Focusing near and far with Bimorphs Mirrors

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ACTOP 2011
April 4, 2011

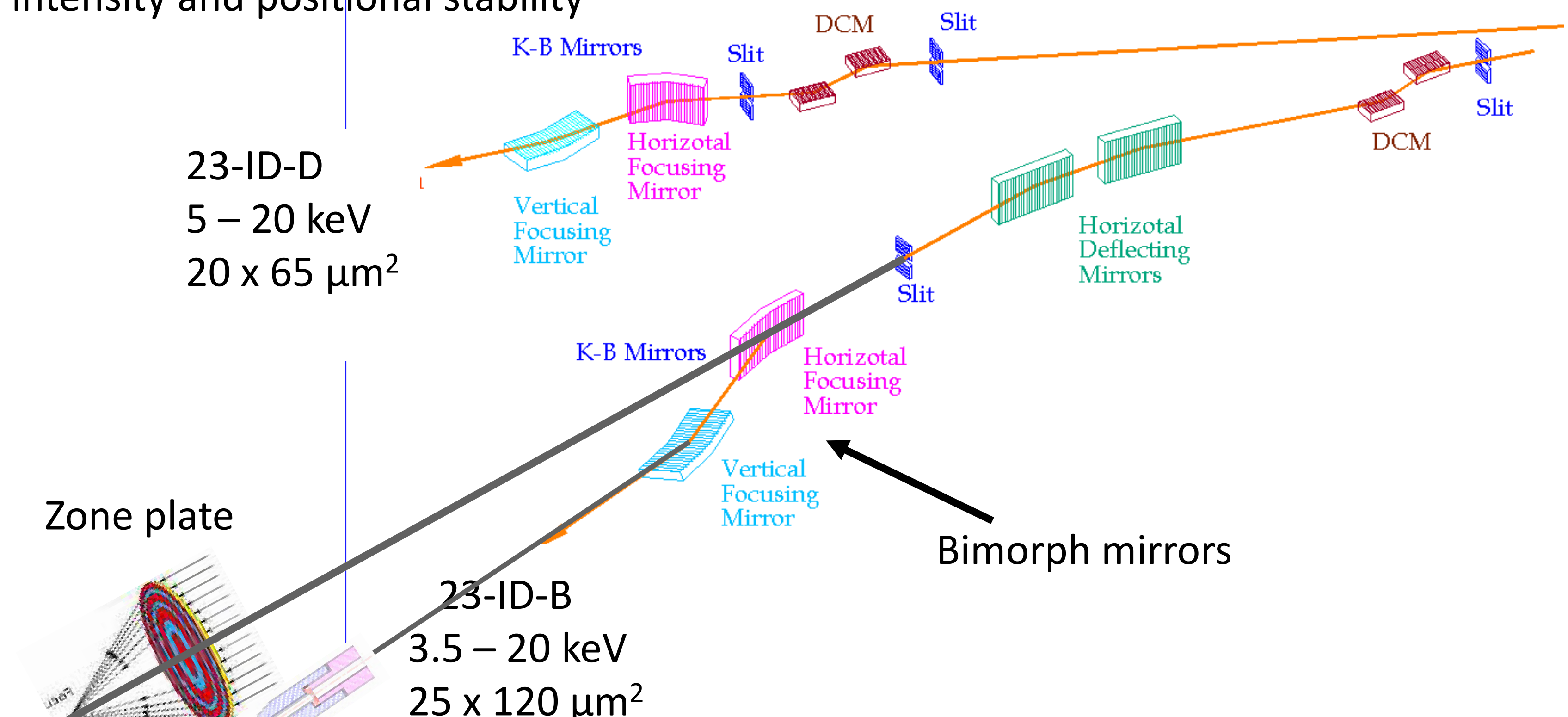
Outline

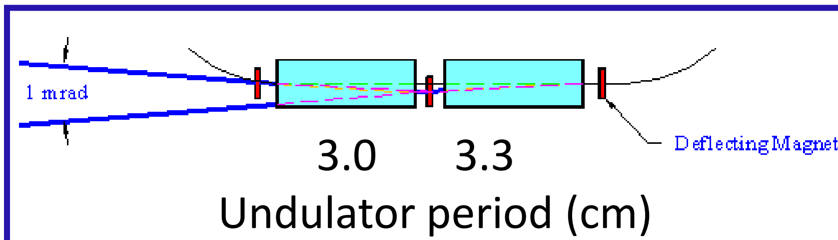
- Current microcrystallography capabilities
- 1-µm beam development for macromolecular crystallography
- In-situ, at wavelength metrology
- Far field beam profile
- Future plans

GM/CA-CAT dual canted undulator beamlines at the APS

Rapid energy tunability

High intensity and positional stability



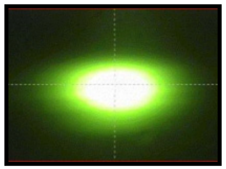
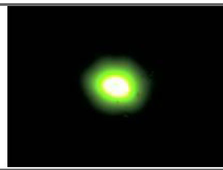
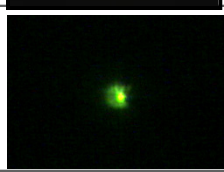


3.0 cm device optimized for Se MAD phasing

Large unit cells of biomolecules

→low convergence optics

Beam properties

Beam		Size at sample, FWHM (µm)	Intensity (Photons/sec)	Flux density (Photons/sec/µm²)	Convergence (µ-radians)
Full		25 x 120 20 x 65	1.0×10^{13} 2.0×10^{13}	3.3×10^{9} 1.5×10^{10}	176 x 95 305 x 172
20-µm		20 ∅	5.0×10^{11} 1.0×10^{12}	2.0×10^{9} 3.0×10^{9}	
10-µm		10 ∅	1.3×10^{11} 5.2×10^{11}	1.1×10^{9} 4.6×10^{9}	103
5-µm		5 ∅	2.7×10^{10} 5.4×10^{10}	9.1×10^{8} 2.1×10^{9}	
1-µm		1 ∅	3.0×10^{9}	2.2×10^{9}	310 (<0.02°)

23-ID-B 23-ID-D

Comparing LTP and at wavelength metrology

Slope error specification

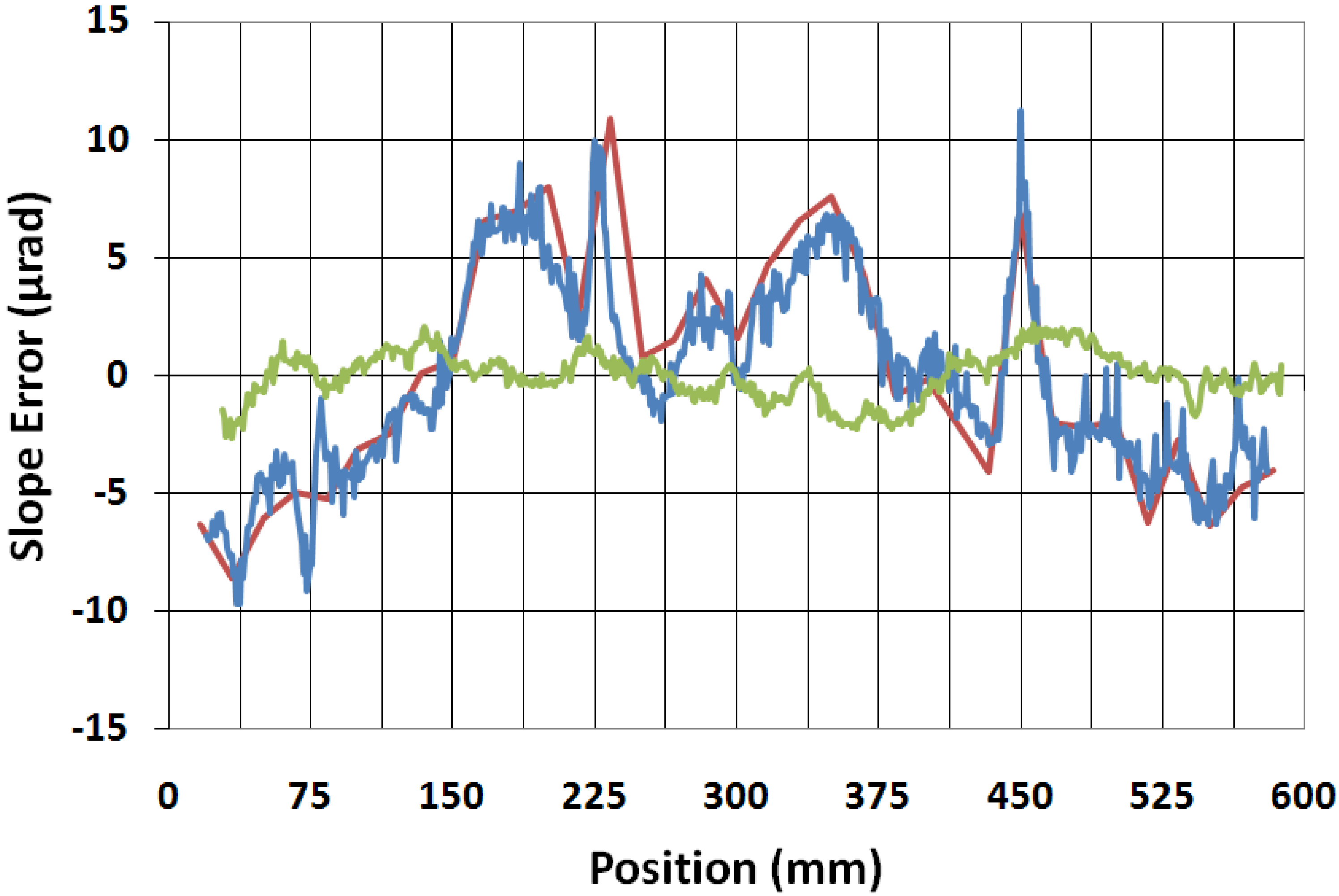
Original specification: 2.5 µrad in 2003

