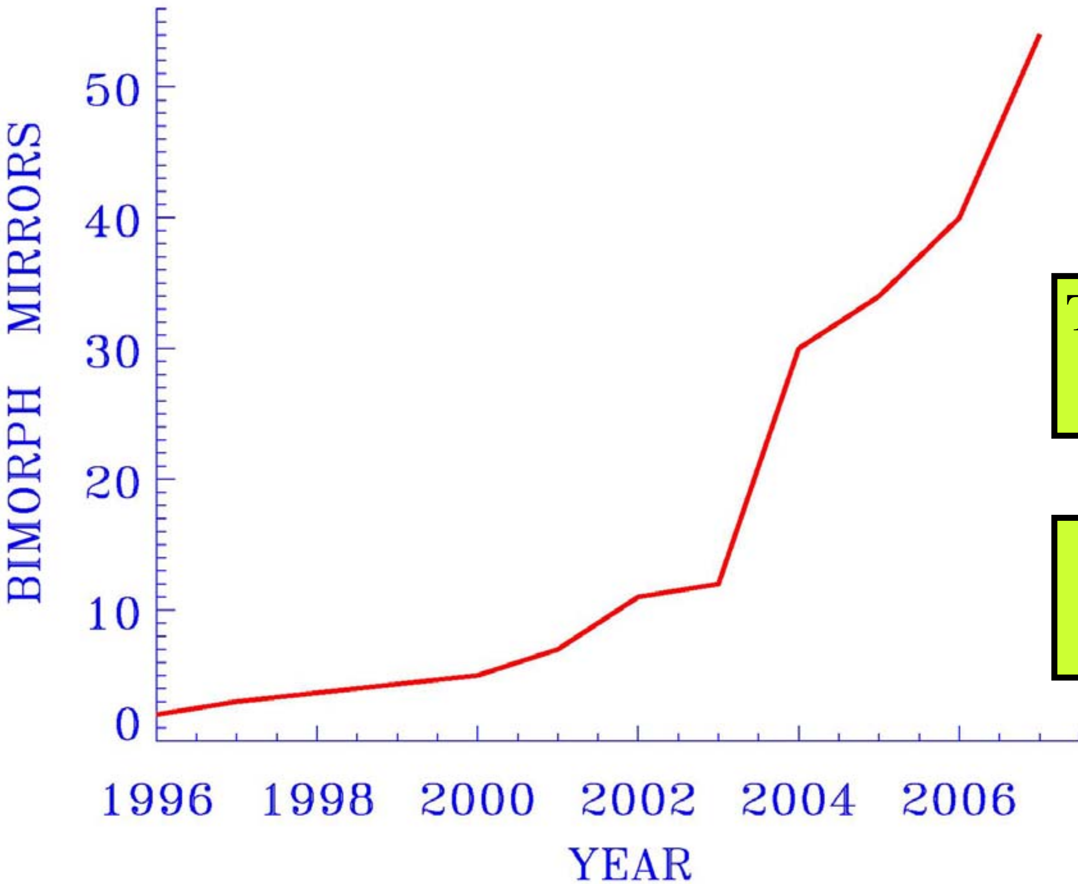
FOCUSING FROM A FEW 100´s of mm to ∞

Bending from R ~ 30 m to flat

Manufactured/Ordered Modular Bimorph mirrors:

Today´s Total: 55

Updated to September 31st, 2008



Total Bimorph Mirror Length

~ 33 m

Total Number of Electrodes

~ 740

Advantages of bimorph mirrors

Fully Modular architecture (from 100 mm to 1650 mm)

Simple, elegant and ***fully standardized*** *design*

Reversibility of global & local bending momentum

Adaptive zonal control → PSD low frequency filtering possible

Easy implementation of different electrodes density

N electrodes → control over N^{th} degree in slope, $(N+1)^{th}$ in shape

Can approximate ***n+1*** *(!) order polynomials → large focusing tunability*

Can improve their own slope error → lower polishing requirements

Mirror performance does not depend on illuminated footprint

- *can freely approximate high order polynomials over any freely selectable illuminated length*

Reconstruction of deformed wavefronts!!!

Correct wavefront aberrations ***due to mirror & other optical elements***

dynamical reconstruction possible → full ´optical flexibility´

In-situ X-ray wavefront reconstruction

Possibility to control beam properties when operating out of focus :

Striations control & High Strehl ratio

Takes into account all possible perturbations sources

No moving parts or mechanisms: bending is intrinsic to the mirror

→ *No Maintenance*

→ *Very Robust*

→ *UHV compatible (no lubricants)*

Compact & lightweight

smaller vacuum vessels – fits in crowded Bl

allows installing fast feedback on fine pitch with pzt linear actuator

Holder has NO effect on mirror operation

NO clamping: *simple 3-points support*

Designed to protect mirror;

to allow simple & safe handling& installation

delivered as a ´ready-to-install´ device

Backlash-free, NO ´lost-steps´ operation

Possibility to use same mirror as HFM / VFM

Gravity compensation not necessary – Isostatic mount possible

Possibility to polish both sides; reflection possible as:

→ *Upwards / Downwards*

→ *Outboard / Inboard*

Pre-polished to shape close to typical working position

No need to have specially shaped substrates optimized for one specific configuration only

No anticlastic effect

"Environmental friendly": mirror can be recycled by:

Repolishing to different radius → adapt to drastic layout changes

Repolishing optical surface → keep up with state-of-the-art polishing

Strip-off & re-coating → remove surface damage due to X-rays

Bimorph bender itself has virtually UNLIMITED LIFETIME

Calibration / Encoding / Resolution

Calibration: *INTRINSIC*

NO effects due to

- ***Transportation*** → ***proven***
- ***Mounting*** → ***proven***
- ***Temperature*** → ***proven***

Encoding: *INTRINSIC*

Use HV supply 16-bit resolution readout

Resolution: " *virtually UNLIMITED* "

limited only by HV supply noise (ripple)

1 - Active Mode

All the electrodes kept at the same voltage

UNIFORM VARIATION (SPHERICAL) OF THE BENDING RADIUS

2 - Adaptive Mode

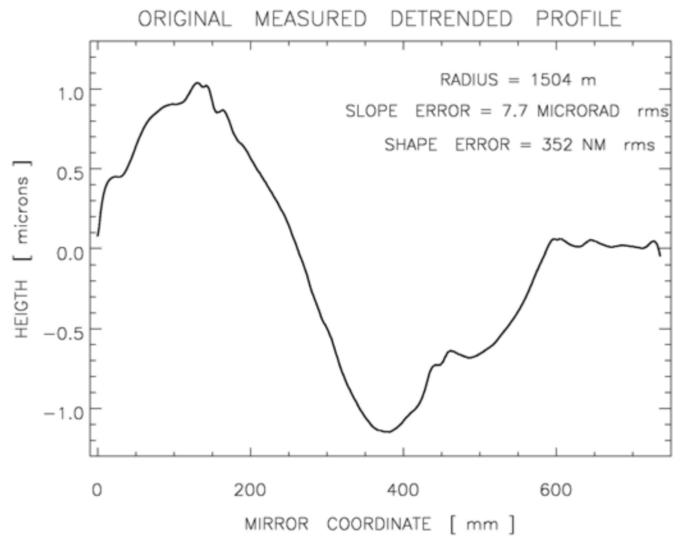
Different voltages applied at each electrode

INTERACTION MATRIX (H)
CONTROL MATRIX (M)
SVD

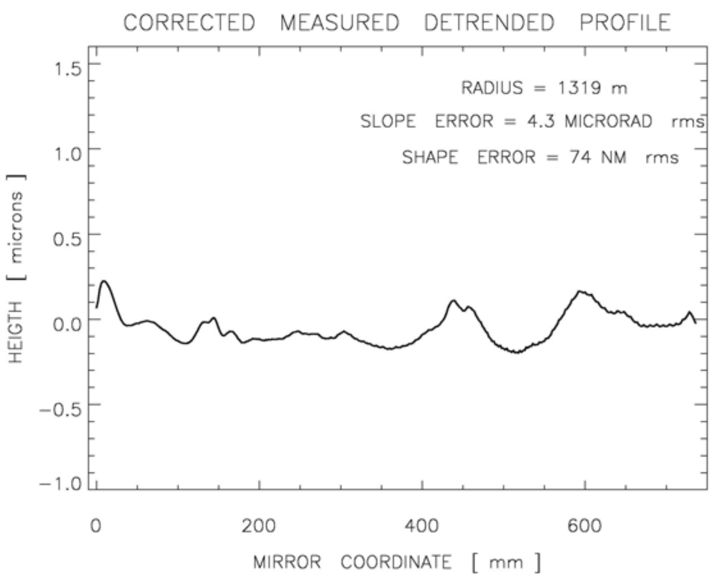
$$\begin{pmatrix} V_{D,1} \\ V_{D,2} \\ V_{D,3} \\ V_{D,4} \\ V_{D,5} \end{pmatrix} = \left(H^T H\right)^{-1} H^T \delta f_0$$

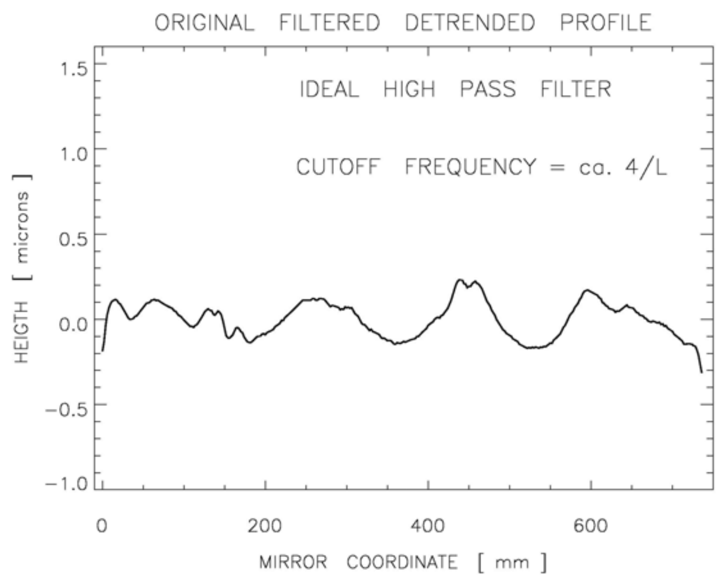
SELECTIVE ATTENUATION OF PSD LOW FREQUENCY COMPONENTS

First proof of Adaptive Correction @ ESRF in 1997



R. Signorato´s PhD thesis



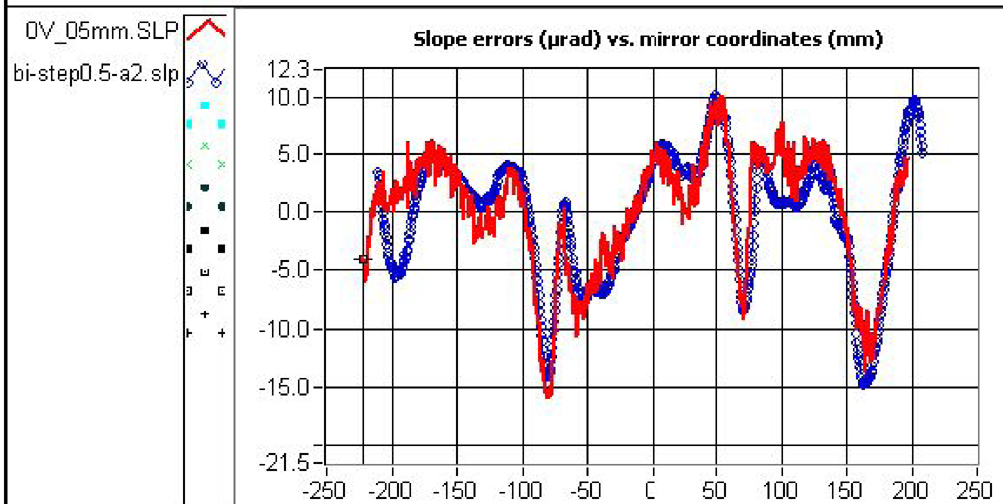


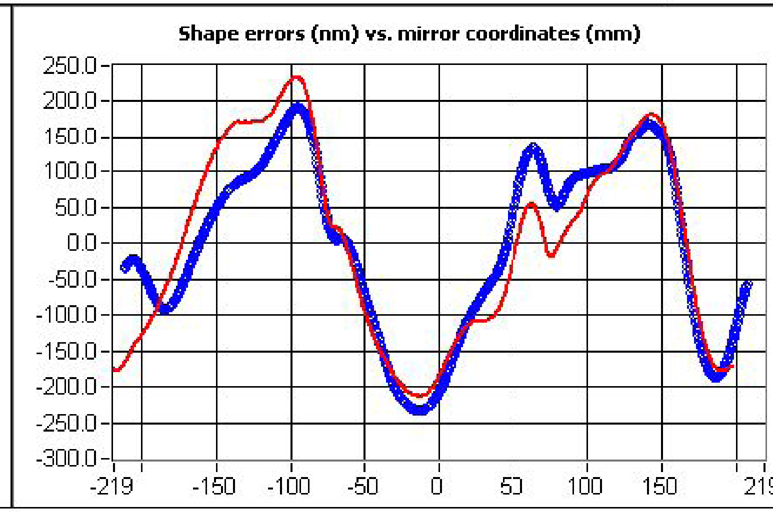
Forensic Metrology

On corpse of long (450 mm) bimorph Prototype No.1
polished in winter 1996 – requiescat in pacem †

Long Trace Profiler results

02/02/2006



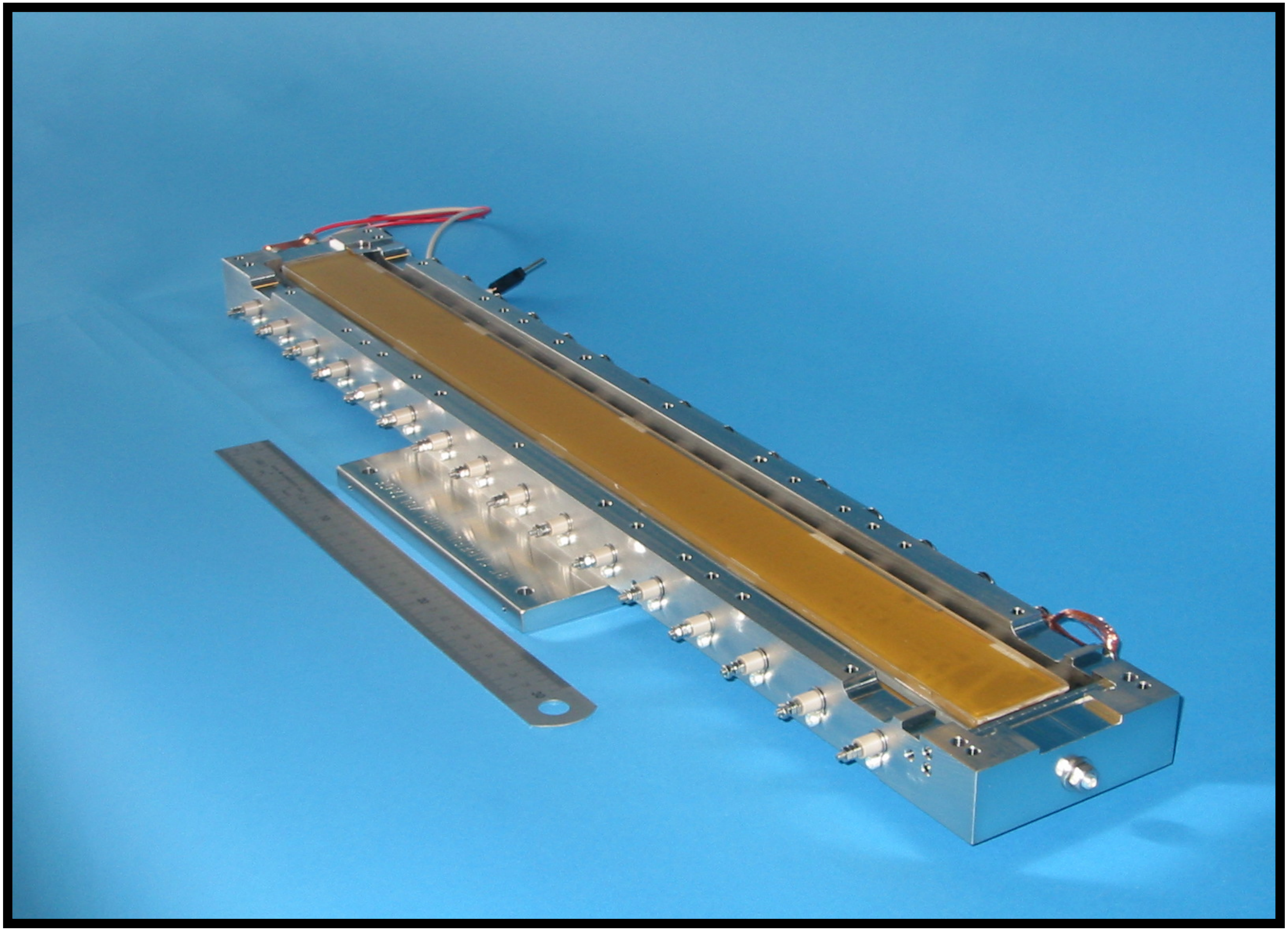


Detrending order 1

Date	Filename	Comment	Step (mm)	Length (mm)	g-re moved	Radius of curvature	Slope error RMS (urad)	Shape error RMS (nm)	Shape error PV (nm)
/99 at 11:	0V_05mm	step 0.5 at 0 Volt	0.5	419.5	yes	4.517 km	5.2	134.6	448
03/11/05	bi-step0	step 0.5 mm	0.5	419.5	yes	3.466 km	5.5	122.3	425

Conclusion : recent measurements are in a good agreement with data obtained in 1999. The figure error of this bimorph mirror has not been changed after few years of exposure to X-rays on ID32 beamline.