Repolished : 1.0 µrad in 2007

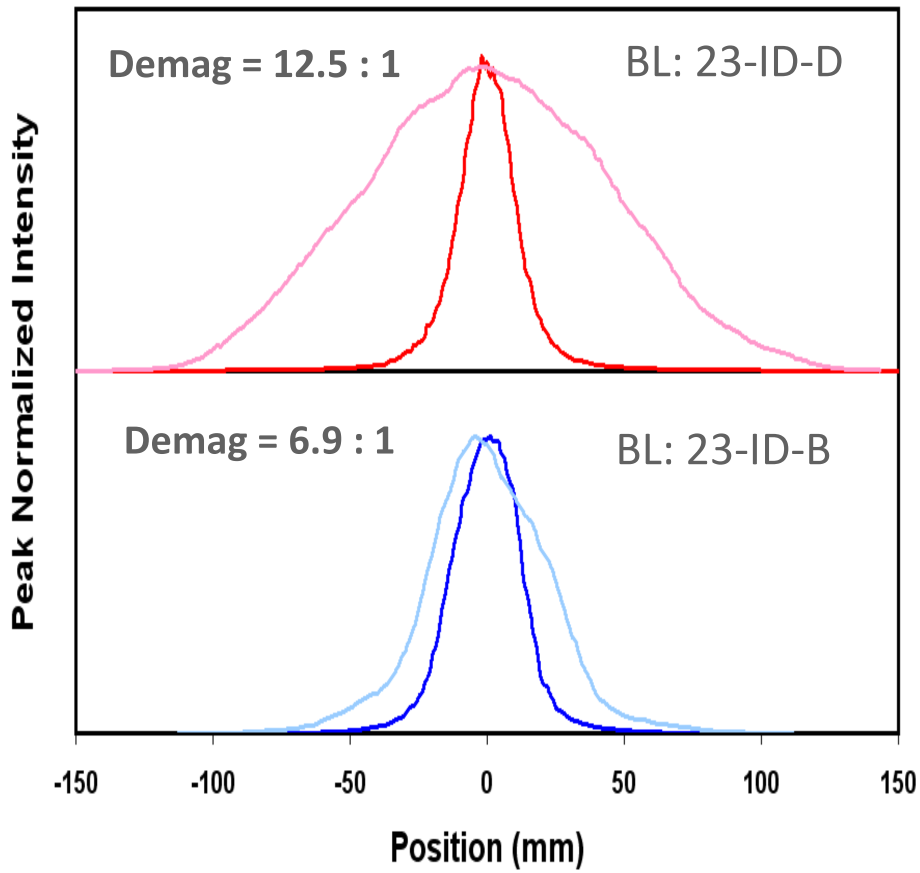
Blue – LTP before repolish

Red – in situ; before repolish

Green – LTP after repolish



Vertical focusing with “bi-morph” mirrors: unstructured profile at and off focus, automated focusing



- ❑ State-of-the- art slope error for 600mm long mirrors
  - <1.0 µrad RMS – uncorrected
  - ~0.5 µrad RMS – corrected
- ❑ Auto-focusing algorithm implemented
- ❑ Gaussian beam shape on/off focus
- ❑ Residual slope error
  - Determines minimum beam size
  - Effects beam positional stability
- ❑ GM/CA-CAT designed gravity compensator is better than the one provided by SESO

Derek Yoder

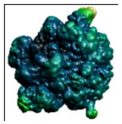
Relative Dimensions of small to largest Macromolecules Studied by X-ray Crystallography

Science August 27, 2010
3.5 Å resolution
Vijay Reddy and Glen Nemerow
The Scripps Research Institute

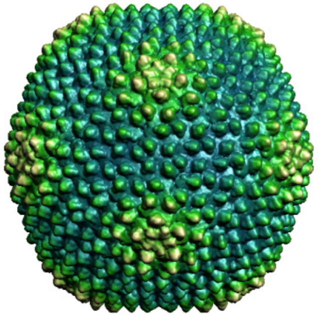
a=854.03 Å
b=855.17 Å
c=865.24 Å,

Myoglobin (2W6X)

Ribosome (70S; 2X9S)

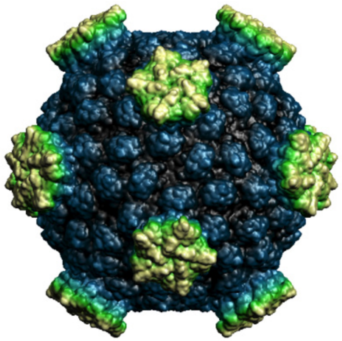


Bacteriophage PRD1; 1W8X



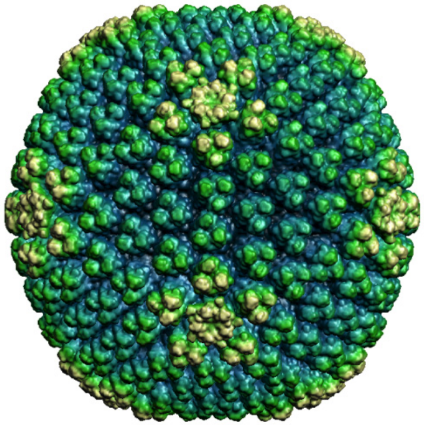
pT=25

Reovirus core (1EJ6)



T=1

Adenovirus (1VSZ/2BLD)



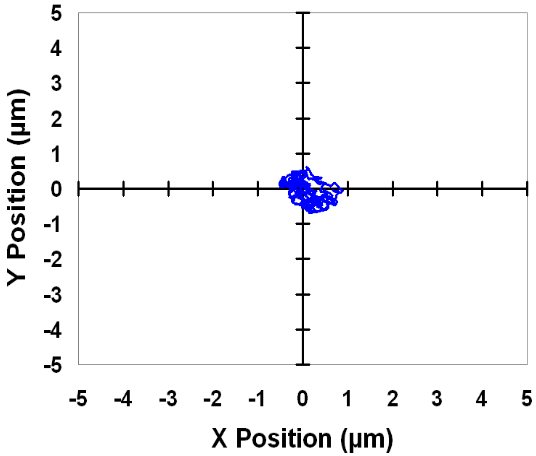
pT=25 ←T number

Dia. (Å):	42	280	702	754	960
# a.a. in IAU:	153	3,394	4,915	4,370	15,155
DNA/RNA (Kbp):	N/A	3.3	14.9	23.5	35.9

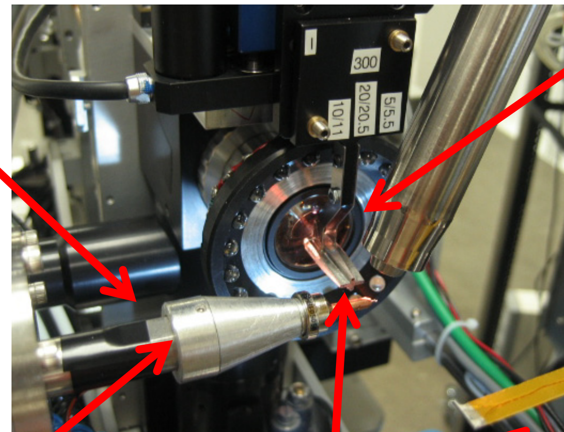
Micro-crystallography developments

Goniometer:

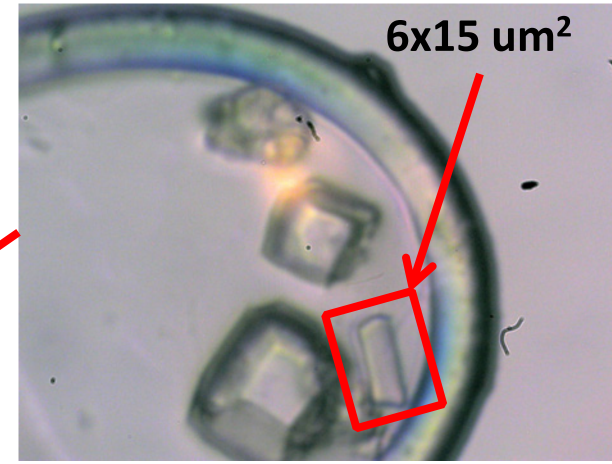
1 µm SOC peak-to-peak

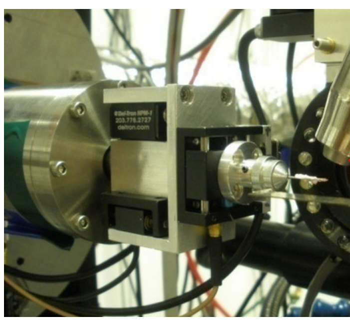


Sample environment

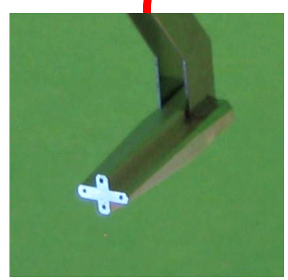


On-axis sample visualization

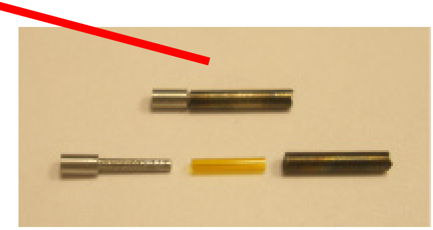




Goniometer head:
nano-positoning

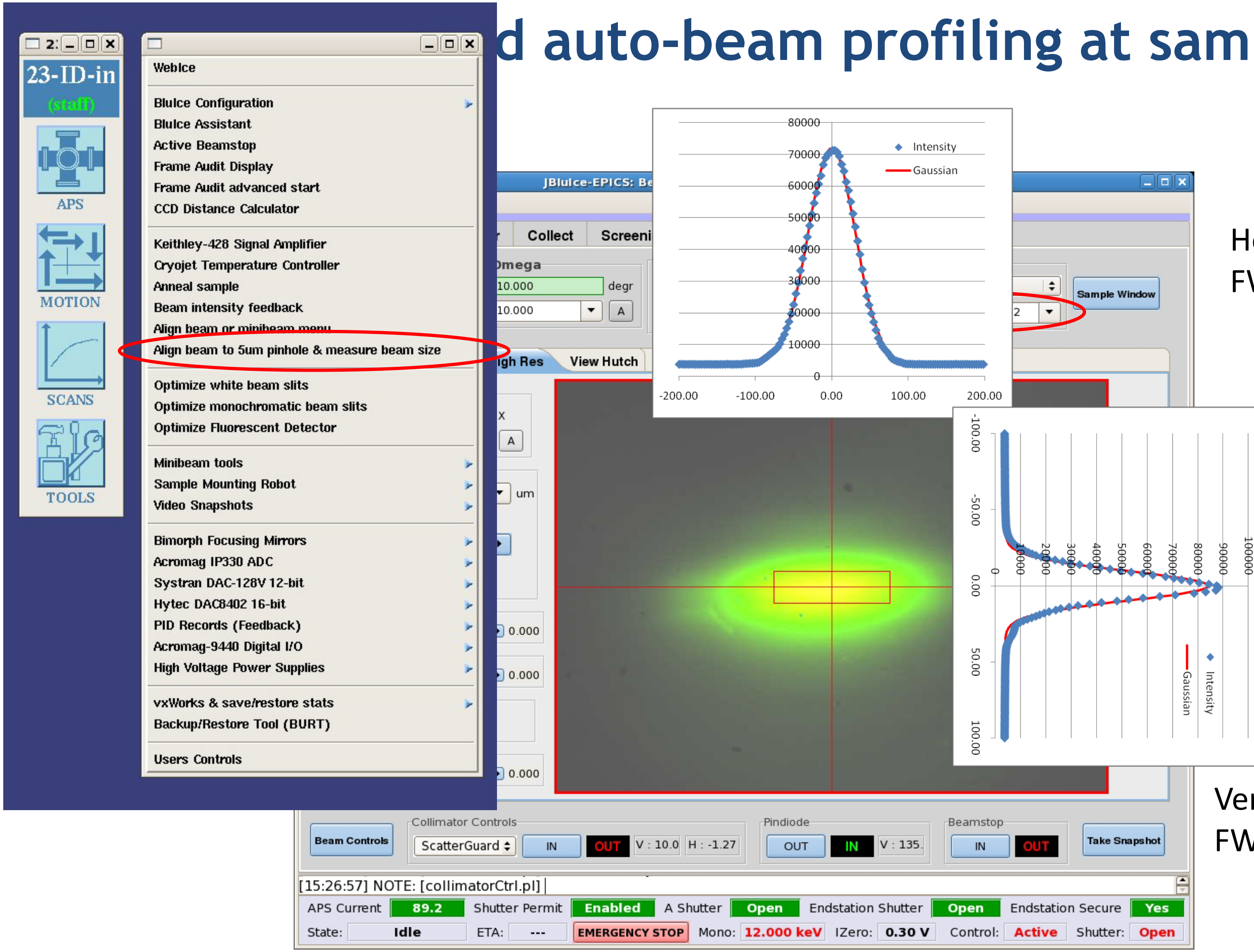


Quad mini-beam collimator:
5, 10, 20-µm beams and
300- µm scatter guard



Active beamstop:
Photoelectric effect

d auto-beam profiling at sample



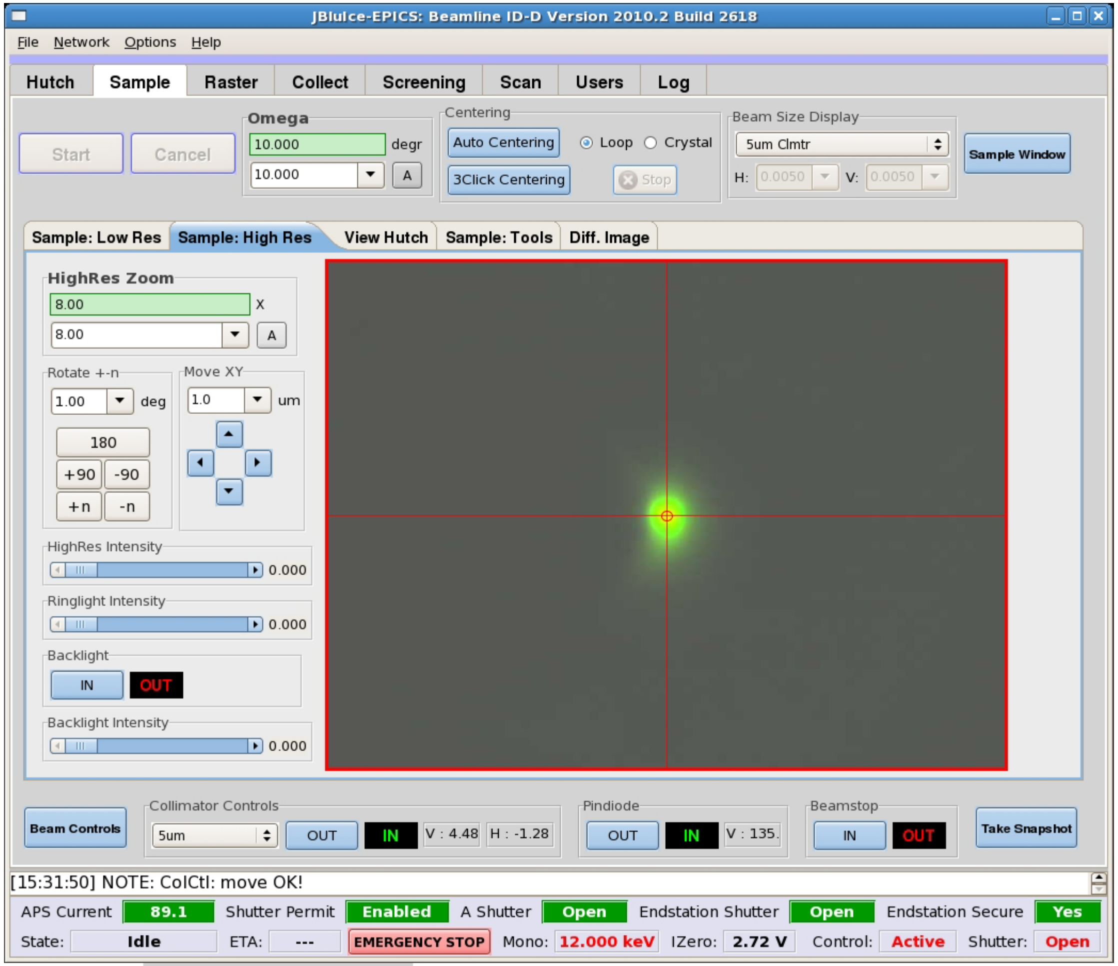
Horizontal
FWHM = 62.5 µm

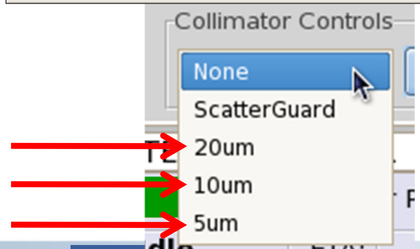
Vertical
FWHM = 18.8 µm

Reduce the beam size to 35 x 15 μm^2 with slits

National Institute of General Medical Sciences
GM/CA CAT
NATIONAL CANCER INSTITUTE