@ APS, BESSY II, DLS... (third generation)



Mirror installed at GM/CA CAT *Photo courtesy of SESO*

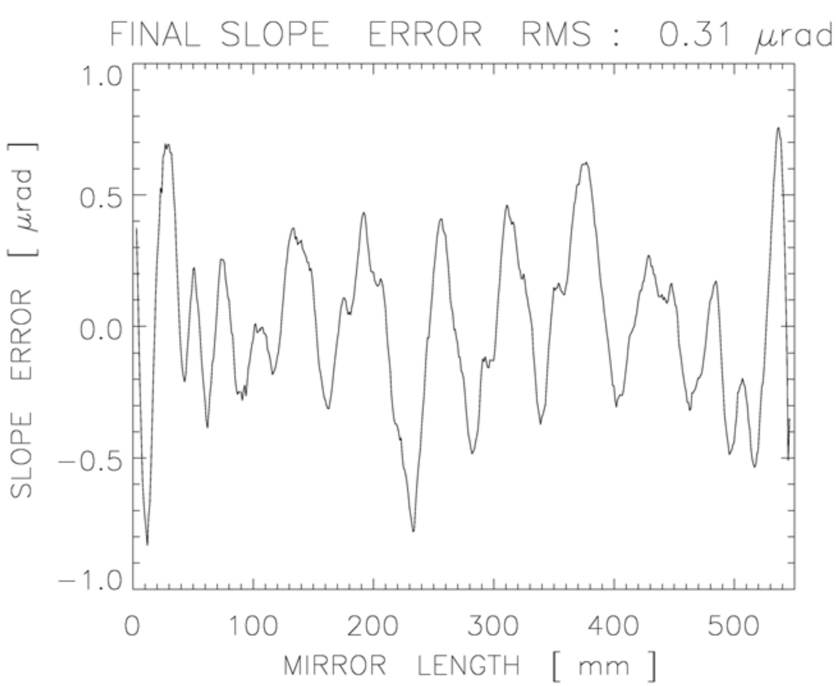
State-of-the-Art Metrology Data

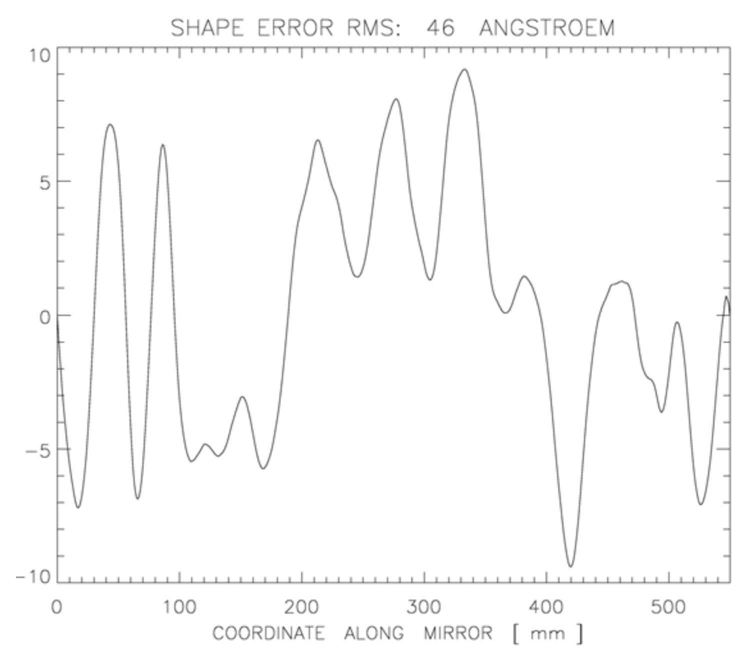
(courtesy of ELETTRA Trieste)

Tangential Slope Error – measured on <u>550 mm over 600</u>

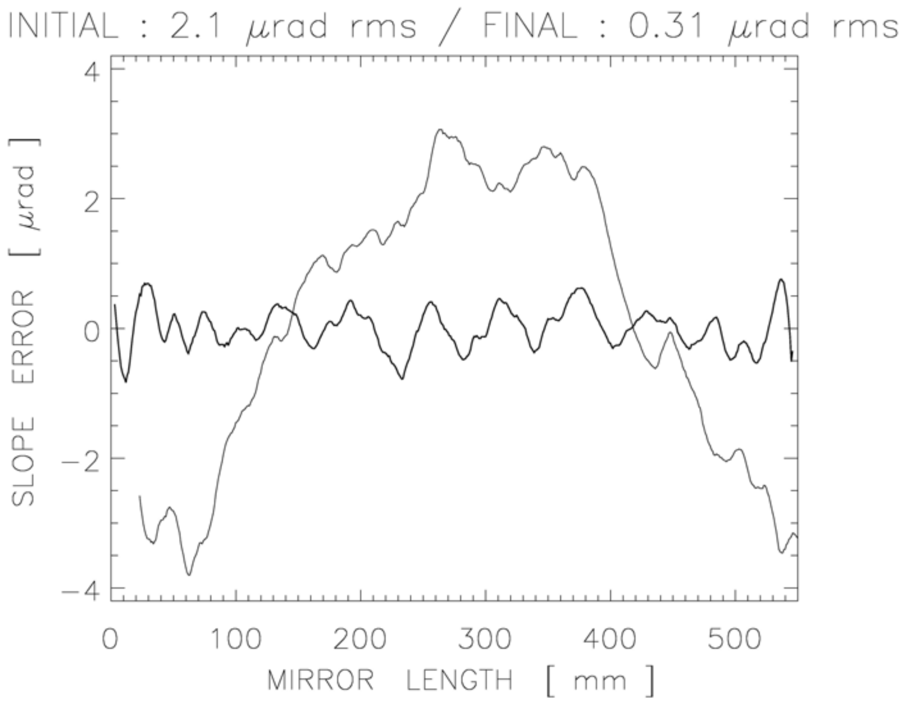
<u>APS mirror (16 electrodes) = 0.3 μrad rms (shape: 46 Å rms)</u>

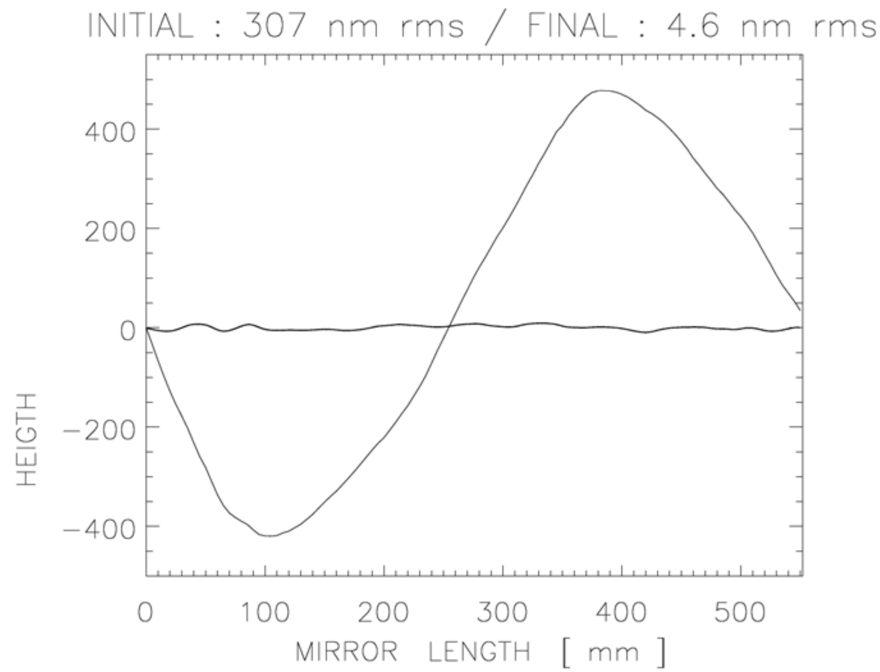
Dynamical Range: Flat - 0.8 km





Before and after ...





Repeatability & Hysteresis (1)

Monodirectional

Delta R / R < **± 0.1%**

Bidirectional

Delta R / R < ± ***0.25%***

Long Term Repeatability
@ SESO @ 1000V → *437 m!*

Similar behaviour @ SP8

Voltage (V_D)	*Spherical best fit radius (m)*
0 / 0 / 0	632.0 / 631.1 / 631.7
+500	**516.8**
+1000	**435.7**
+500	**517.7**
+1000	***436.4***
+1500	374.2
+1000	***434.1***
+500	**517.0**
0	634.6
-500	842.5
+500	**515.8**

Data taken at APS metrology laboratory – Dr. L. Assoufid and Mr. J. Qian

Repeatability & Hysteresis (2)

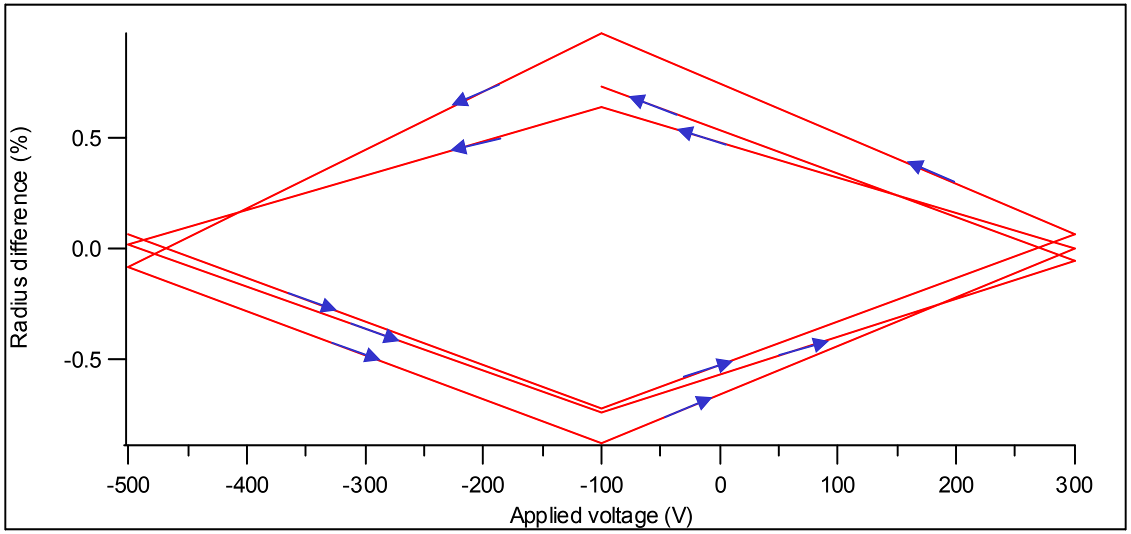
Voltage	Radius of curvature	Percentage difference
(V)	(m)	(%)
-500	2276.71	0.0624096
-100	3257.42	-0.723827
300	5989.88	0.0593018
-100	3313.21	0.976481
-500	2273.36	-0.0848244
-100	3252.35	-0.878345
300	5986.25	-0.00133638
-100	3302.07	0.636968
-500	2275.79	0.0219752
-100	3256.86	-0.740894
300	5982.85	-0.0581324

Monodirectional

Delta R / R < **± 0.05%**

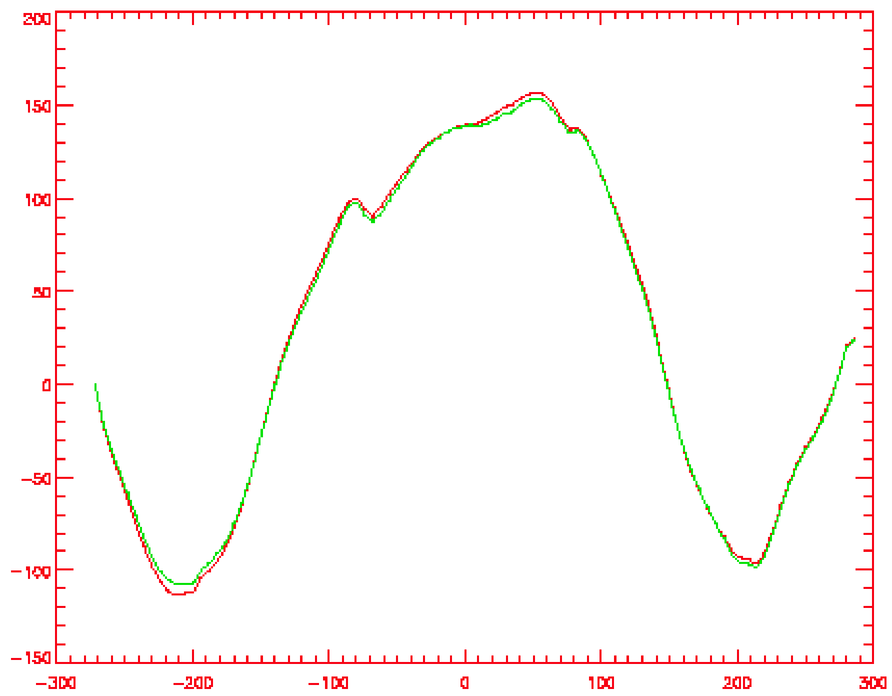
Bidirectional

Delta R / R < ± ***0.5%***

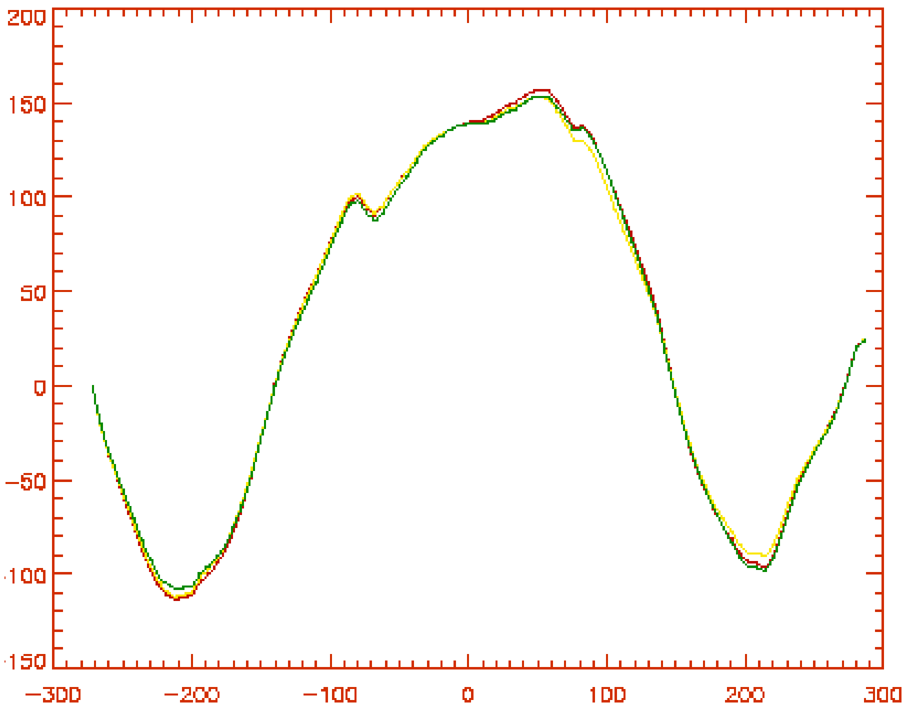


Data taken at ELETTRA metrology laboratory – Dr. D. Cocco and Mr. G. Sostero

Repeatability & Hysteresis (3a)



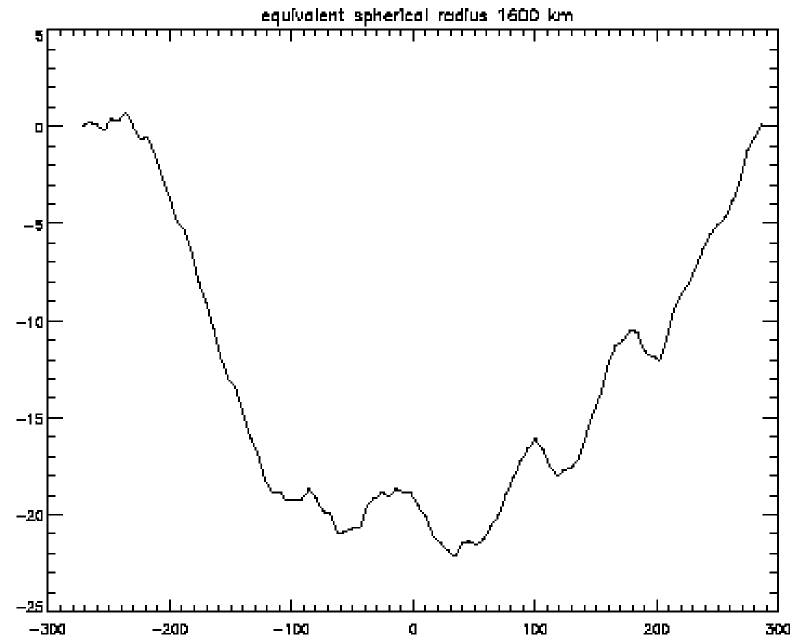
Over 2 days

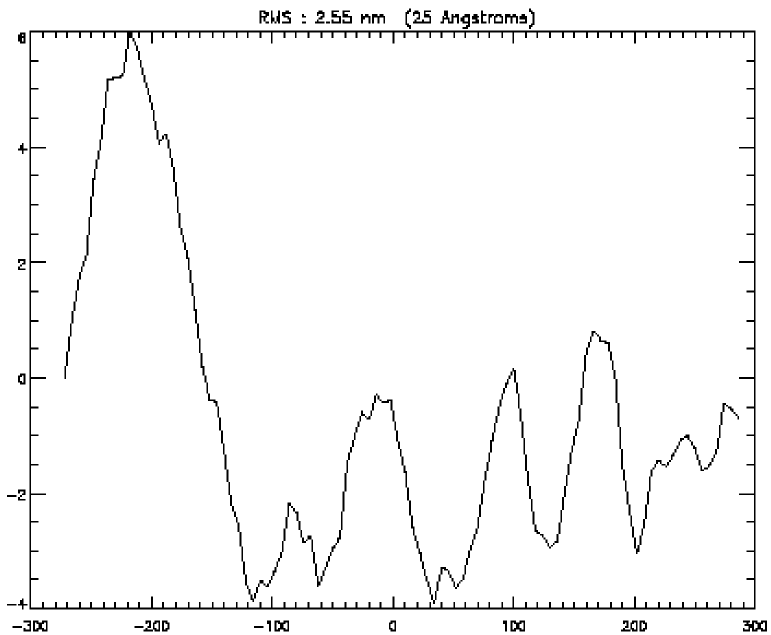


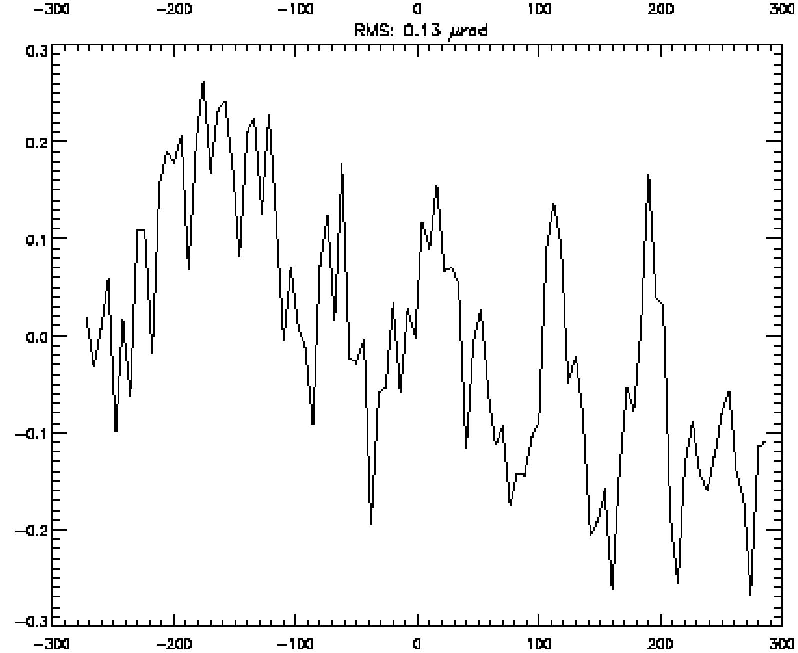
Over 3 days

Data taken at <u>Diamond metrology laboratory</u> – Dr. S. Alcock

Repeatability & Hysteresis (3b)







Data taken at <u>Diamond metrology laboratory</u> – Dr. S. Alcock

BESSY

Repeatability of shape:

Voltage off: (shortly after delivery) **:**	R = 2020,1m	Slope = 0,303 arcsec rms
Voltage on: (19 days after delivery)	R = 2306,1m	Slope = 0,233 arcsec rms
Voltage off: (20 days after delivery)	R = 2018,6m	Slope = 0,294 arcsec rms
Voltage on: (20 days + 5h after delivery)	R = 2310,5m	Slope = 0,233 arcsec rms