Rapid beam size selection





GM/CA-CAT Bimorph Mirrors

- SESO mirrors
- Kirkpatrick-Baez geometry
- SiO_2, Pt, or Rh stripes for harmonic rejection

Horizontal mirror:

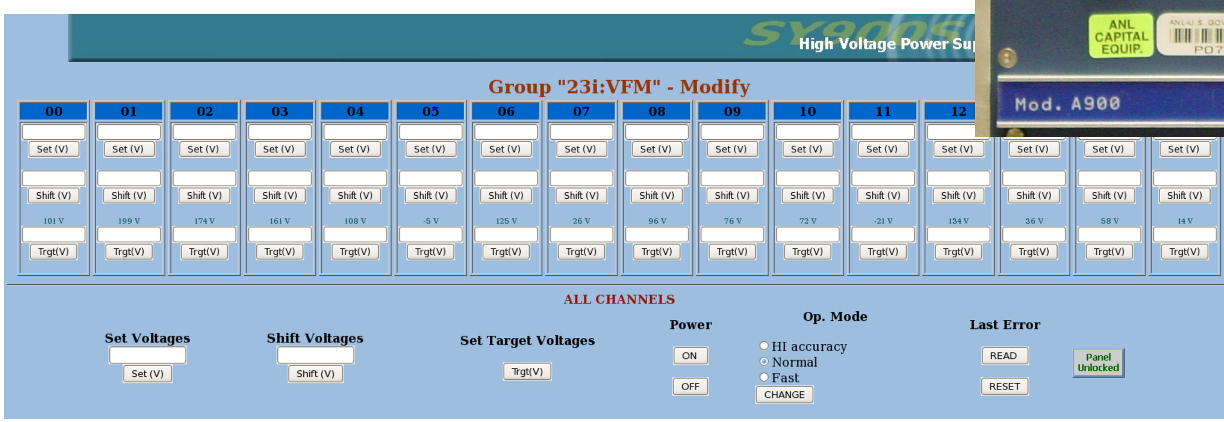
- length = 1.05 m
- 3.15 mm acceptance @ 3 mrad
- 2.5 Å roughness, 2.5 µrad slope error
- 14 electrodes

Vertical mirror:

- length = 0.60 m
- 1.80 mm acceptance @ 3 mrad
- 2.5 Å, 2.5 µrad → 1.0 µrad
- 16 electrodes

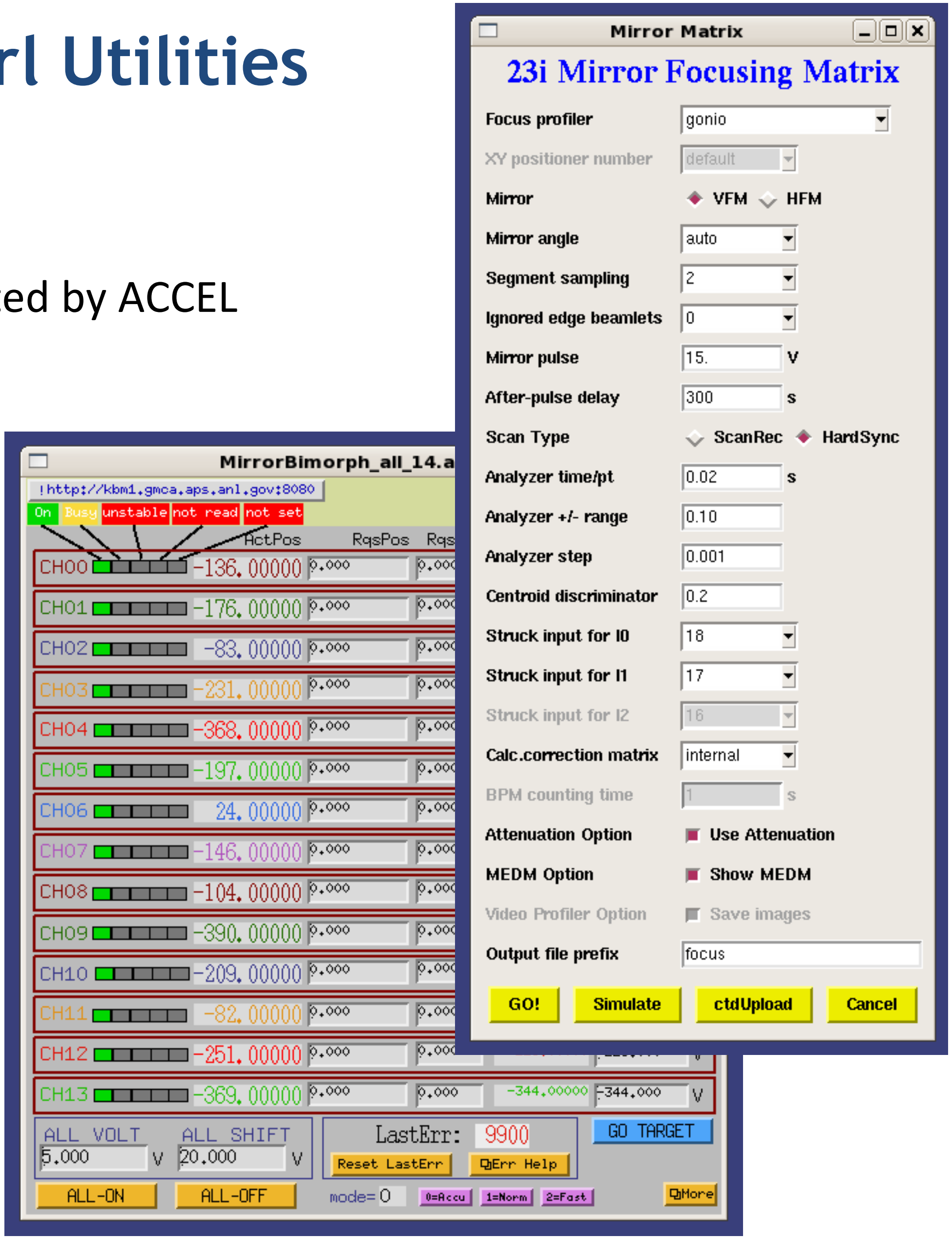
Power Supplies and Web GUI

- Precision, high voltage power supply from Elettra
- Bipolar output to ±2000 V
- Protection for neighboring electrodes (ΔV_{max} = 500 V)
- Controller includes focus software, ethernet connectivity, and web interface



Control via EPICS: via Perl Utilities

- EPICS driver and MEDM screens created by ACCEL and modified by GM/CA
- GM/CA has created a perl script library to facilitate basic mirror functions and has used this library to create a number of mirror utilities:
  - Voltage backup
  - Voltage restore
  - auto-alignment of a mirror
  - Auto-focusing
- Auto-focusing
  - Implemented in 2008
  - Used routinely



Automated Focusing

- A 14- (or 16-) dimension linear minimization problem (see Signorato, et al., *J. Synchrotron Rad.* (1998), **5**, 797-800)

ts). By knowing **H**, the solution to the least-squares
ation of a given measured distortion $\boldsymbol{\delta}\mathbf{f}_0(x_i)$ is given by:

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

^{T} is the standard notation for the transposed matrix. A
inverse singular value decomposition (SVD) method is
avoid singularities of **H**.

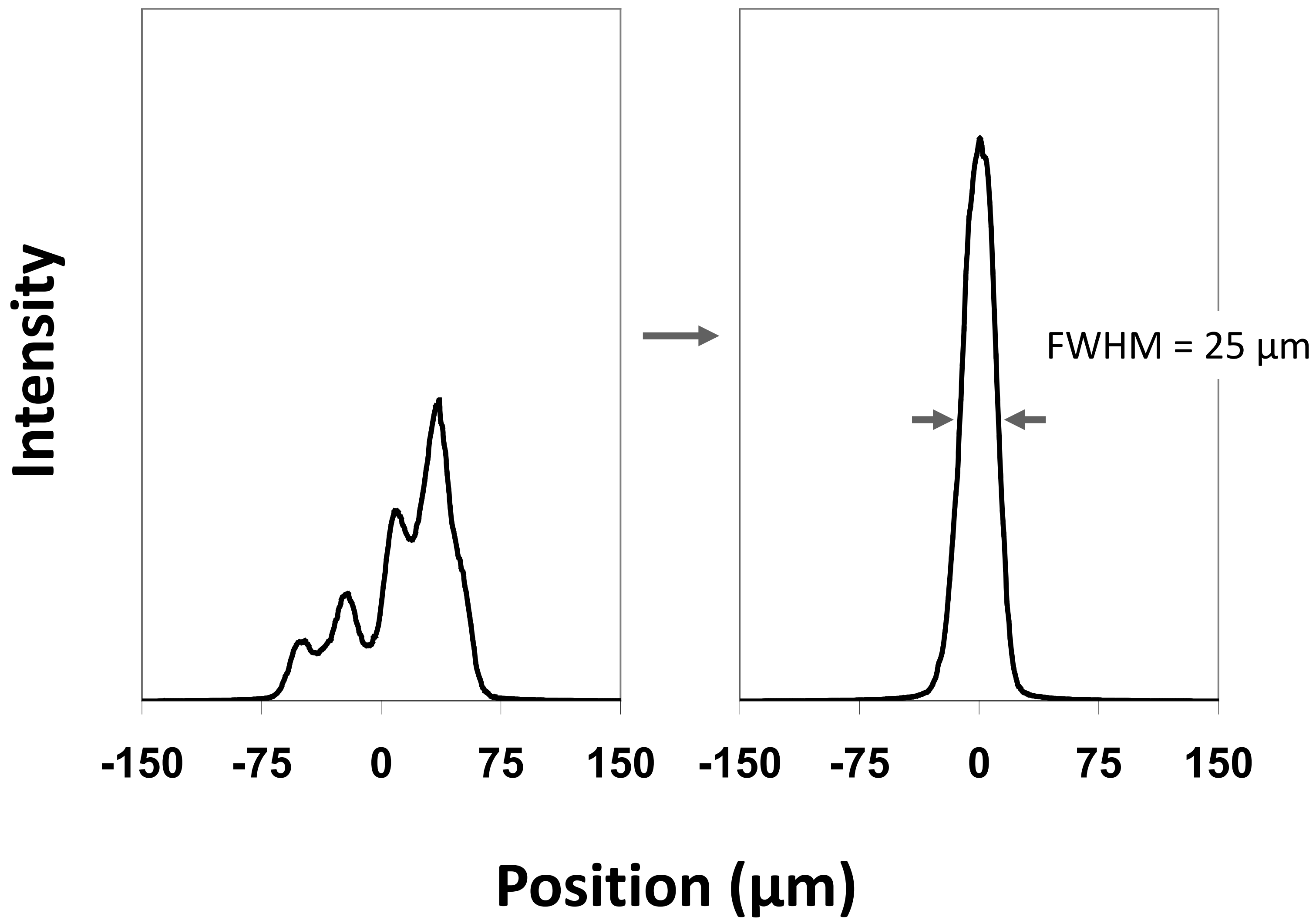
- Obtain the interaction matrix describing the response of each portion of the mirror to voltage pulses

**Interaction Matrix:
Response of
32 positions to
16 voltage pulses**

- The interaction matrix, combined with the error vector describing the current state of the mirror, provides the correction needed to focus the beam

- Typical time for collection of interaction matrix is 2-3 hours

Automated focusing since 2008



Crystallography with micron (and smaller) beams

What are the science drivers for micro-crystallography?

- Smaller crystals
  - membrane proteins
  - protein and RNA complexes
- Inhomogeneous crystals
  - probe to find more ordered regions
- Radiation damage
  - expose fresh crystal
  - reduce radiation damage by understanding behavior of photoelectrons

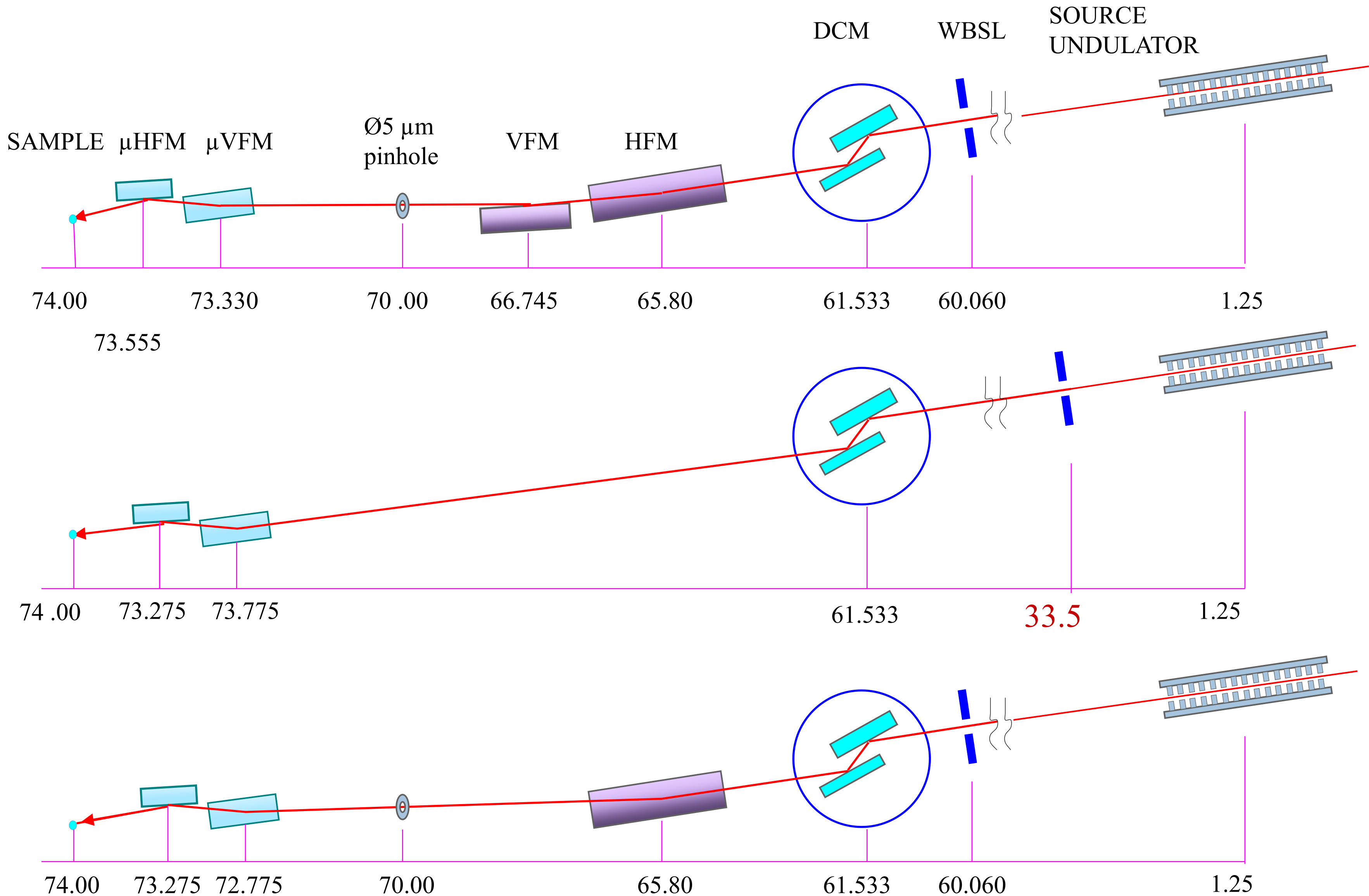
What is so challenging about sub-micron beams?