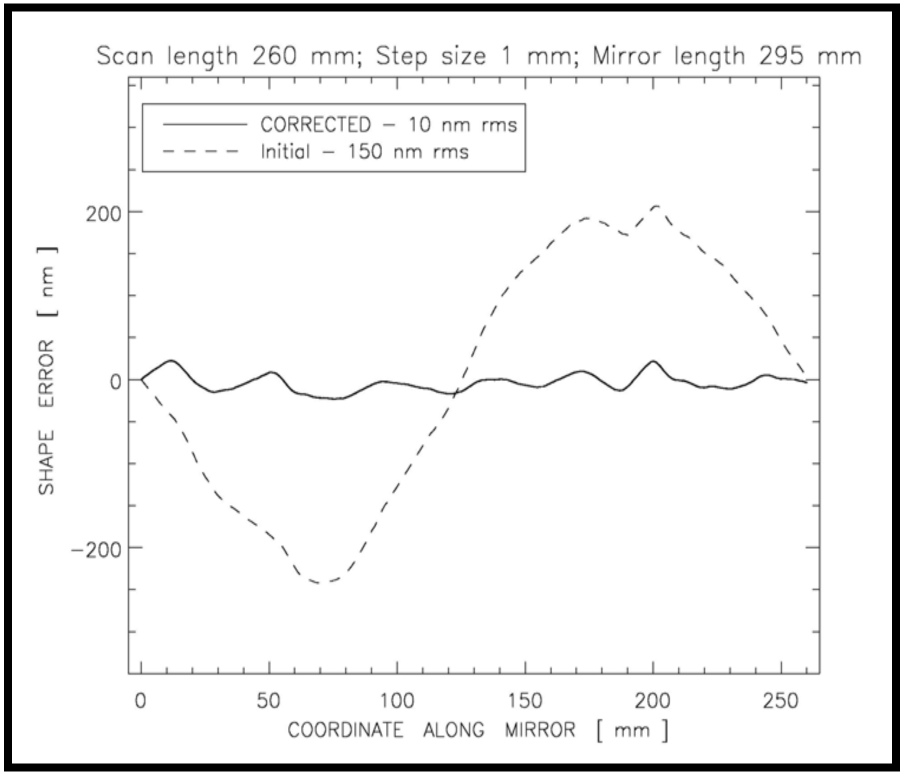
APPLIED VOLTAGES

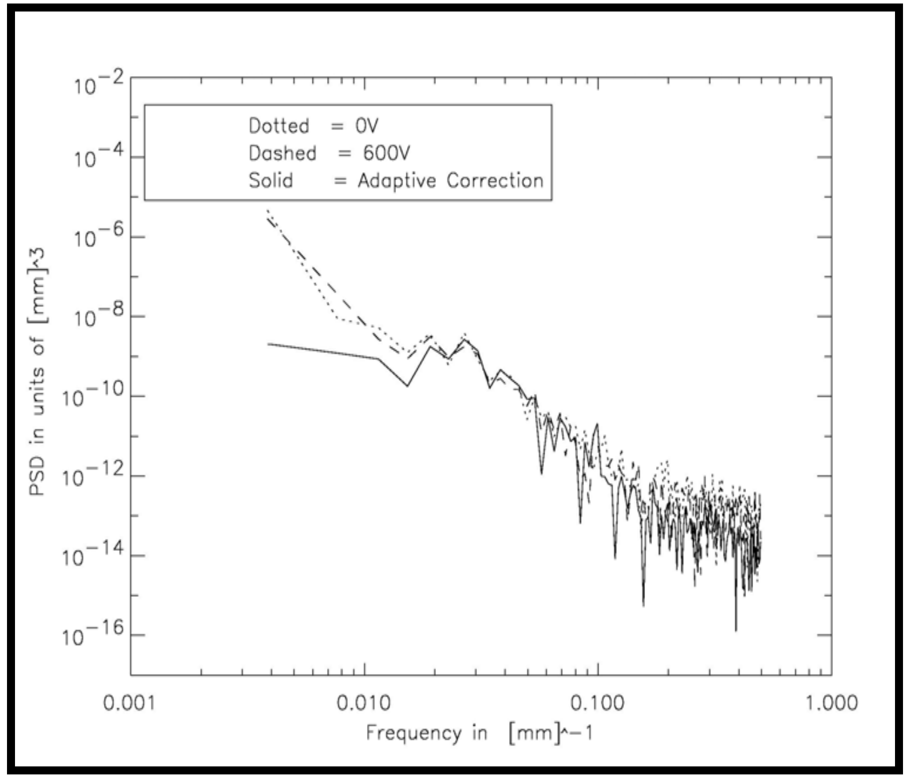
115.65 / 196.91 / 106.96 / 80.87 / 48.22 / 117.78 / 123.16 / 232.41

Data taken at BESSY metrology laboratory – Dr. F. Siewert

PSD Filtering

Data obtained at APS metrology lab
LTP



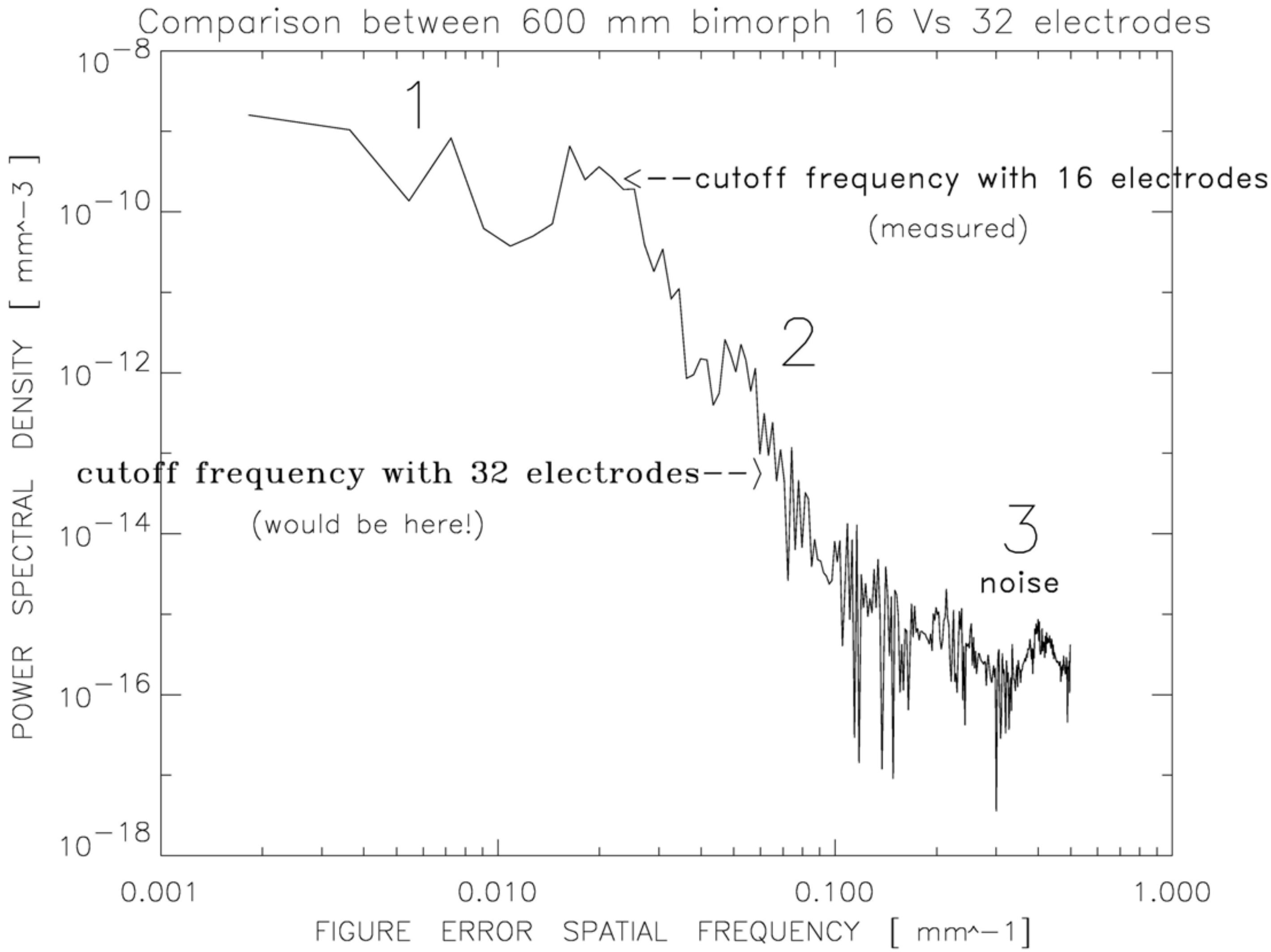


[Top Left] shape error before – dashed - and after – solid - adaptive correction of the mirror shape. The bimorph can be shaped to a perfect sphere with a residual shape error as small as ***100 Å rms****.*

[Bottom Right] PSD function at V = 0V & 600V on all electrodes and after adaptive correction (each electrode is independently set at a different V_i*). Low frequency components of the PSD could be reduced by as much as* ***4 orders of magnitude****.*

PSD Filtering - Limits ??

(LTP data courtesy of ELETTRA)



…*LAST BUT NOT LEAST :*

High Voltage Bipolar Power Supply fully developed and tested

- *linear fully bipolar state-of-the-art power supply (- 2000 V → + 2000 V)*
- *compact: up to 32 channels in a single 19" crate*
- *dedicated ´user-proof´ software for safe operation*
- *standalone operation (WEB interface) possible*
- *easily interfaced with EPICS, TANGO …*
- *flexible, expandable, highly customized system*
- *dedicated high level software being continuously updated*

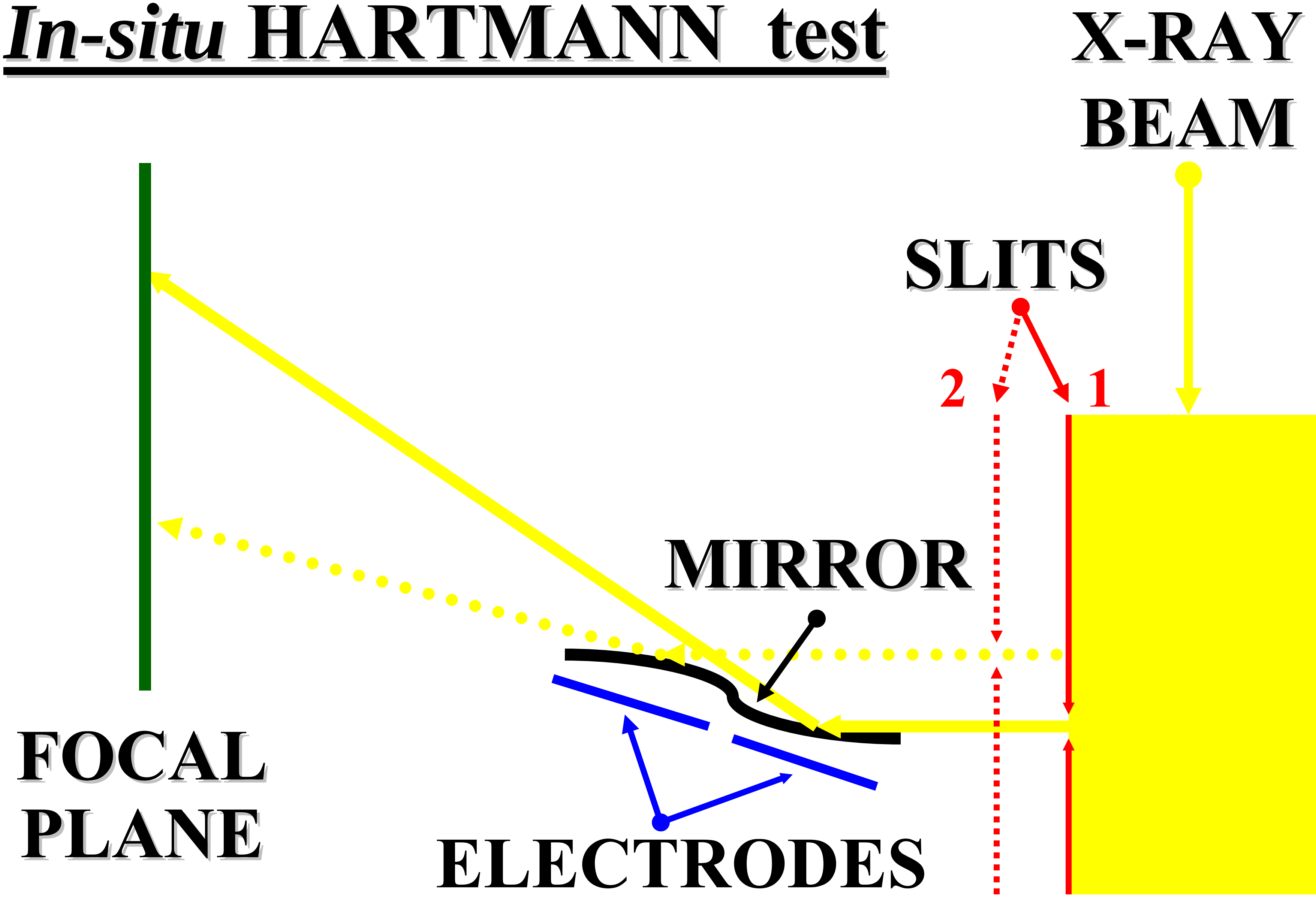
Features

- Ethernet and GPIB full remote control
- RS232C remote configuration
- Fully encased on 19"-wide, 6U-high Euro mechanics rack

Main software features

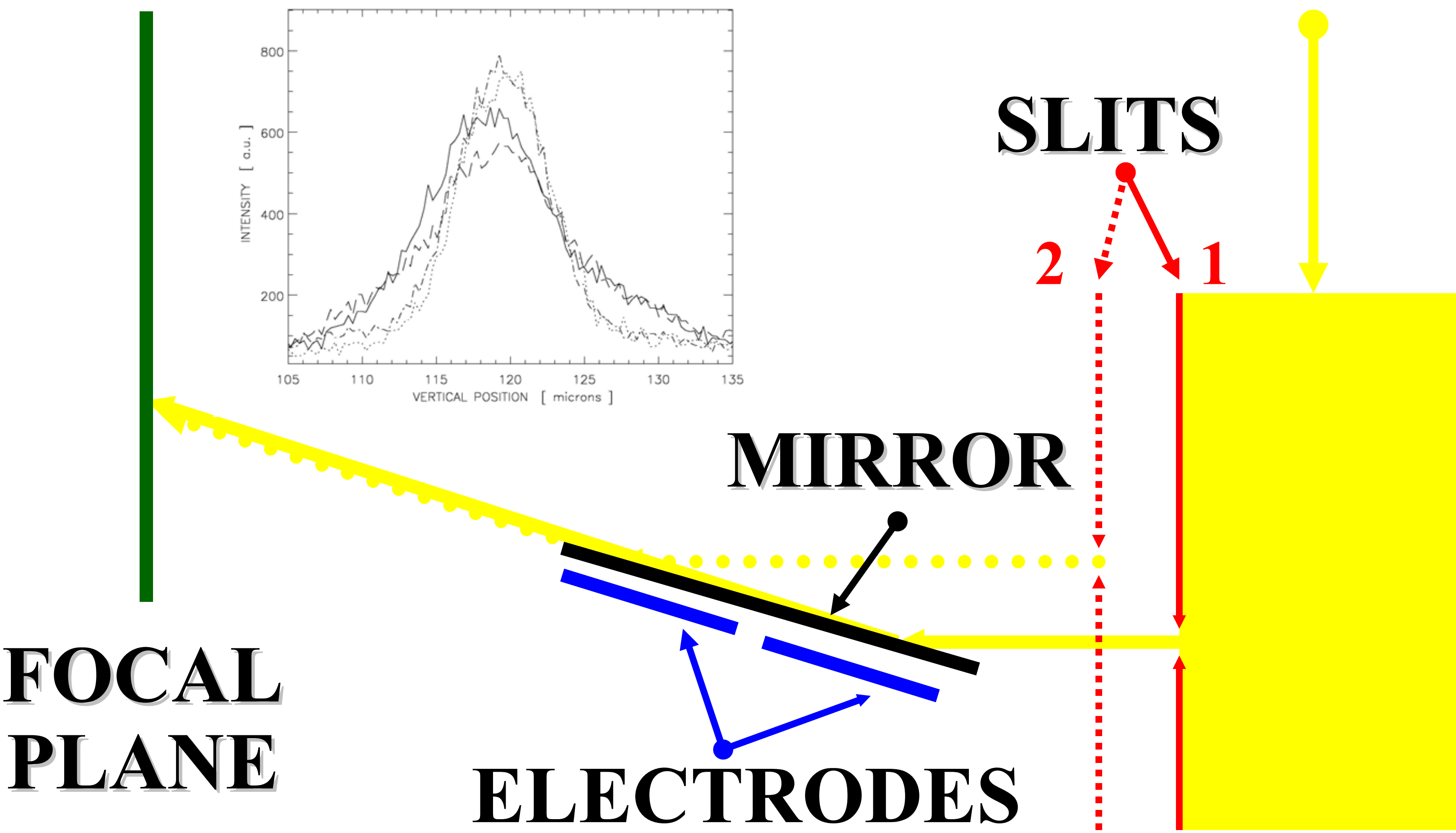
- Multitasking embedded system supervisor
- System Configurator (via RS232C port)
- Self Diagnostic Test
- Remote Firmware Upgrade
- Communication Modules
  - IEEE488.2 (SCPI) Standard Command Syntax on Eth, GPIB, RS232C
  - TCP/IP communication (Labview, Python and Java libraries, EPICS)
  - HTTP Interface via standard Web Browser

In-situ HARTMANN test



In-situ HARTMANN test

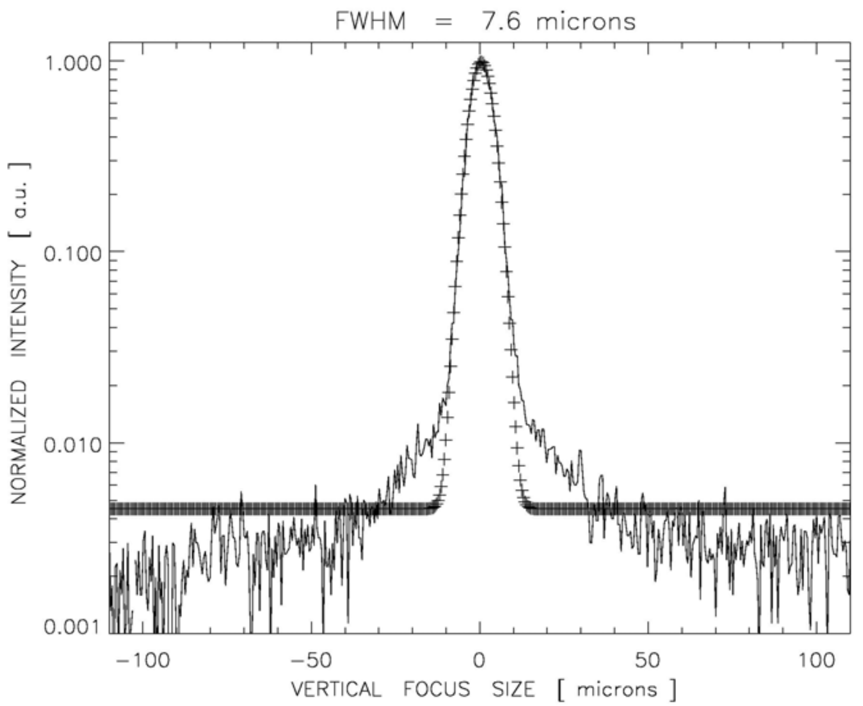
@ Spring - 8



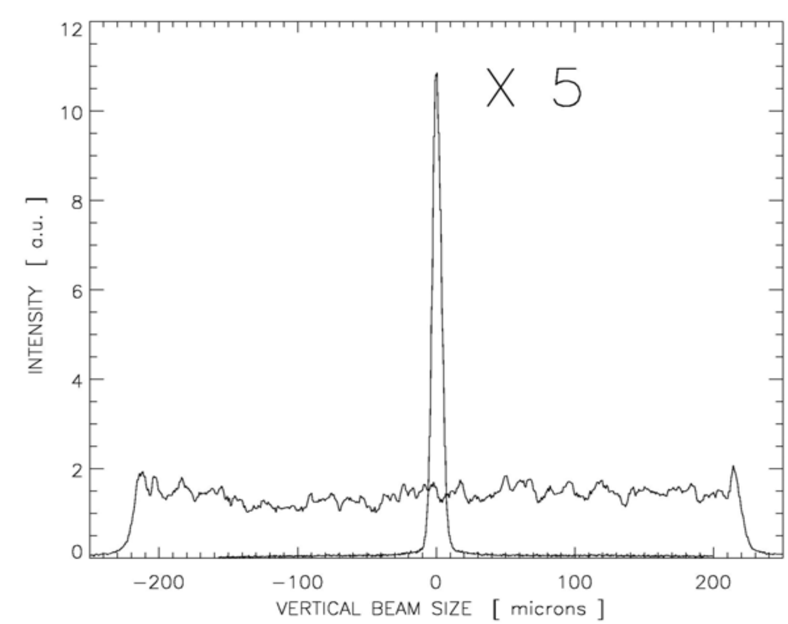
@ SPring - 8

Data obtained at 1km long Bl in year 2000

Source-to-Sample distance = 990 m
Focusing Distance = 1 m
q = 2 mrad
Illuminated footprint = 225 mm



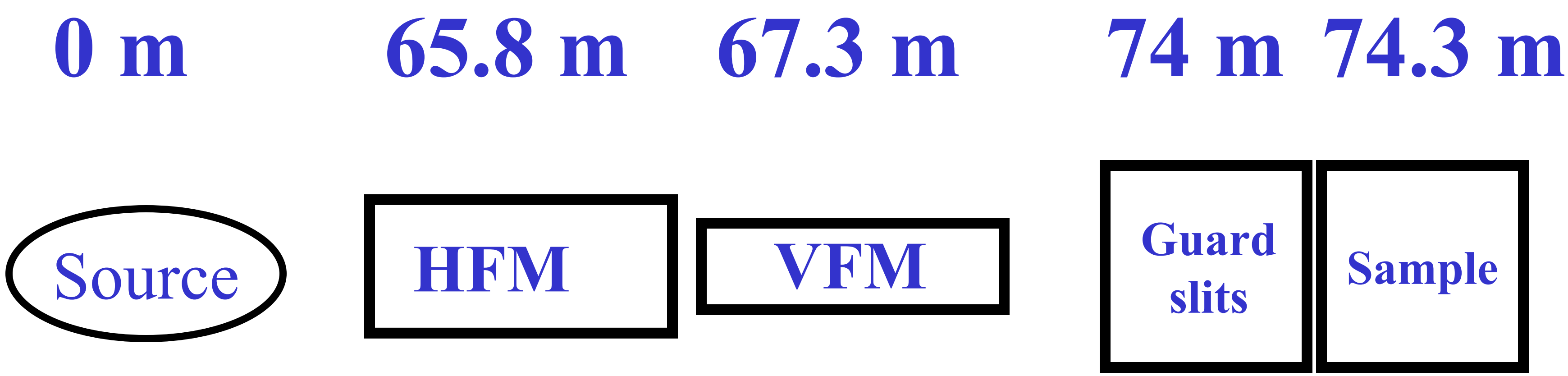
Data in
SEMILOGARITHMIC
scale!