- Achieve the desired size ***while maintaining a small divergence***
  - Large divergence prevents resolution of diffracted spots

- What is a small divergence?
  - Good cryo-cooled crystals have a mosaicity of about 0.1° = 1.7 mrad
  - Ideally, would like to keep divergence below 200 - 300 μrad

- Considerations:
  - Trade-off: % beam collected by focusing optic vs. beam divergence
  - Increasing focal length
    - keeps divergence low
    - reduces the demag
    - amplifies the effects of slope error
      - beam blur
      - source motion

ID-in beamline option-1, 3and 5



Summary beam properties for micro-focus layouts

	Option 1a		Option 3		Option 5c	
Energy = 18.5 keV	**Horz**	**Vert**	**Horz**	**Vert**	**Horz**	**Vert**
Source size (FWHM) (µm)	642	21	642	21	642	21
Source divergence (FWHM) (µrad)	21	10	21	10	21	10
2nd source size (FWHM) (µm)	5	5	40		5	
2nd source divergence (FWHM) (µrad)	362	238			362	
Working distance (m)	0.37		0.575		0.52	
Mirror RMS slope error (µrad)	0.15	0.15	0.15	0.15	0.15	0.15
Focal size (FWHM) (µm)	0.99	0.63	0.89	0.94	0.99	0.89
Focal convergence (FWHM) (µrad)	894	1008	792	584	1343	612
Final flux (photons/sec)	1.39E+11		1.27E+12		1.36E+12	
Focal brilliance (ph/sec/mm^2/mrad^2/**0.0141% BW**)	2.45E+17		3.3E+18		1.85E+18	

“Optimized” micro-focus configurations

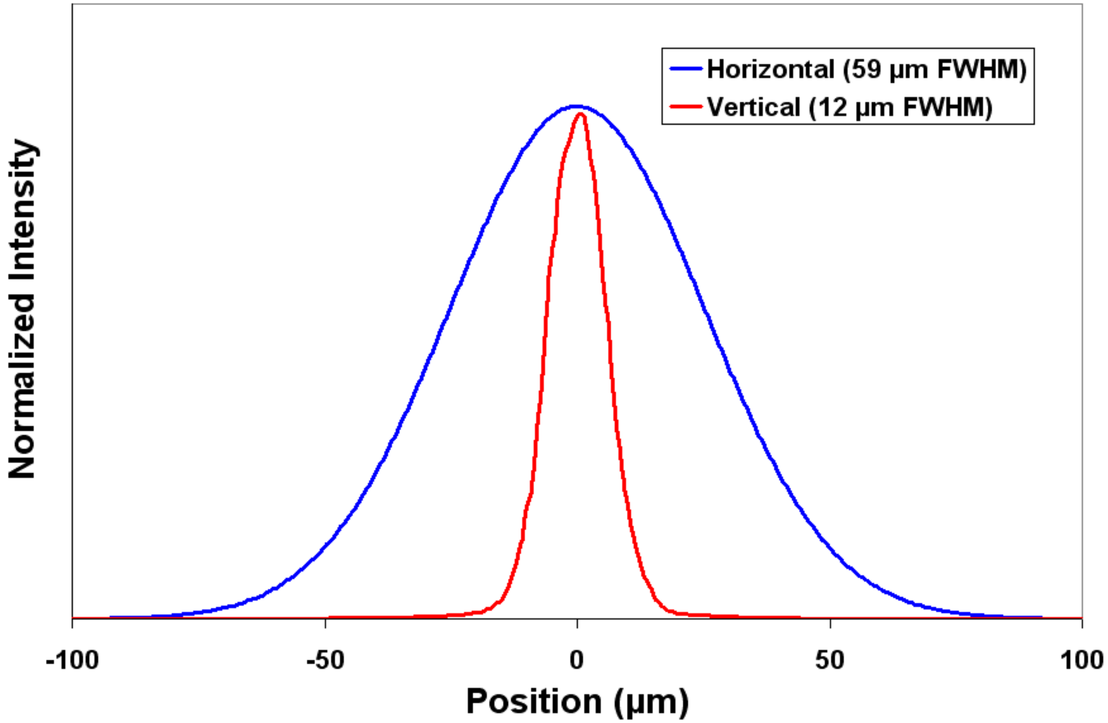
- Option 1 – KBM, MBSL 2nd source, µKBM
  - Pros
    - Proven
    - Seemed more stable than option 3 over period of hours
    - Lowest cost
  - Cons
    - Lowest intensity and brilliance
    - Very short working distance
- Option 3 – WBSL 2nd source, µKBM
  - Pros
    - Lower horizontal convergence
    - Variable horizontal beam size is easy
  - Cons
    - More expensive - requires adding a WBSL
    - Experience showed alignment tended to drift
- Option 5 – HFM, MBSL 2nd source, µKBM
  - Pros
    - Highest intensity
    - Variable horizontal beam size is easy
  - Cons
    - Highest convergence

“Dynamic” micro-focus configurations

- Option 6 – similar to option 5 but push HFM focus downstream
- WBSL 2nd source issues
  - Options:
    - » Fixed or movable mask(s) in the FE at 22 m
    - » Invert existing IDA mask, then add a fixed mask for IDout somewhere
    - » New, shorter, IDin mask at 27.313 m for 150 mA
    - » New mask at >33.5 m, possible only horizontal defining
  - Add water cooling and monitoring into EPS
- MBSL 2nd source issues
  - Need to design precision adjustable slits

Large K-B bimorph mirrors focused tightly

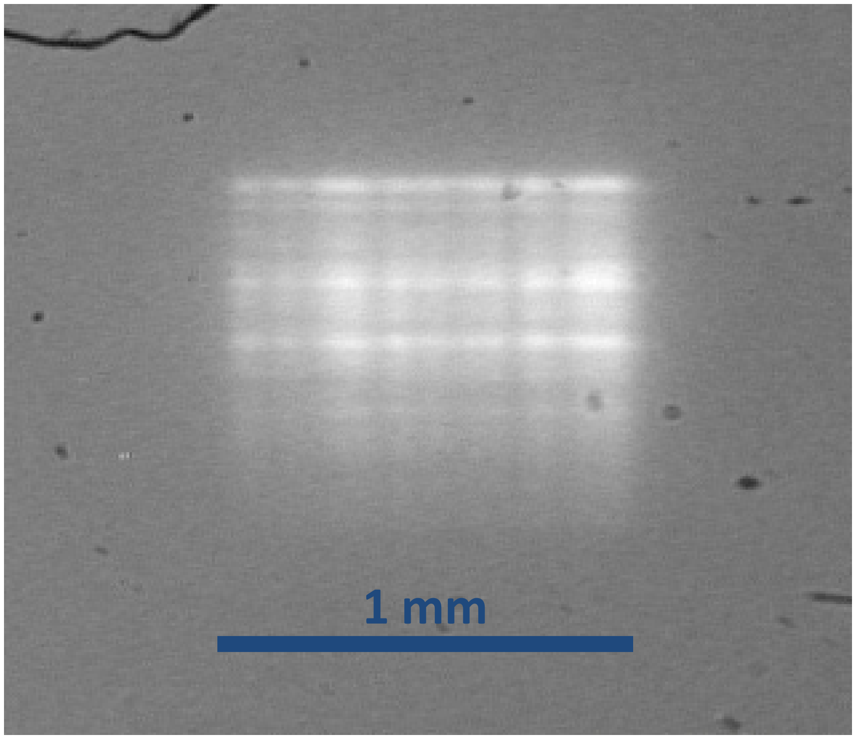
2nd source: 59 × 12 μm²



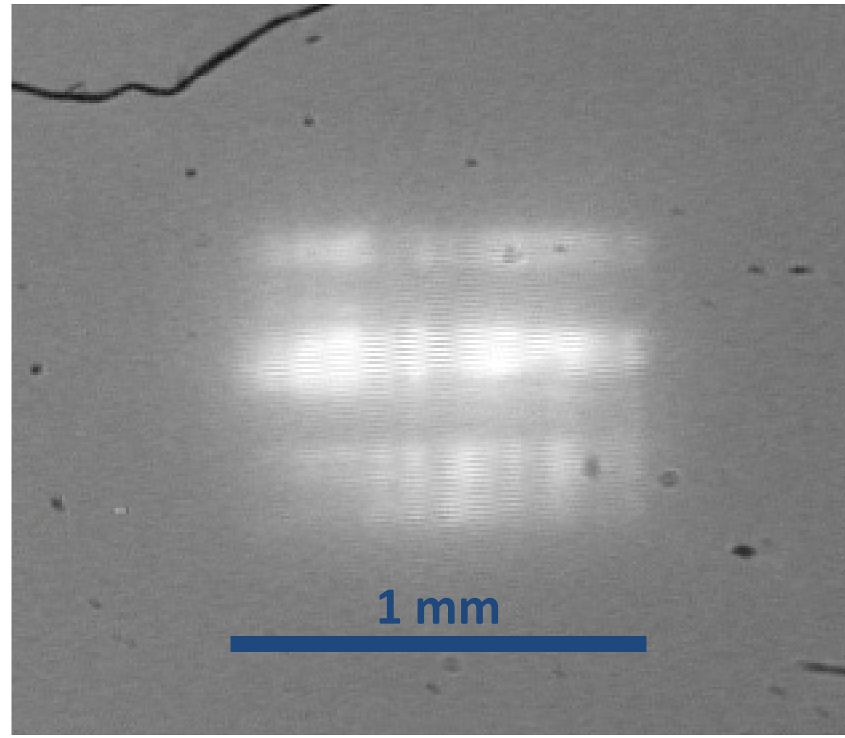
Mirrors are bent to neat their elastic limit