Intensity Gain: 40 x
Elliptical bending
slope error rms ~ 1 µrad rms
Checked ´a-posteriori´ with LTP

OPTICAL GEOMETRY OF GM/CA IDin BL

(Beamline dedicated to protein crystallography)

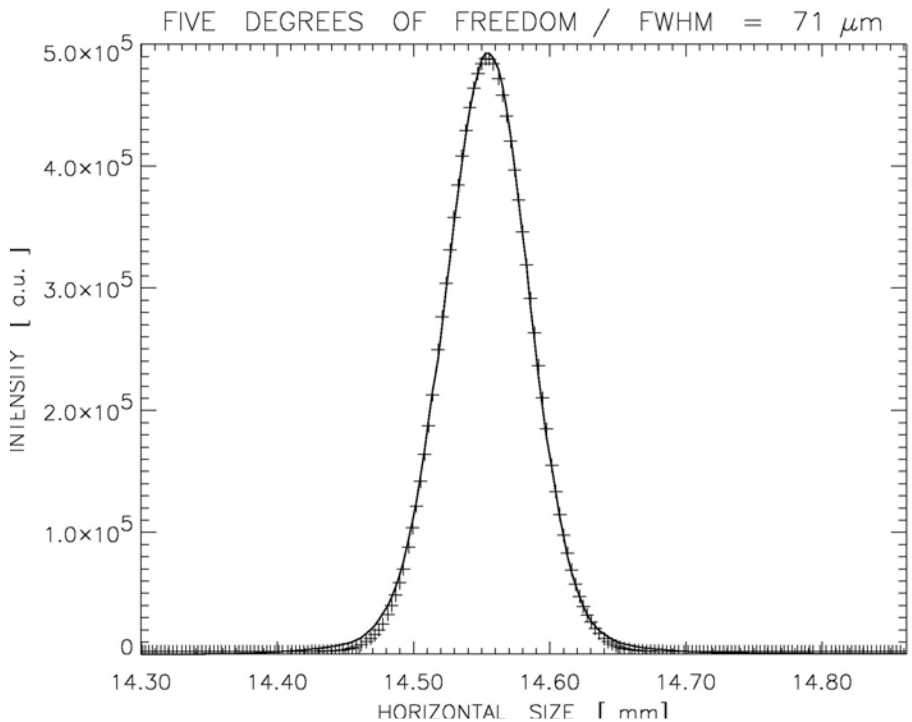


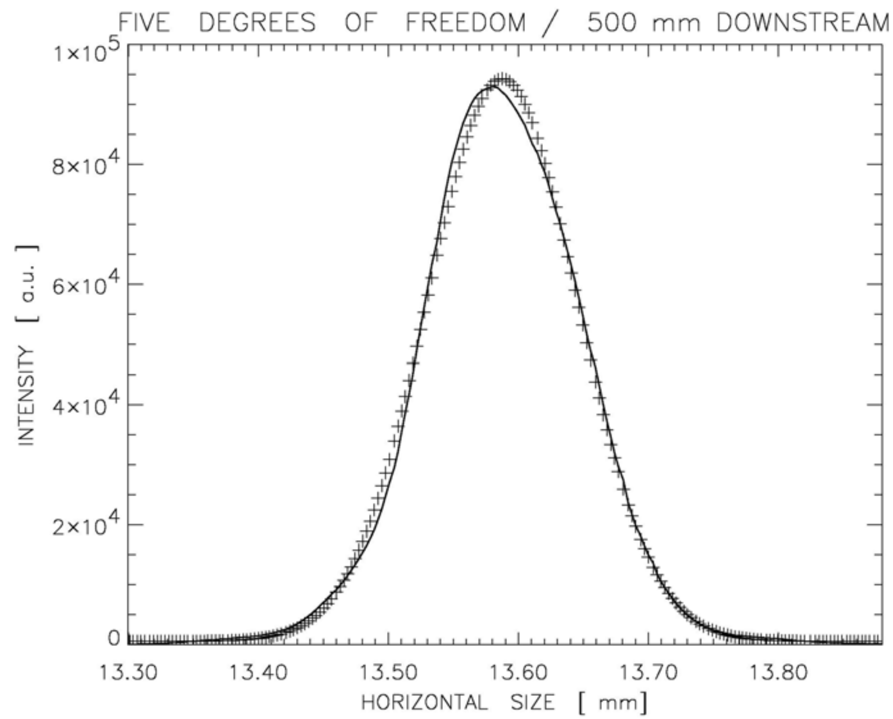
HFM → 1050 mm long (1000 mm useful)

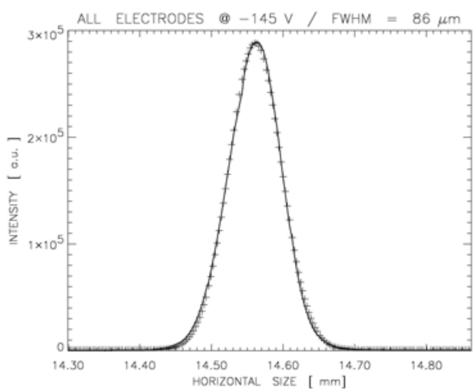
→ 14 Electrodes → 14 Degrees of freedom !

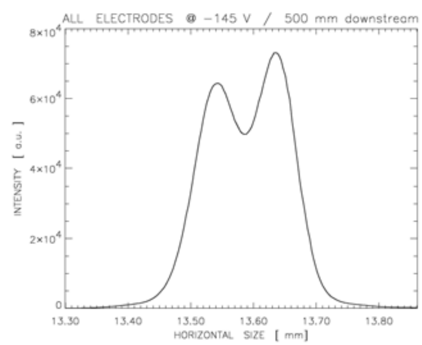
VFM → 600 mm long (550 mm useful)

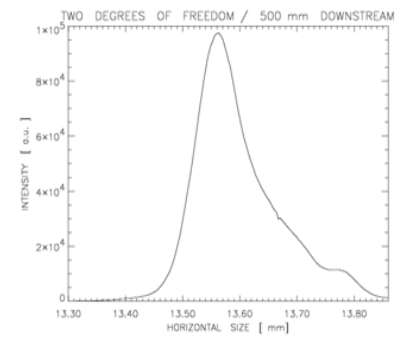
→ 16 Electrodes → 16 Degrees of freedom !









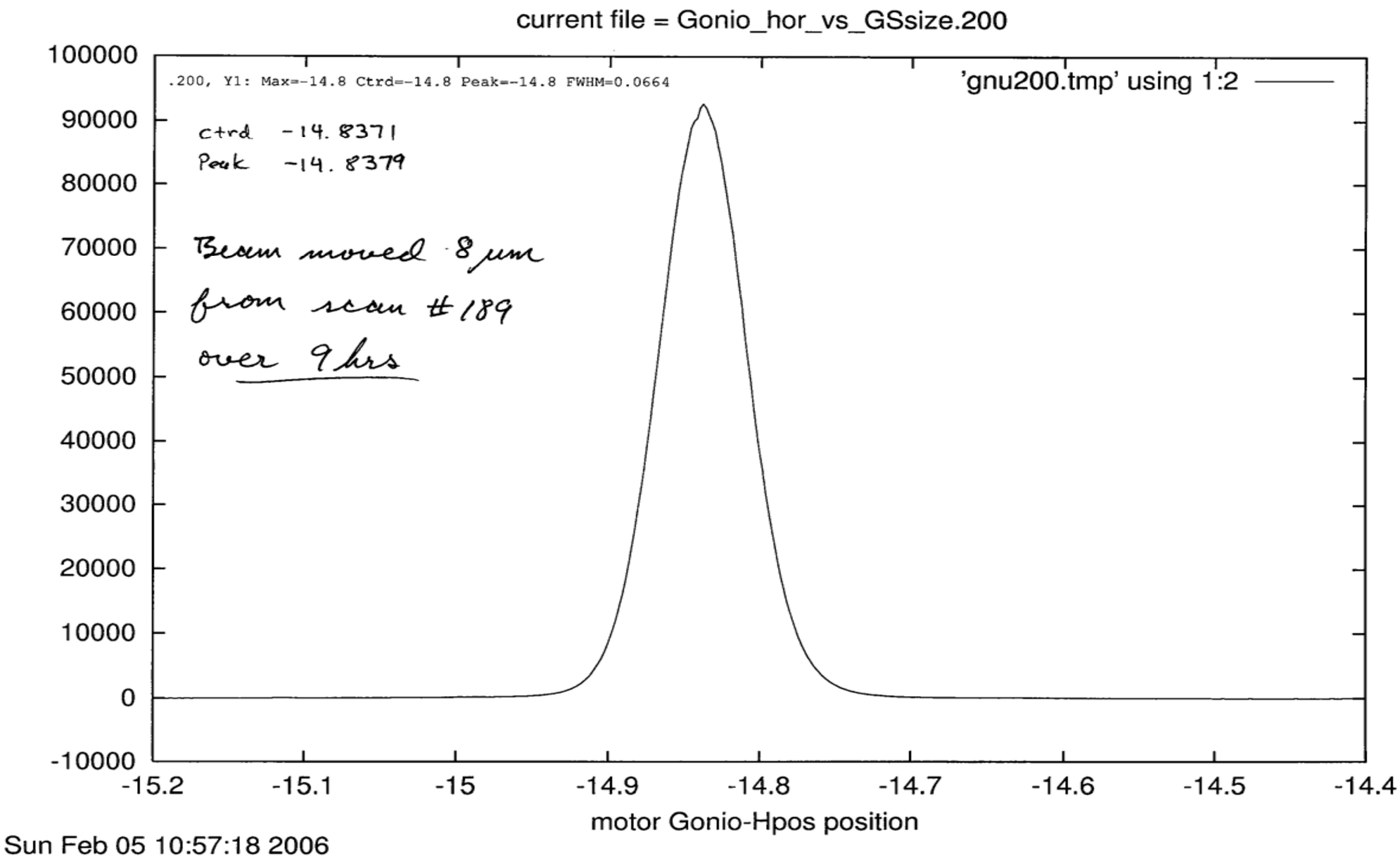


…and still **9** degrees of freedom available

Data taken @ GM/CA CAT – UNPUBLISHED RESULTS

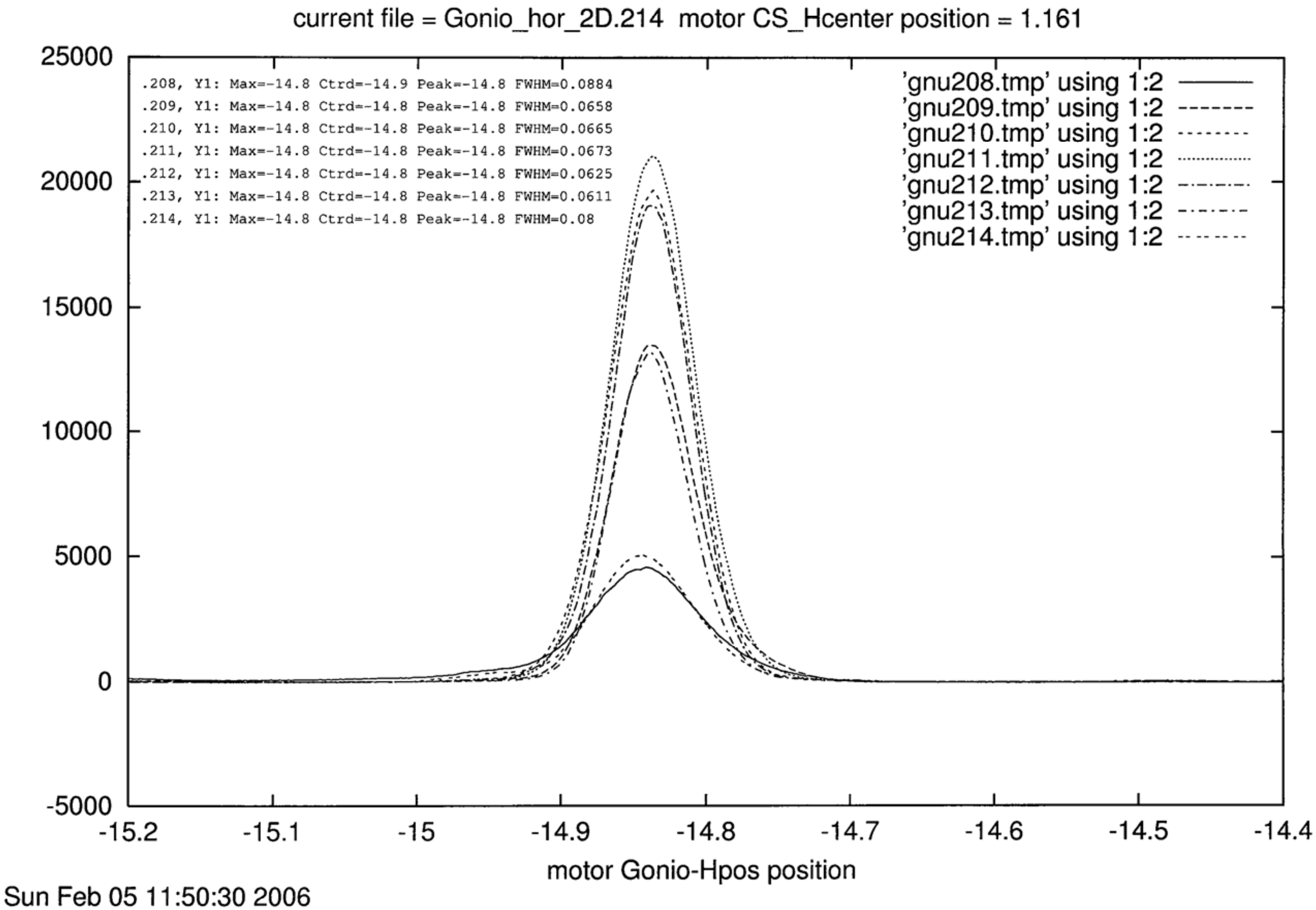
HFM - At focus

Focusing Distance = 8.5 m



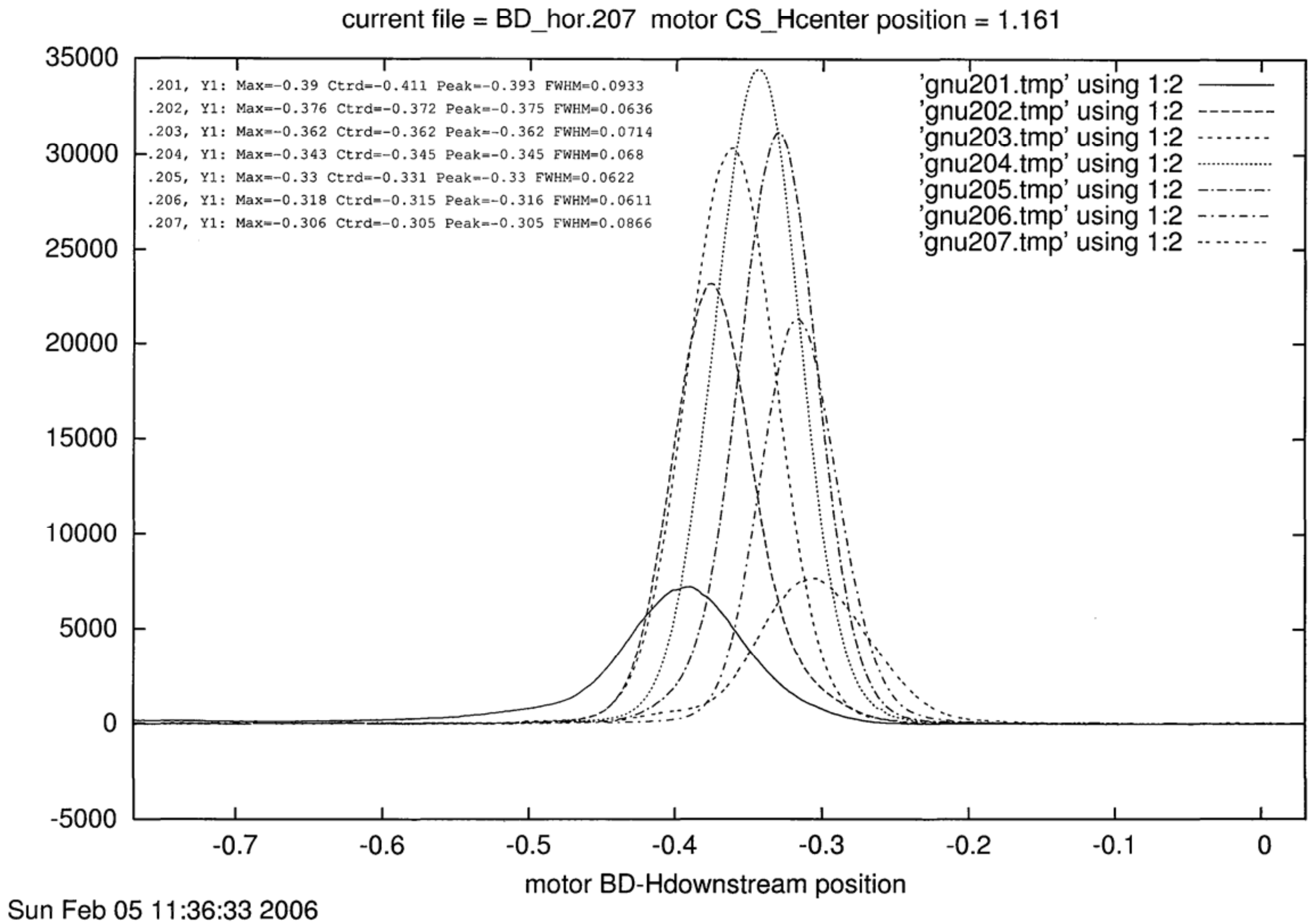
Data courtesy of GM/CA CAT – UNPUBLISHED RESULTS

HFM - At focus



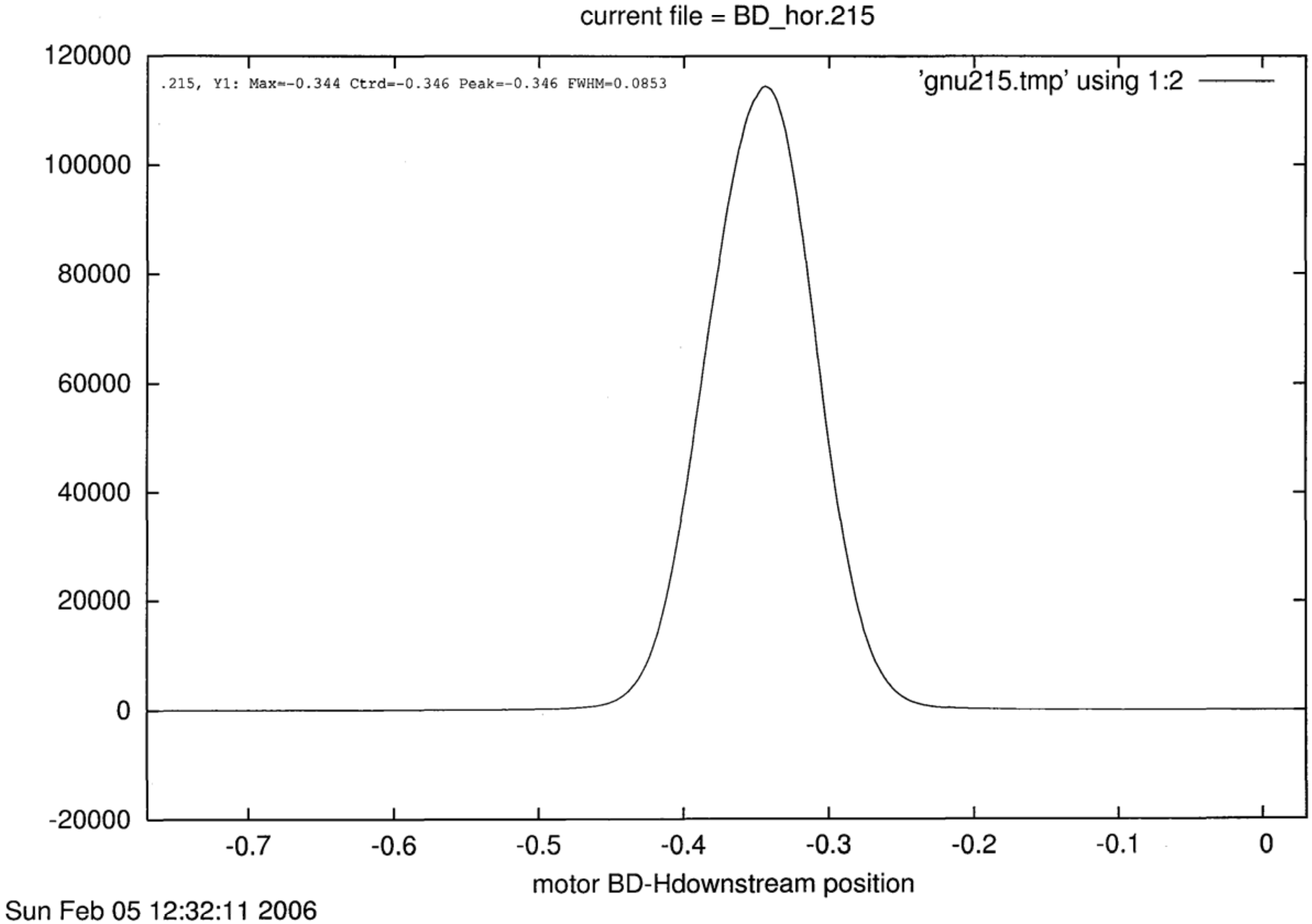
Data courtesy of GM/CA CAT – UNPUBLISHED RESULTS

HFM - Out of focus – 350 mm upstream



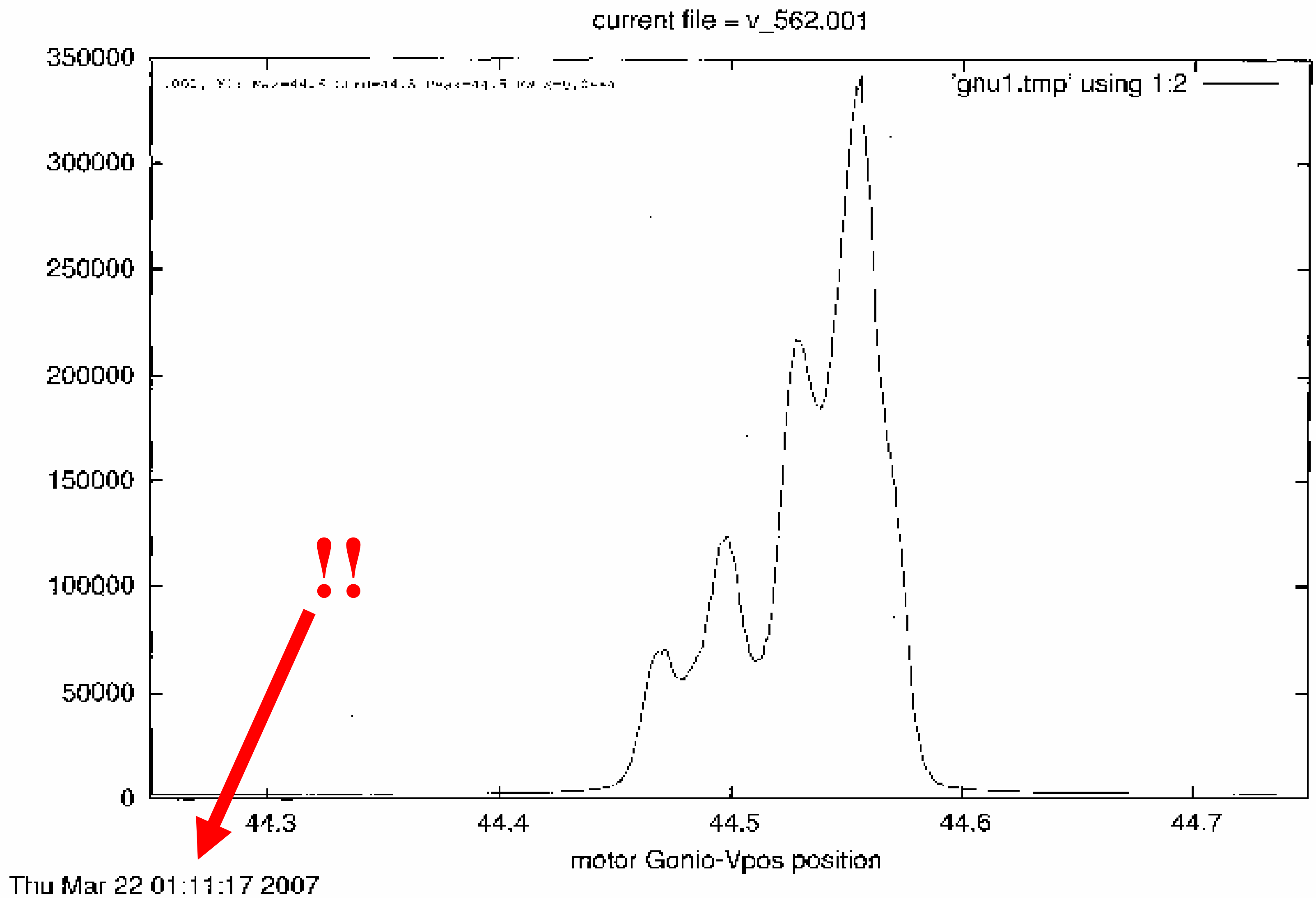
Data courtesy of GM/CA CAT – UNPUBLISHED RESULTS

HFM - Out of focus – 350 mm upstream

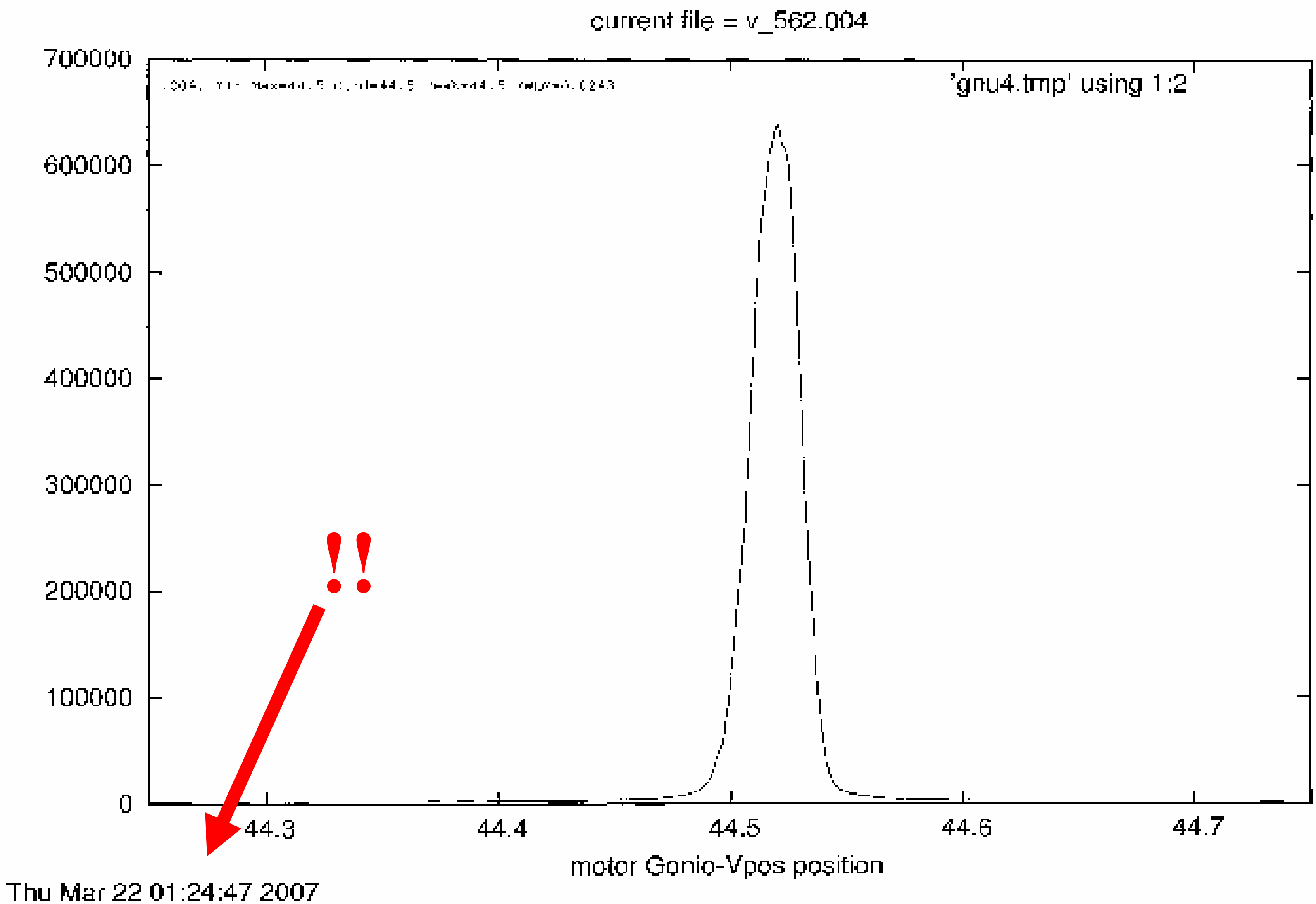


Data courtesy of GM/CA CAT – UNPUBLISHED RESULTS

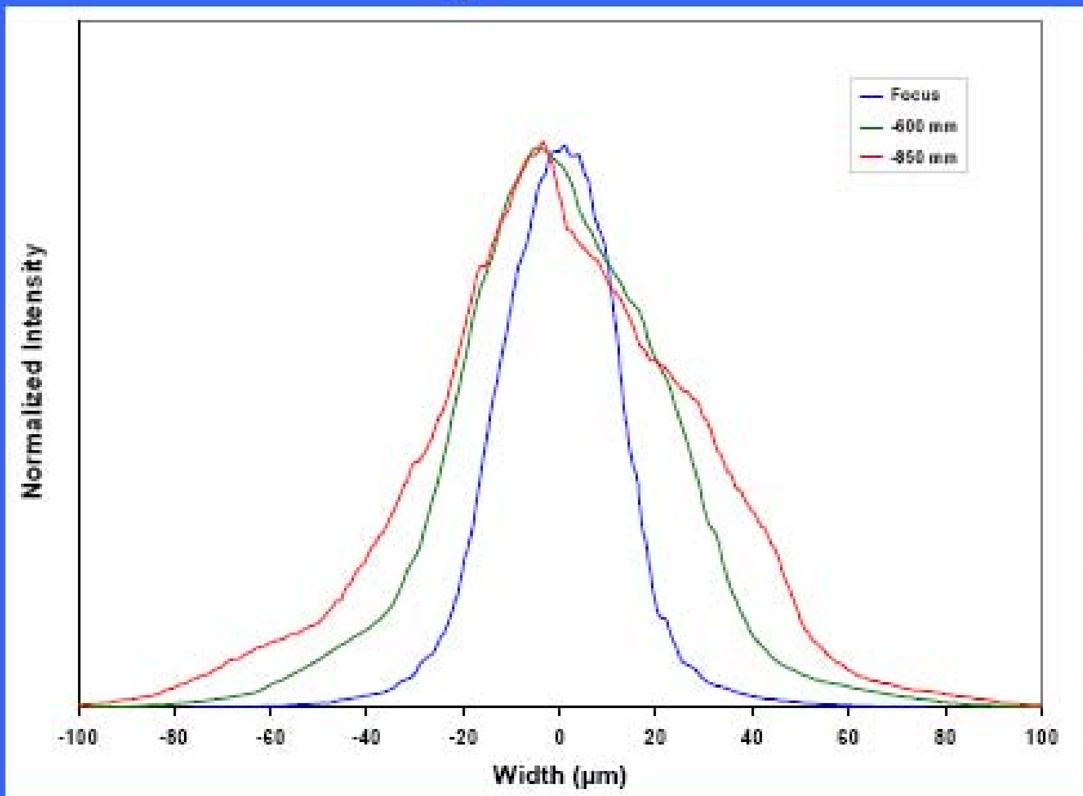
VFM - Automated Focusing - Starting Point



VFM - Automated Focusing - **One Shot**



Vertical beam profiles over 850 mm range



Position	Distance (mm)	Beam Profile FWHM (µm)
Focus	600	30
Sample	0	48
Slits	-250	53

To shift the beam focal position:

- Using automated focusing tools for a new position → 3 – 4 hours
- Using a lookup table for a previously determined position → minutes

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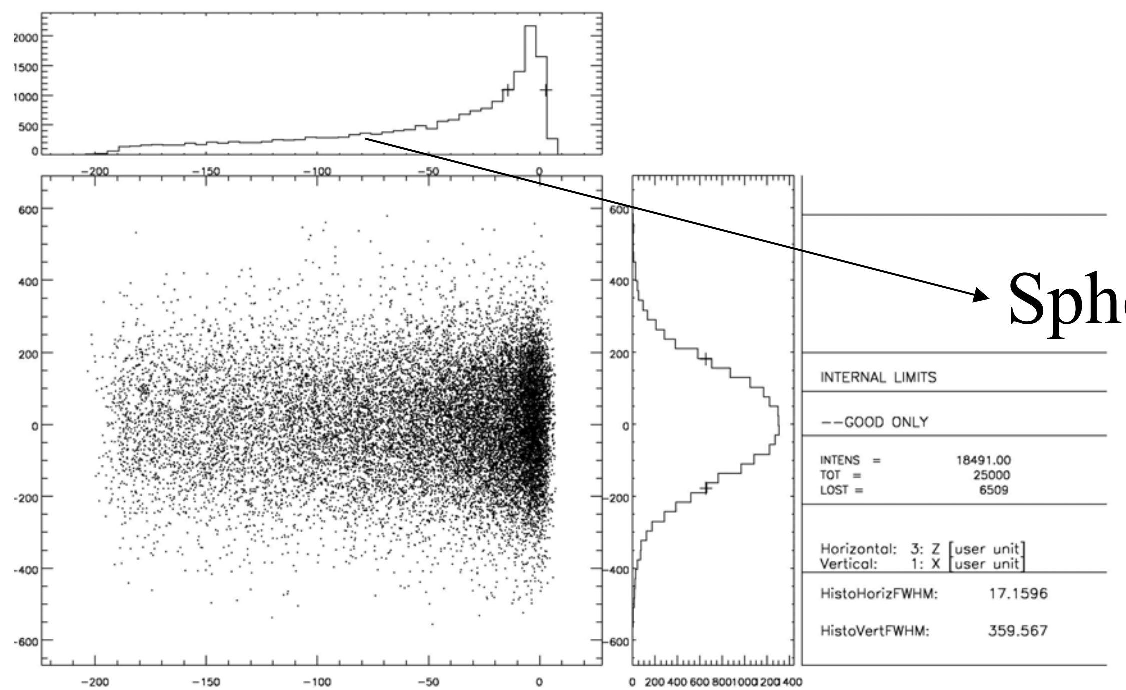
SUPER-bent Mirror / APS Sector 3

Focusing geometry	p = 33 m; **q = 0.57 m** → demagnification **58:1**
Incident angle	2.2 mrad
Coating	2/3 (24 mm) Pd , 500 Å thick , 1/3 (12 mm) Pt 500 Å