Clean focus

Visual image of beam off-focus



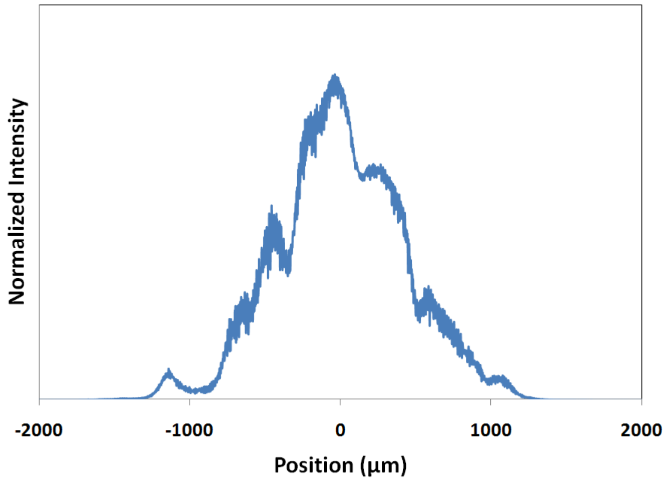
Without pinhole



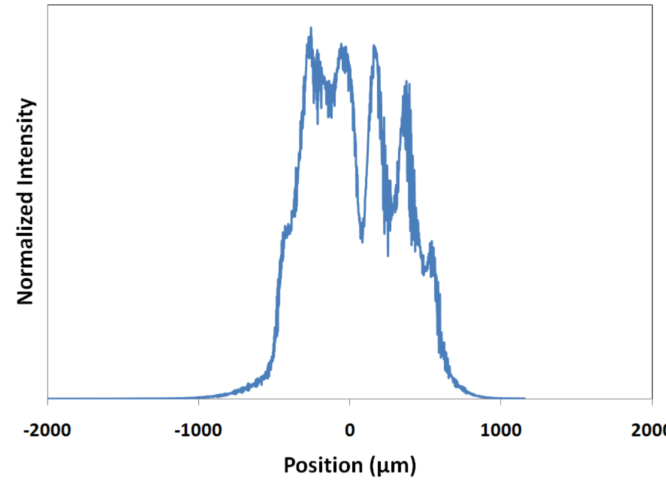
With pinhole

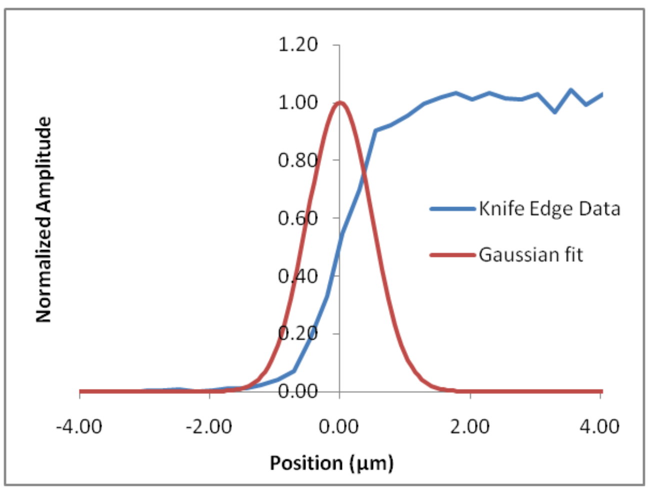
Beam profile at Zone Plate and final focus

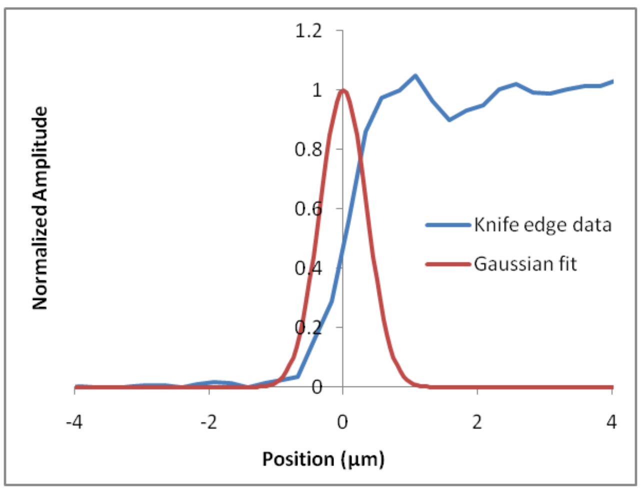
Horizontal



Vertical





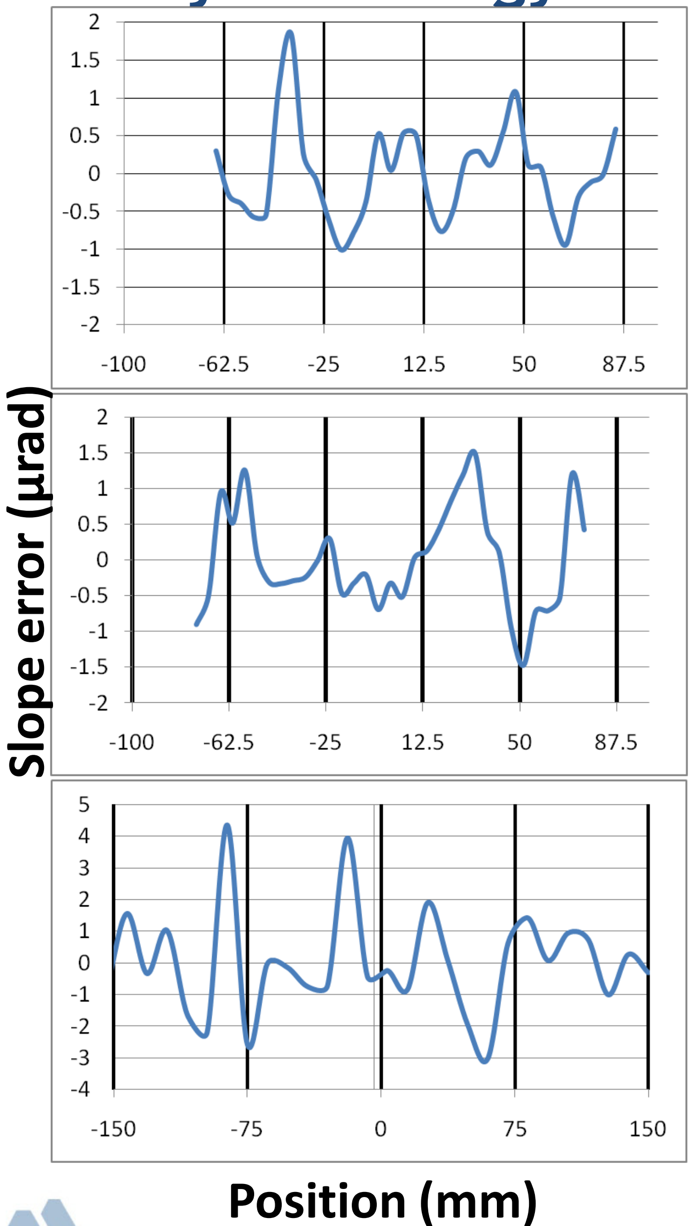


FWHM = 1.16 µm

FWHM = 0.81 µm

Structure not observed at focus!