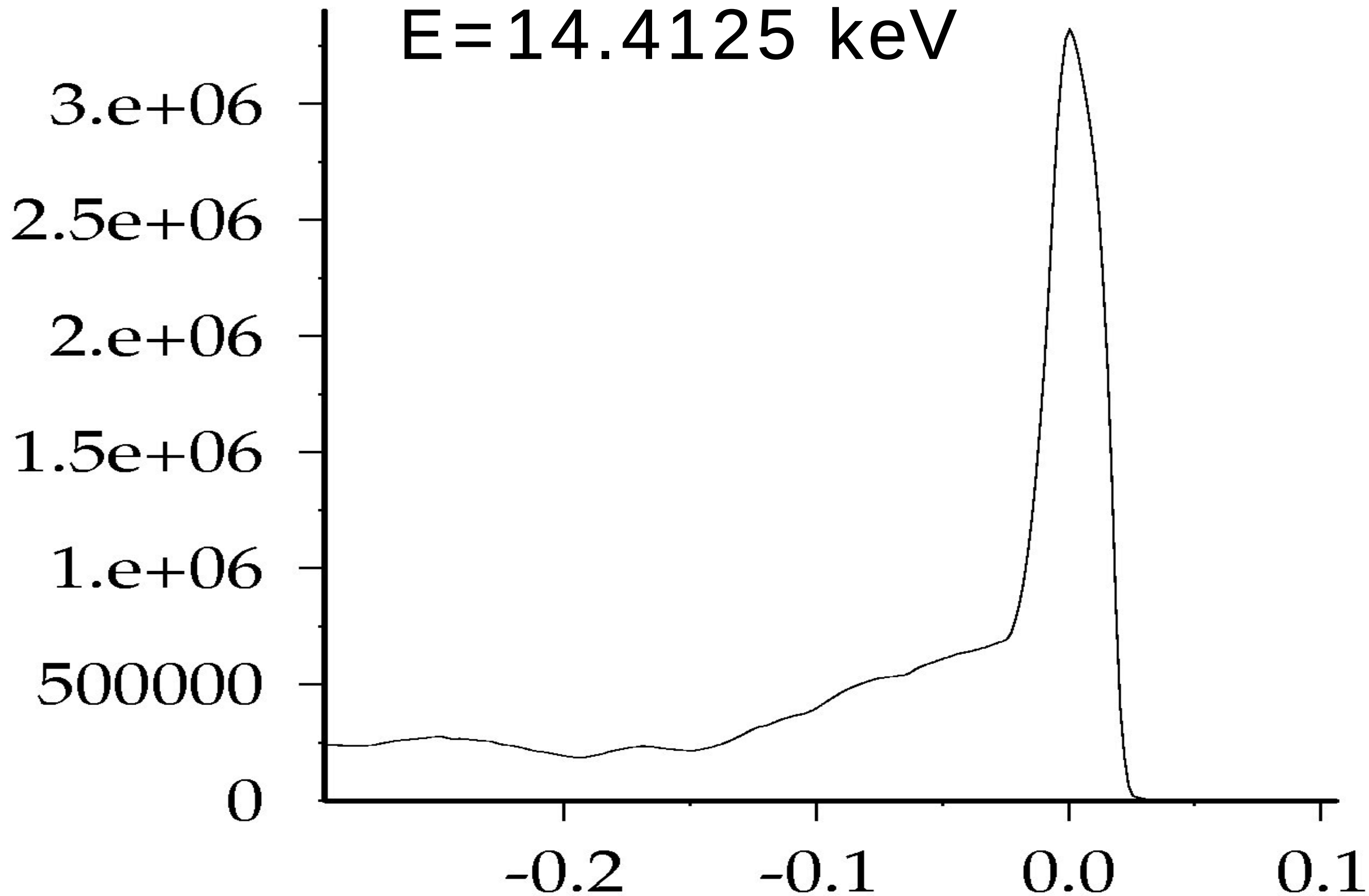
Mirror length: **600 mm** / HFM / **16 Electrodes**

0V = 250 m; -2000V = 135 m; +1700 V = 1000 m

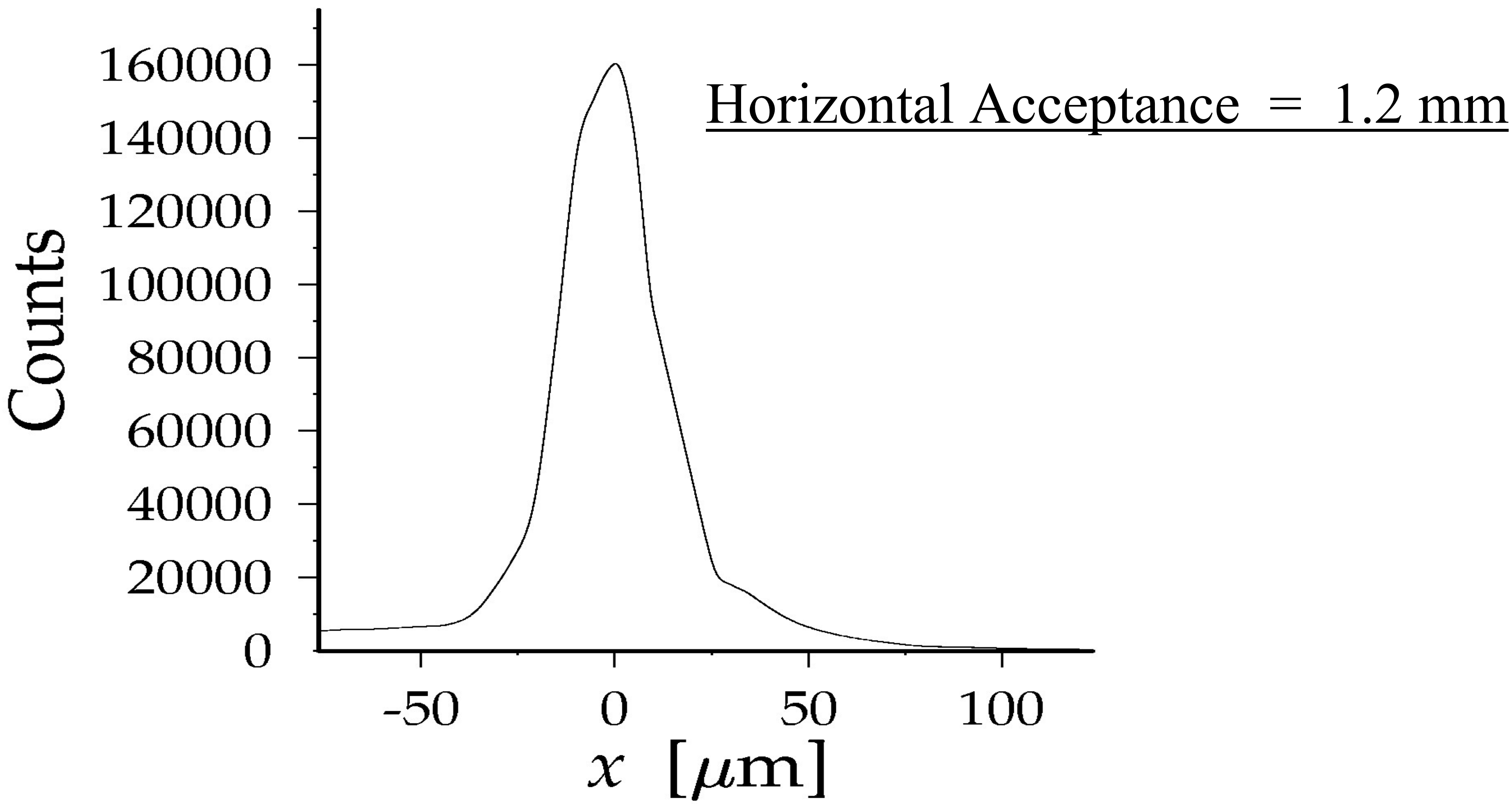


Spherical Aberration

~ 200 µm



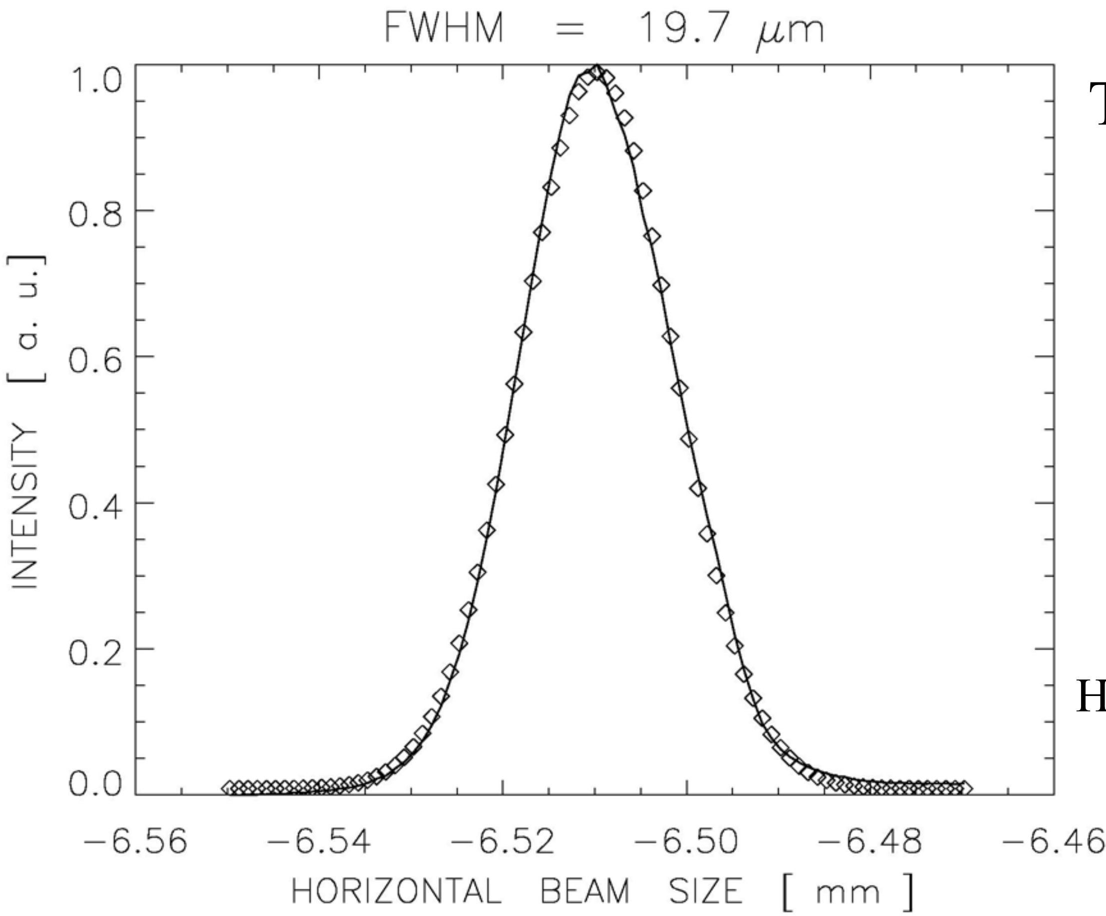
Best focus with all electrodes at same voltage +100 V



Best focus with visual optimization on a YAG

Voltages: 1430 1430 1140 1010 830 630 130 -360

E=14.4125 keV



Theoretical Reflectivity
95.7 %

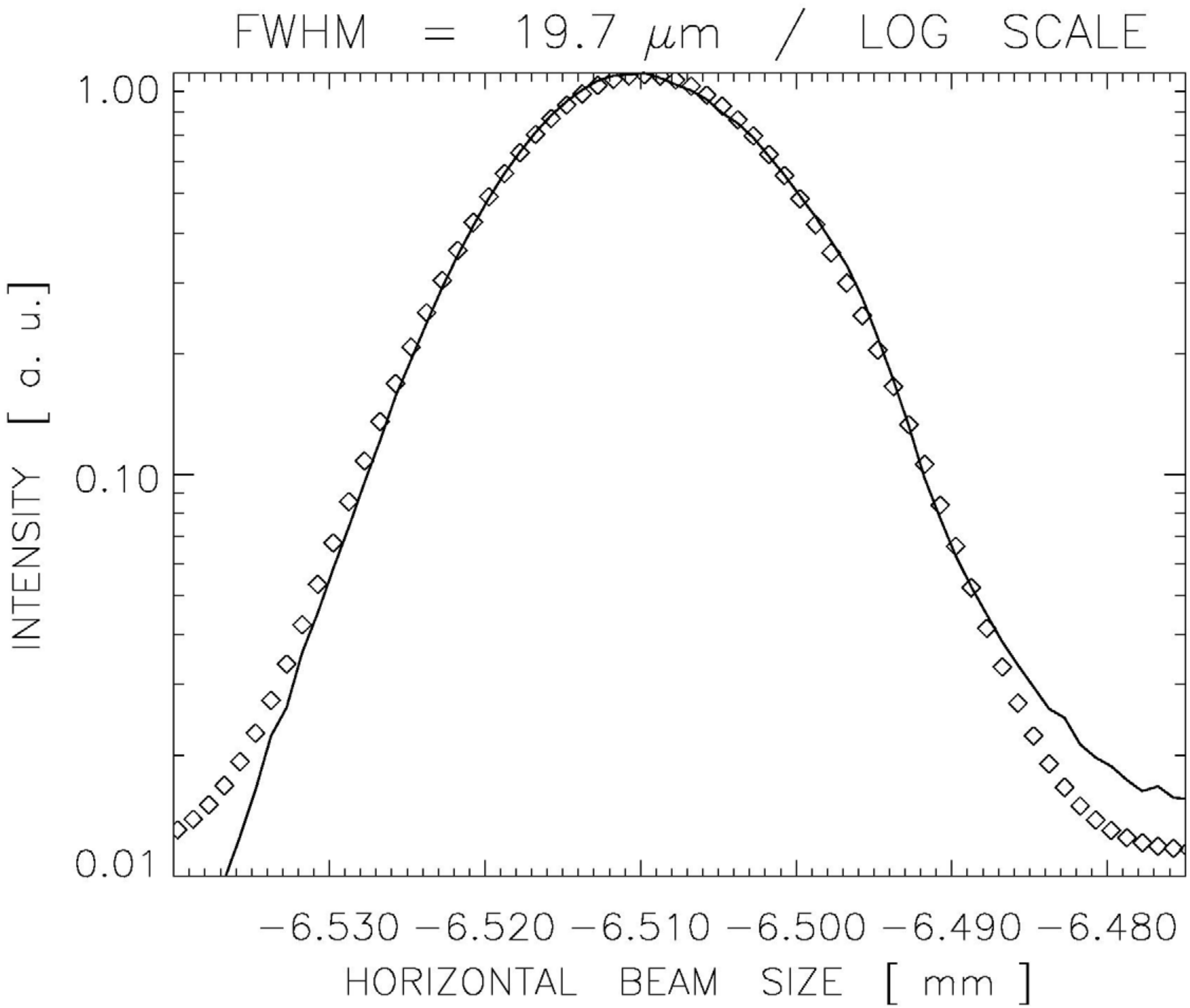
Measured Reflectivity
94 %

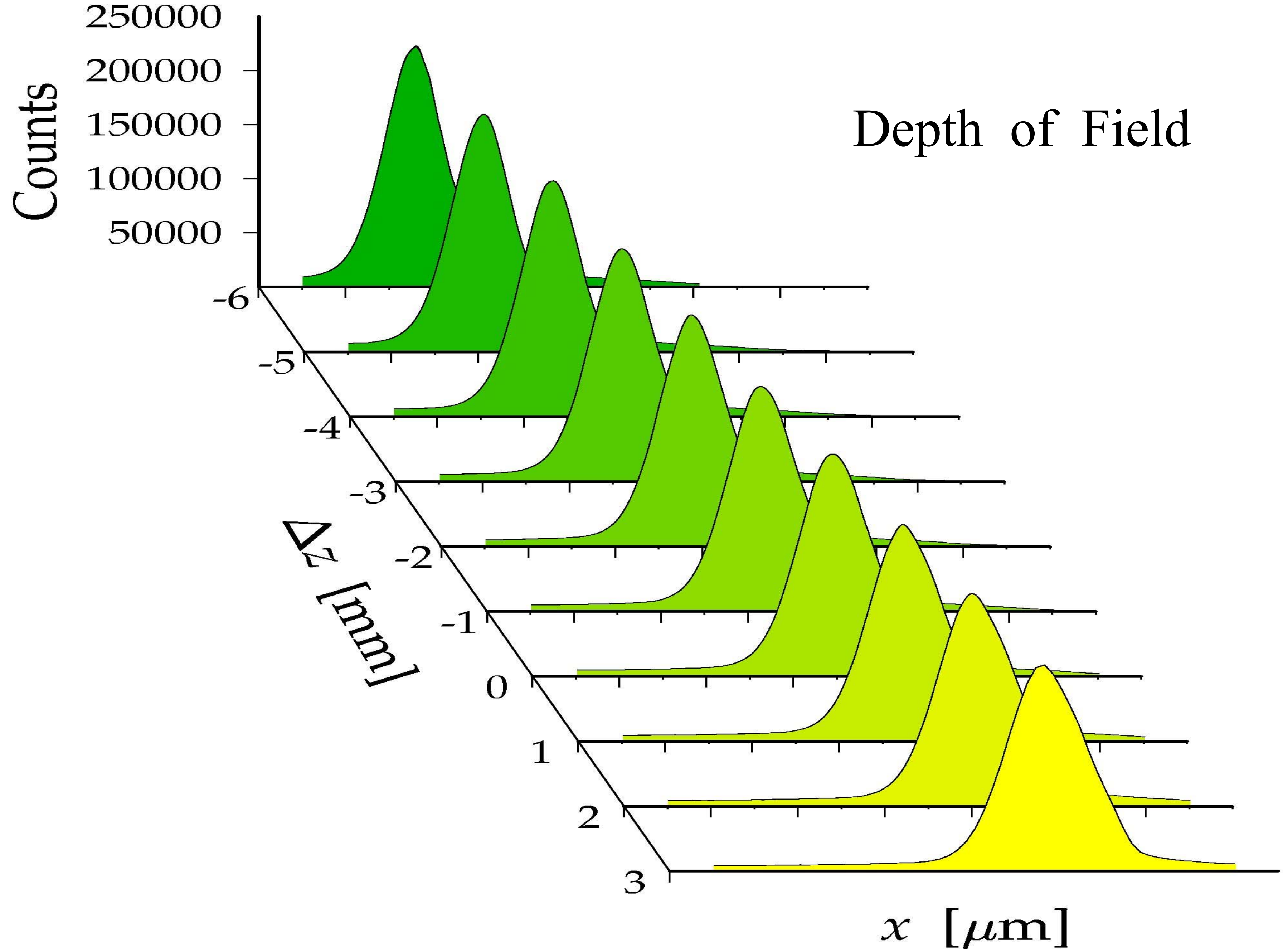
I_{REFL} / I_0

Horizontal Acceptance = 1.2 mm

Best focus with **FOCUSING SOFTWARE TOOL**

Voltages:	1351.3	1510.8	1010.8	1003.5	899.9	400	-100	-108.5
´manual´:	1430	1430	1140	1010	830	630	130	-360

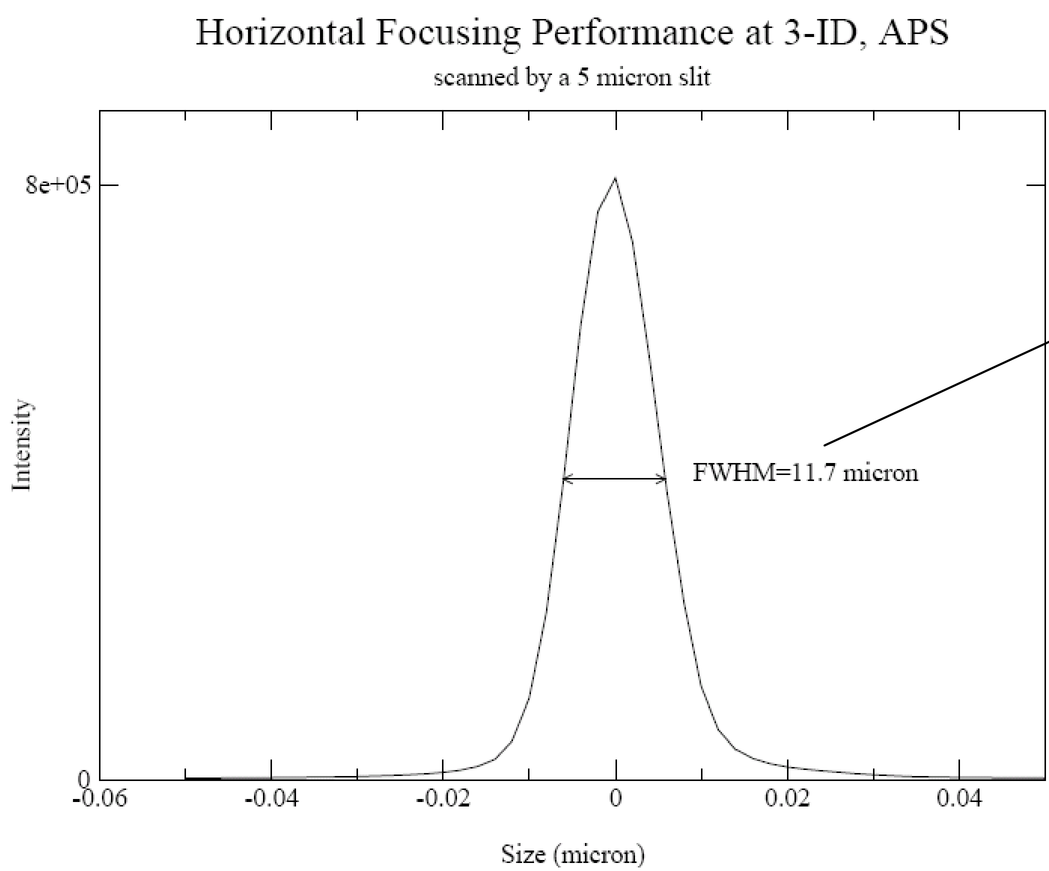

FWHM = 19.7 μm / LOG SCALE
1.00
0.10
0.01
INTENSITY [a. u.]
−6.530 −6.520 −6.510 −6.500 −6.490 −6.480
HORIZONTAL BEAM SIZE [mm]



Depth of Field
Counts
250000
200000
150000
100000
50000
Δz [mm]
-6
-5
-4
-3
-2
-1
0
1
2
3
x [μm]

… after upgrade to full 16 HVBPS channels:

Focusing geometry	p = 33 m; **q = 0.53 m** → demagnification **62:1**
Incident angle	2.8 mrad
Horizontal acceptance	1.6 mm



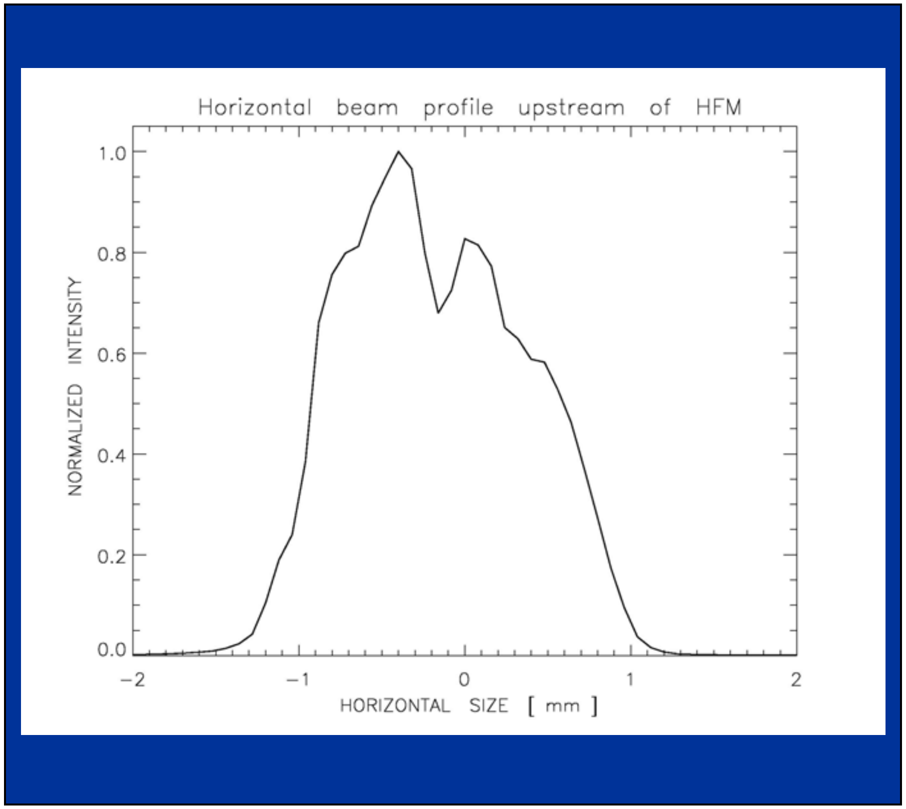
~10 µm FWHM
After scanning slits size deconvolution

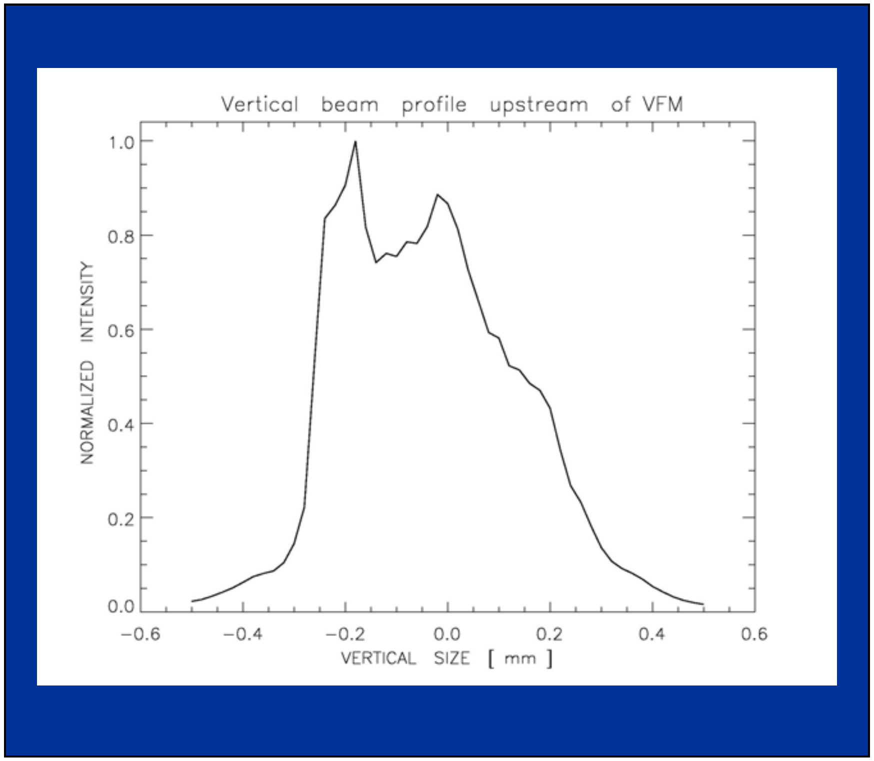
Gain: ~Factor of 2 in spot size

Voltages: 1492.3/1301.3 817.5/707.8 1109.4/619.2 509.1/628.4 353.5/327.3 63.6/-118.7 -530.6/-820.1 -1320/-1697

1351.3 1510.8 1010.8 1003.5 899.9 400 -100 -108.5

BEAM PROFILES Upstream of KB´s





Sometimes beam can be ´Ugly´

THE PRESENT ...

1) Make sure that the beam is ´clean and stable´
2) Make sure that the beam is ´clean and stable´
3) Make sure that the beam is ´clean and stable´
4) If it vibrates... Quantify it!
5) If you can stabilize it... Do it!

→ BEAM DIAGNOSTICS is KEY !!

The new HVBPS system is built following an *´integrated approach´* incorporating:

- Fast 4-channels low noise picoammeter
- ´On-line´ BPM readout with statistics calculation
- ´Real –time´ FFT available
- Triple PID/feedback available (hor., vert. & intensity)
- Remote support available via WEB-based GUI

THE FUTURE ...

1. Use a ´Condenser + Corrector´ approach ?
2. Deterministic superpolishing ?
3. nm-level surface control capability ?
4. Denser electrodes ?
5. Simple wavefront measurement tools available to ´non-optician´ BI scientist ?
6. In-situ feedback ?

→ Can adaptive optics be...

SIMPLE??

AdaptoGyzmotron needed?

...To be continued at the Rocca Bernarda castle Round Table !!

Automated Focusing at GM/CA-CAT

Bob Fischetti
Associate Director, GM/CA-CAT,
Biosciences Division,
Argonne National Laboratory

ACTOP 2008

Trieste, Italy

October 9, 2008

Design Parameters for the ID lines

- **Energy range** — **3.5 – 35 keV**
- **Energy resolution** — **ΔE/E < 0.02%**
- **Harmonic rejection** — **< 0.01% at all energies**
- **Intensity** — **>1 x 10^{13} photons/sec/0.1%BW**
- **Energy scan rate** — **0.3°/sec, 350 – 3500 eV/sec**
- **Focal size** — ~~**50 x 200 µm**~~ → ~~25 x 60 µm~~ → 5 x 5 µm
- **Goniometry sphere-of-confusion** — ~~**10 µm**~~ → 0.5 µm

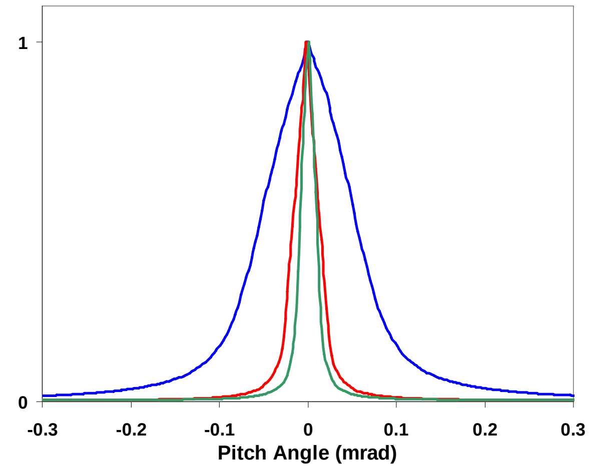
- **High degree of beam intensity and positional stability**
- **Appropriate beam convergence/divergence angles for protein crystals**
- **200 mA beam current**

Delivering a stable beam monochromatic beam

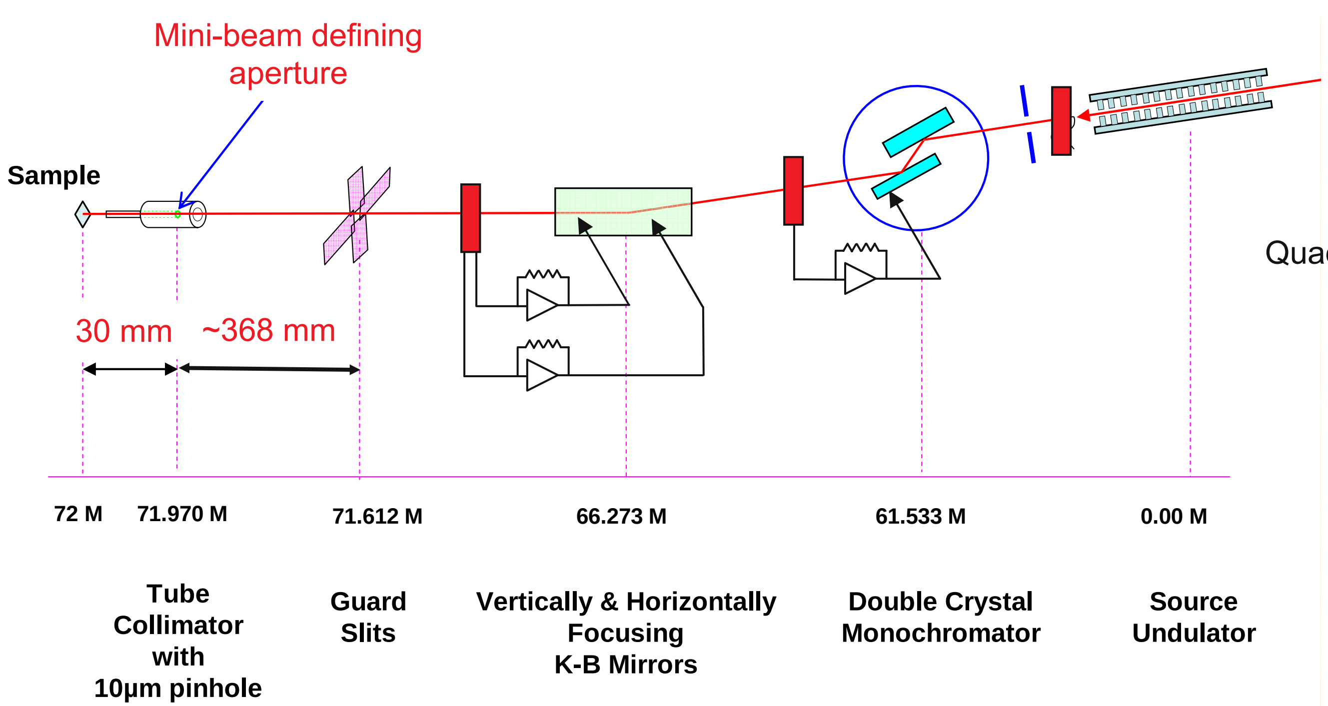
- Independent supports of vacuum and optical structures

- Double Crystal Monochromator stabilization
  - Vibration characterization and dampening
  - Both crystals cryogenically cooled to avoid dispersion
  - Compton scatter shields around 1st and 2nd crystals
  - Thermal stabilization of DCM mechanics
  - No detuning of 1st and 2nd crystals vs. energy
  - Beam position stable to +/- 5 µm over the range 4 – 20 keV

- Beam Position monitors after each optical component
  - Intensity feedback
  - Positional feedback



Beam Position Monitors – after each optical component

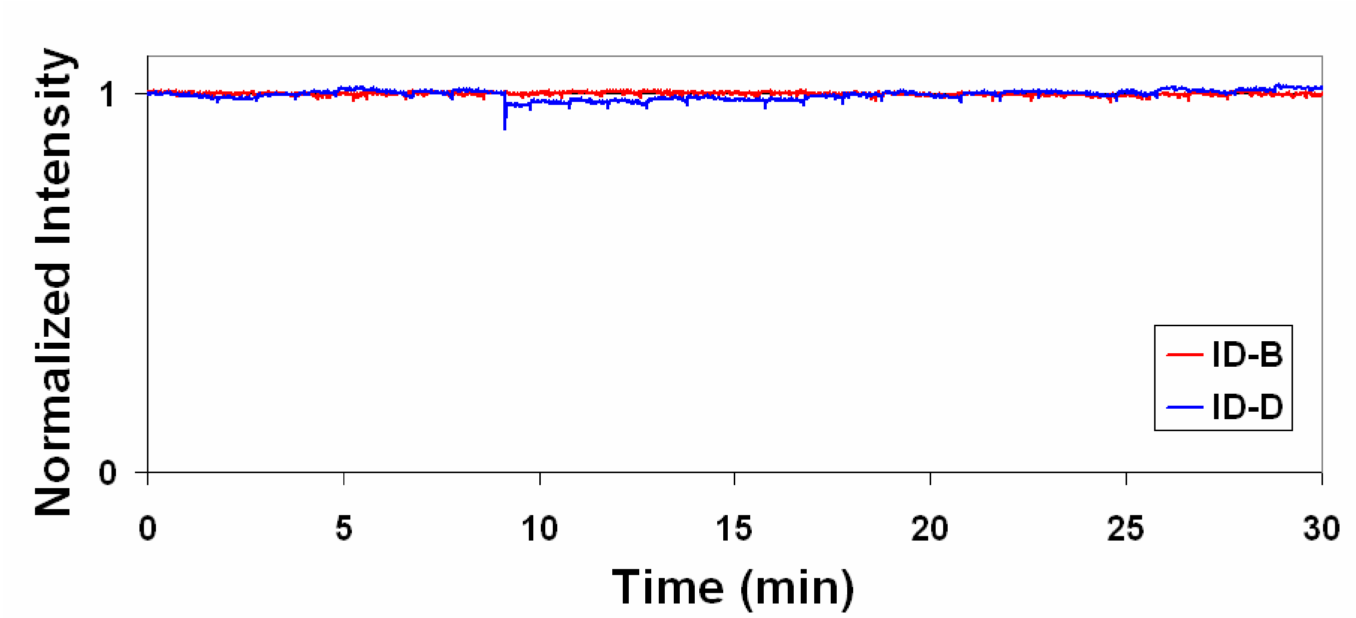


Beam position monitor: R.W. Alkire, G. Rosenbaum, G. Evans *J. Synchrotron Rad*. (2000) **7**, 61-68

Real time image of beam: Xu, S., Fischetti, R.F**.**, Benn, R., Corcoran, S., (2007) Synchrotron Radiation Instrumentation, J.-Y. Choi, S. Rah, eds., American Inst. of Phys. 1403-1406.)

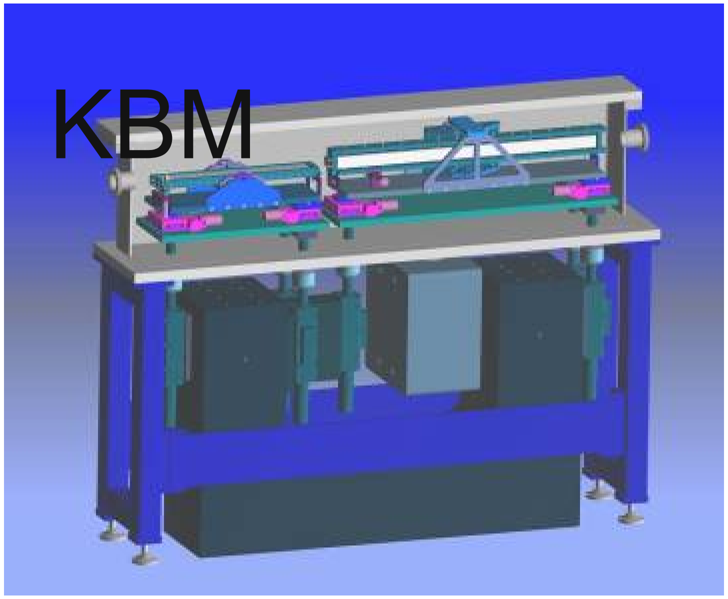
Beamline Stability is Very Good!