X-ray Metrology when bent near the elastic limit



Focused to 9 µm
Slope error = 0.76 µrad
Corrected slope error = 0.64 µrad

Focused to 12 µm
Slope error = 1.21 µrad
Corrected slope error = 0.72 µrad

Focused to 52 µm
Slope error = 1.91 µrad
Corrected slope error = 1.68 µrad

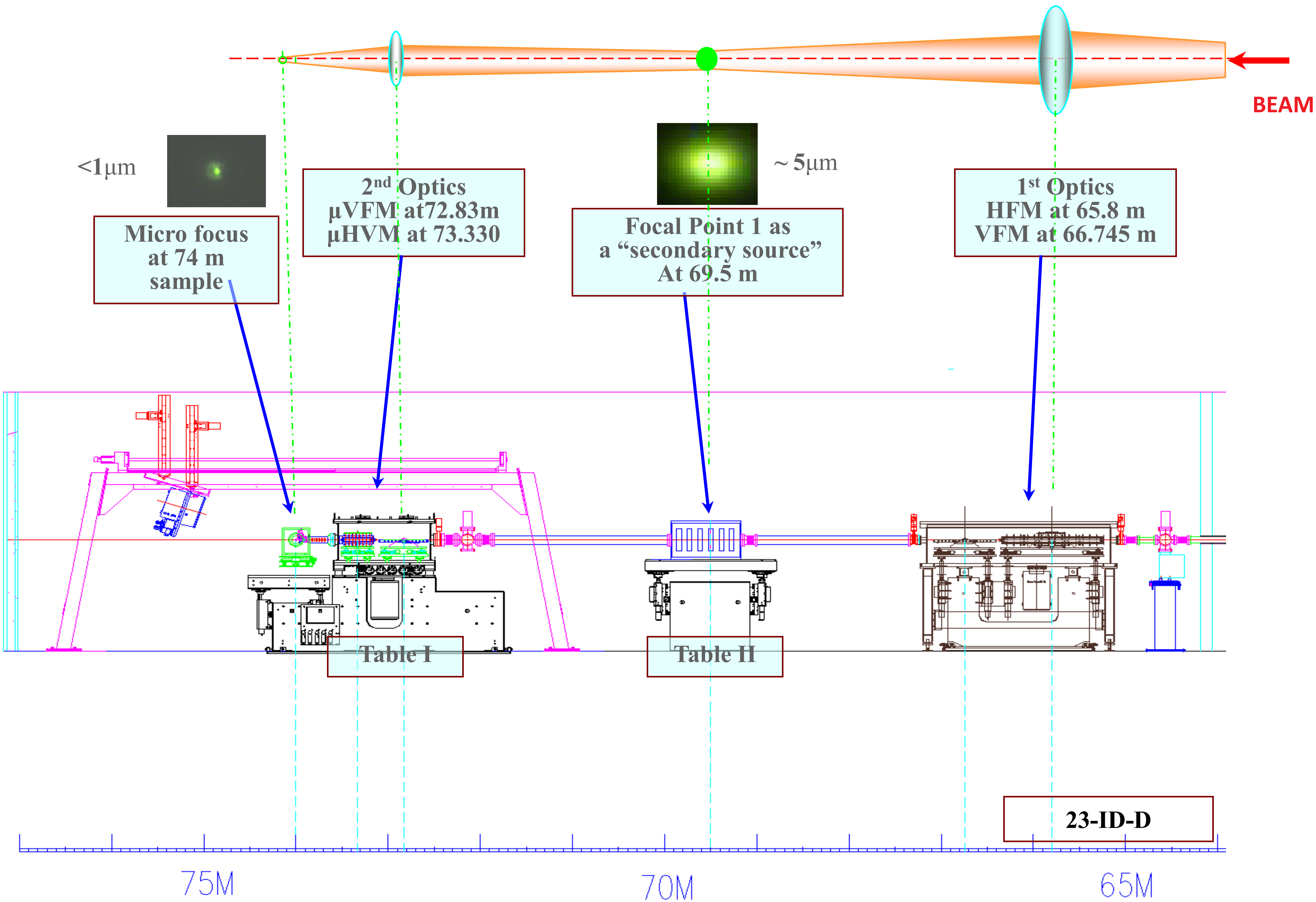
Operational micro-diffraction capabilities

- **GM/CA CAT**
  - 23ID-B,D: 5, 10 , 20 microns
- **Diamond**
  - ID24: 5 microns
- **ESRF**
  - ID-13: 0.3 microns for crystallography (not dedicated)
  - ID23-2: micro-diffraction (7 microns)
- **SPring-8**
  - BL32XU: 1-micron
- **Swiss Light Source**
  - X06SA: micro-diffraction (5 x 25 microns)

Planned/under development

- **NSLS-II: partial funded**
- **Petra-III : under construction**
- **Soleil: under construction**

GMCA Micro-Focus endstation



Conclusions

- Bimorph mirrors
  - provide state of the art focusing capabilities
  - clean off focus profiles
  - beware of bending to extreme **AND** looking far downstream of the focus
- Micro-focusing for MX
  - obtaining a 1 μm beam is "easy"
  - beware of high convergence
  - designing the optics to provide 1- 50 μm QUICKLY can be difficult

Acknowledgements

GM/CA Staff

Derek Yoder - optics

Nukri Sanishvili - rad. damage measurements

Shenglan Xu - mechanical design

Oleg Makarov – instrumentation development

Sergey Stepanov – computing and controls

Richard Benn – mechanical engineering

Steven Corcoran – electro/mechanical integration

Nagarajan Venugopalan – sample visualization

Craig Ogata – sample automounter

Mark Hilgart – software development

Sudhir Pothineni – software development

Michael Becker – mini-beam characterization

Janet Smith – CAT Director

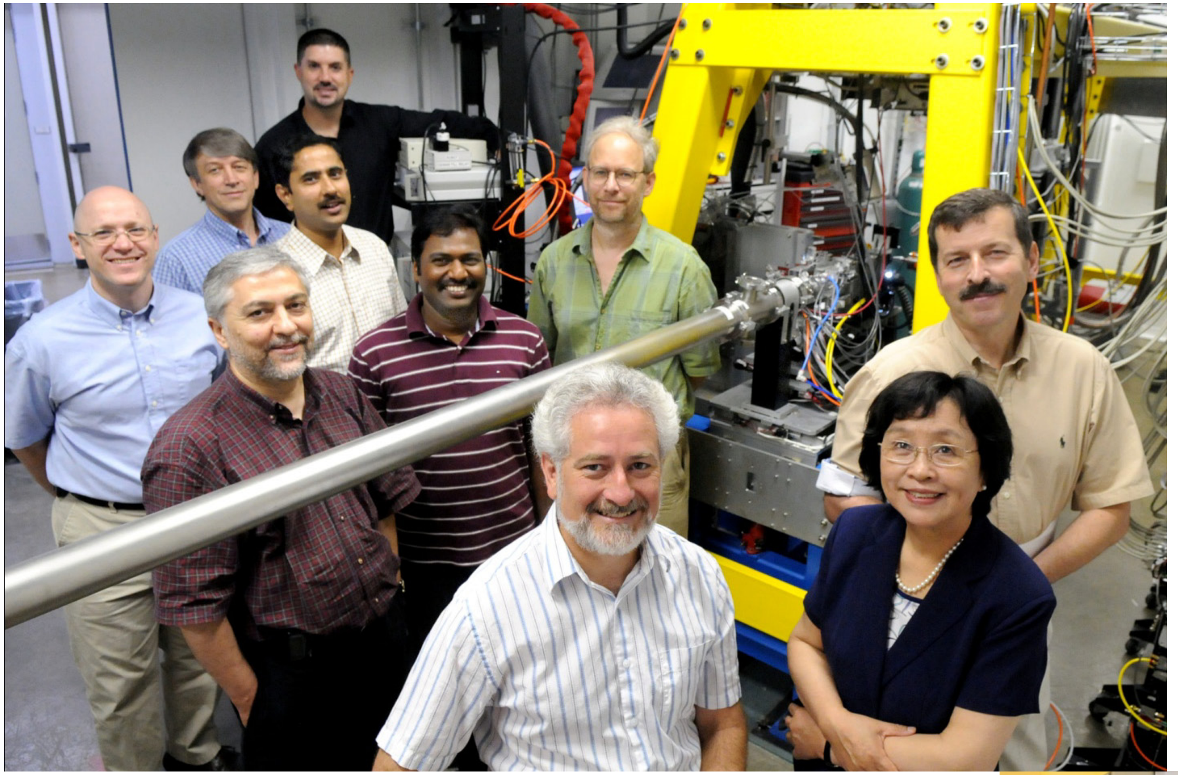
Bruker ASC GmbH (formerly ACCEL)

Riccardo Signorato

Wolfgang Diete

GM/CA CAT is funded by the National Cancer Institute and the National Institute of General Medical Science. The Advanced Photon Source is supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science.

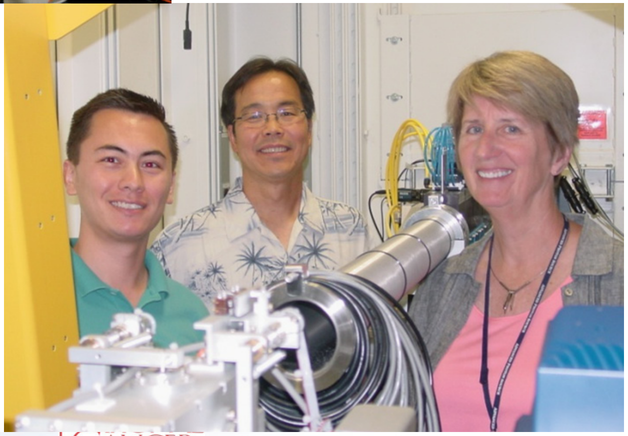
GM/CA CAT Staff



Steve Corcoran
Oleg Makarov
V. Nagarajan
Mike Becker
Derek Yoder
Sudhir Potheneni
Nukri Sanishvili
Sergey Stepanov
Shenglan Xu
Bob Fischetti
Dale Ferguson
Zunping Liu

Dale Ferguson

Mark Hilgart
Craig Ogata
Janet Smith



Thank you for your attention

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