Normalized beam intensity through a 10 μm slit



- 1-2% RMS intensity fluctuation at low heat load (time scales up to ½ hour)
- Better crystallographic data are collected *without* intensity feedback
- Positional stability has not been quantitatively measured, although some conclusions can be drawn from the intensity numbers
  – 2% intensity fluctuation → 3 μm beam motion

Compact K-B "bimorph" mirrors

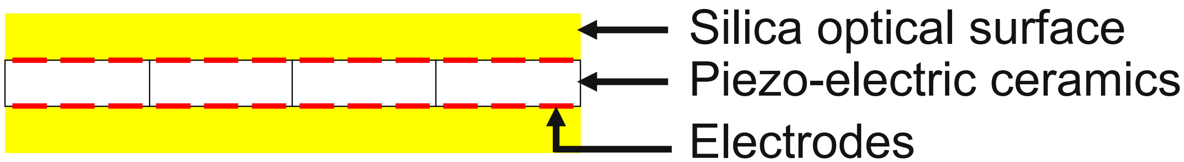


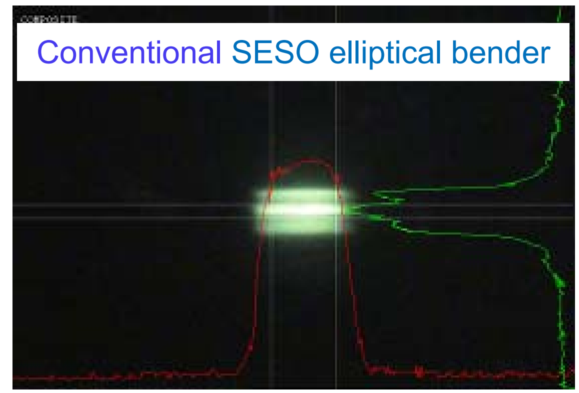
Why use bimorphs mirrors

- In situ adjustment of slope error
- Not just small beam
- Uniform profile "off-focus"

Uniform electrode voltages – sets curvature

Differential electrode voltages – correct slope error

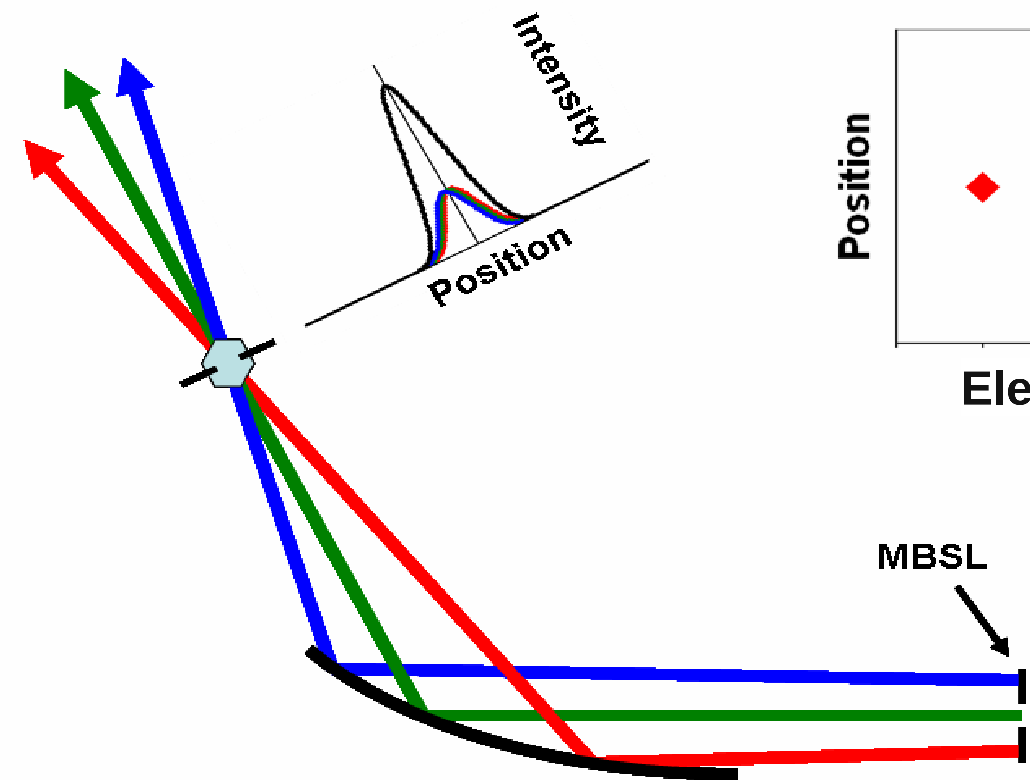


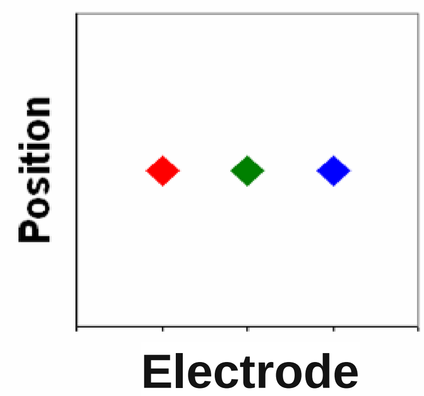


	Length (mm)	# of segments	Electrodes / segment	Total Electrodes	Demag
HFM	1050	7	2	14	6:1 – 10:1
VFM	600	4	4	16	7:1 – 12.5:1

Focusing Technique

- Focusing in almost completely automated via deterministic matrix inversion
- Time to collect data for new matrix and focus using slit scans about 3 hours
- Can refocus using look up table or matrix
- BPM would take about 1 hr to collect matrix and focus



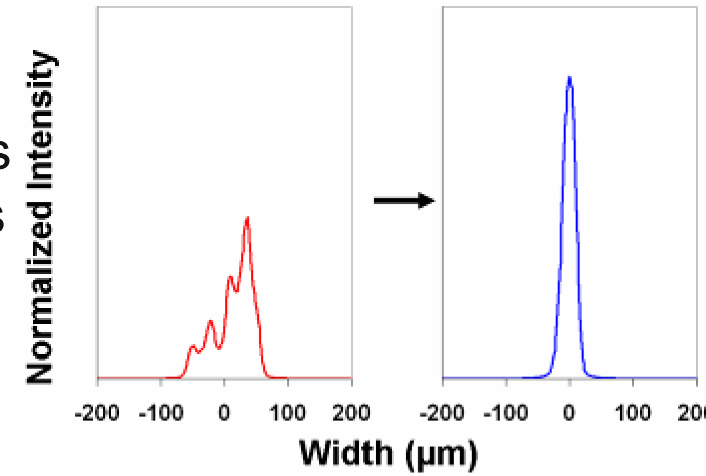


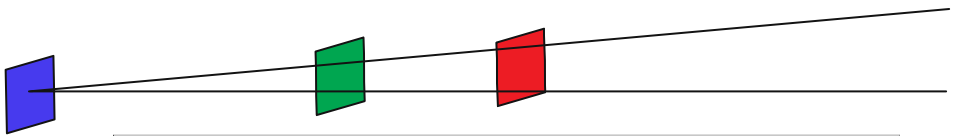
- Beamlets converge at one location
- Beamlets are of equal width
- BPM detects all at the same location
- Focal slit scan shows that beamlets originating from different electrodes overlap at the focal position

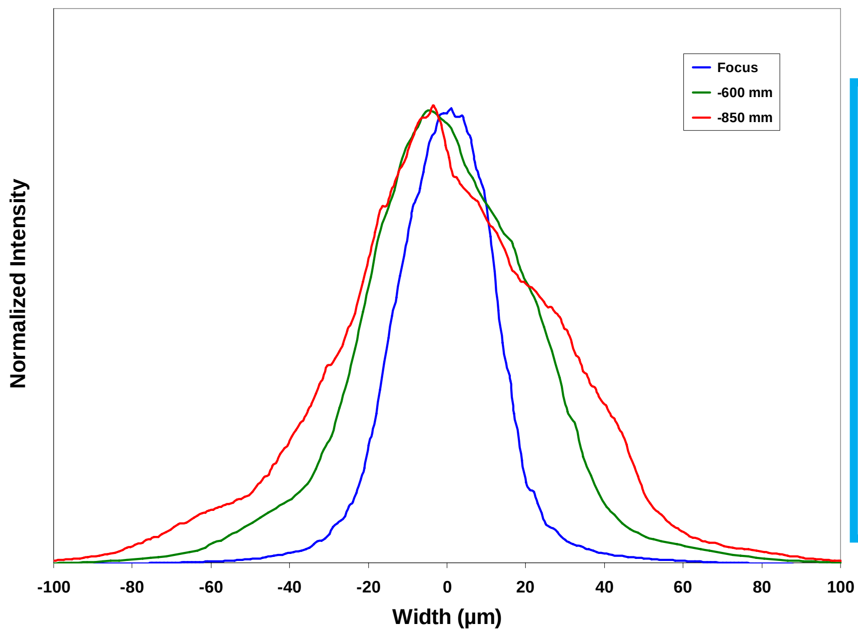
Automated focusing and beam profile homogeneity

To shift the beam focal position:

- Generate new interaction matrix → 3 – 4 hours
- Use existing interaction matrix → 15 minutes
- Load voltages from lookup table → 2 minutes



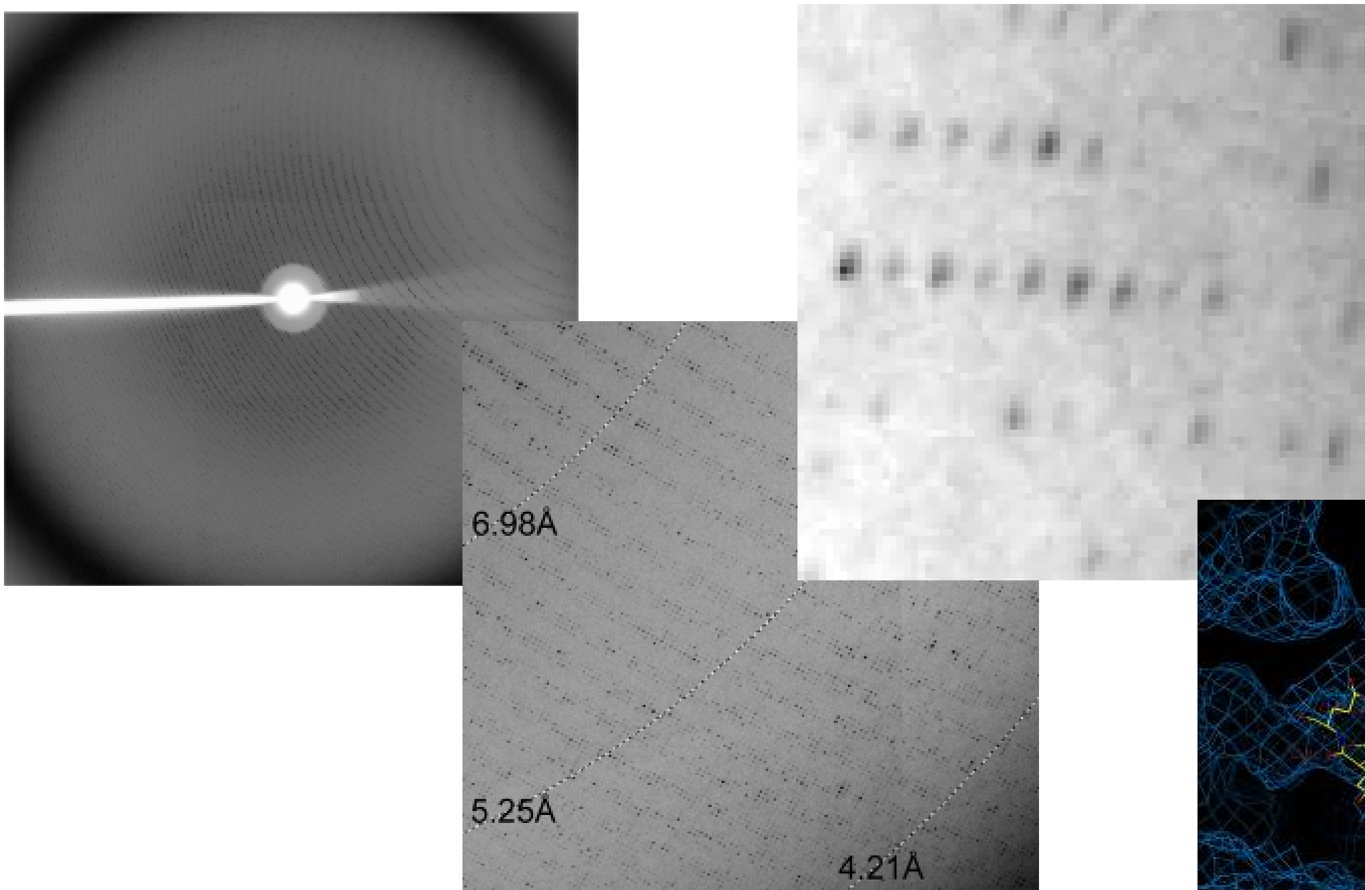


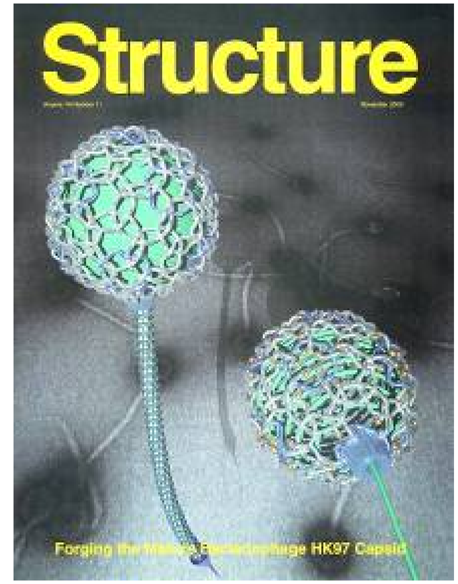


Position	Distance (mm)	Beam Profile FWHM (μm)
Focus	600	30
Sample	0	48
Slits	-250	53

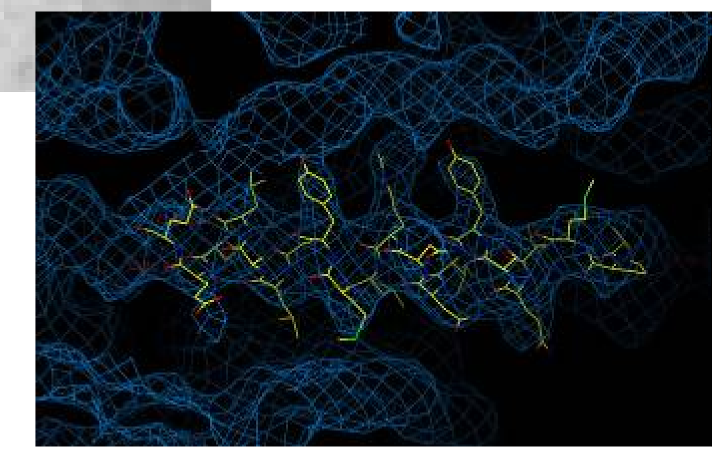
Full Beam Application - Large Unit Cells

Diffraction pattern from HK97 virus capsid.
Unit cell dimensions: 1010 x 1010 x 732 Å





4.2Å map of Head II side-chains



L. Gan, *et al*. & J. E. Johnson *Structure* 14, 1655-65 (2006)

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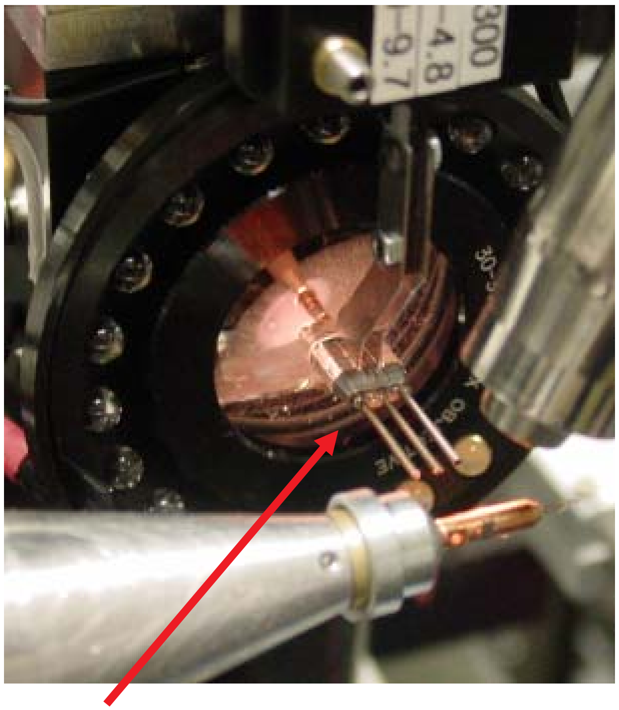
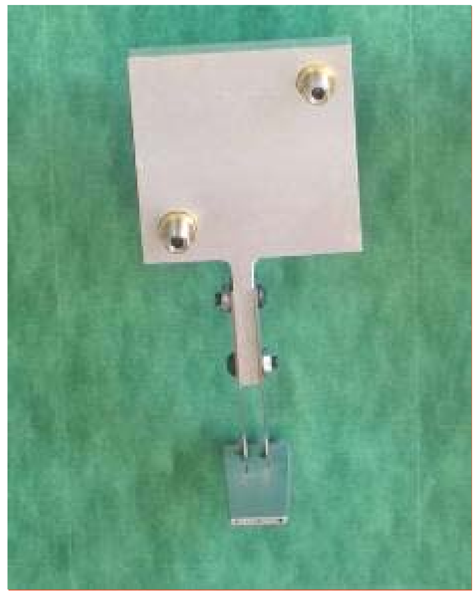
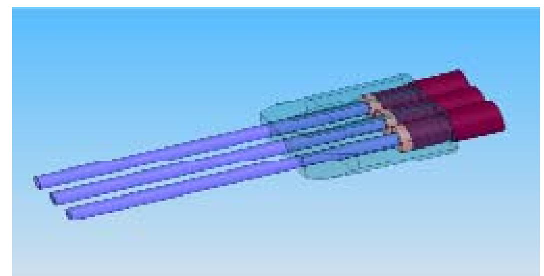
MAR 225, S-D distance 680 mm

Triple mini-beam collimator
5 and 10 micron mini-beam defining apertures, and
300 micron scatter guard aperture



Triple collimator





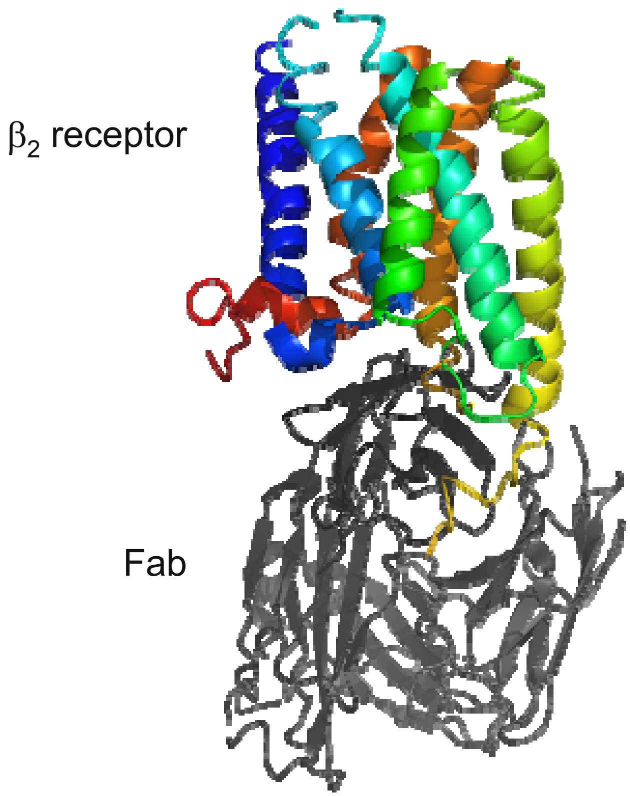
User selectable via BluIce buttons
Prealigned
Highly reproducible

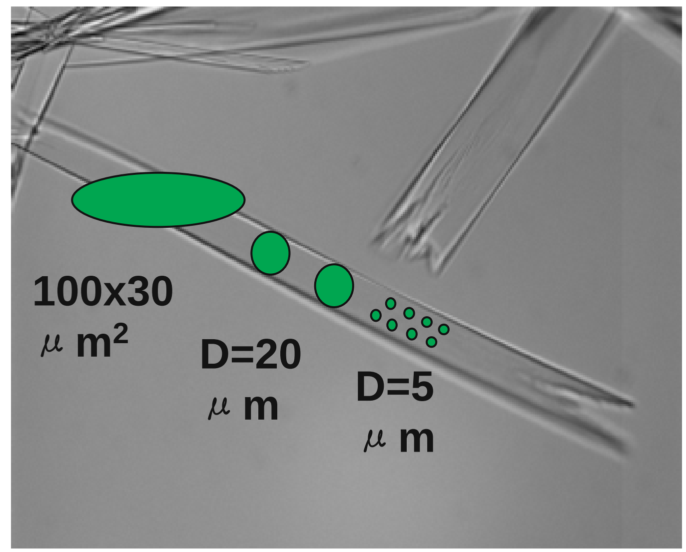
Fischetti *et. al.* submitted

Shenglan Xu

Mini-beam Application - Radiation Sensitivity

β2 adrenergic G-protein-coupled receptor at 3.4 Å resolution





Images courtesy Brian Kobilka and Bill Weis, Stanford University.

S. G. F. Rasmussen, H.-J. Choi, D. M. Rosenbaum, T. S. Kobilka, F. S. Thian, P. C. Edwards, M. Burghammer, V. R. P. Ratnala, R. Sanishvili, R. F. Fischetti, G. F. X. Schertler, W. I. Weis, B. K. Kobilka, "Crystal structure of the human β_2 adrenergic G-protein-coupled receptor", *Nature* **450**, 383-387 (2007).