

Workshop: X-Ray Echo Spectroscopy – Opportunities and Feasibility  
September 8-10, 2016, APS, Argonne National Laboratory.

# The Ultrahigh Resolution IXS Beamline at NSLS-II: Current Status and Performance

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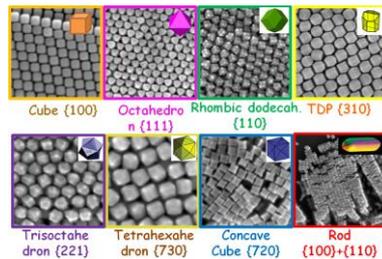
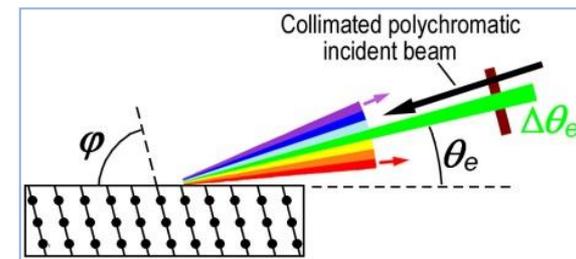


# Outline

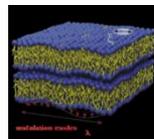
- A Brief Overview
- Advances in Crystal Optics & Beamline Development
- Performance, Recent Results & Early Experience
- Outlook

# The Ultrahigh Resolution IXS Beamline at NSLS-II

- Designed to Achieve Best-in-Class Performance for vibrational dynamics by IXS :
  - Angular dispersive crystal optics for cutting-edge resolution ( $0.1 \sim 1 \text{ meV}$ ) with sharper tails in resolution function and high Q resolution ( $0.1 \text{ nm}^{-1}$ ).
  - Medium operation energy ( $9.1 \text{ keV}$ ) capitalizing on NSLS-II's strengths in flux and brightness
- Scientific Applications
  - Mesoscopic dynamics in liquids, soft matter, and biological systems
  - Phonons in single crystals, surfaces, interfaces and systems under extreme conditions



Programmable Nanoparticle Assemblies

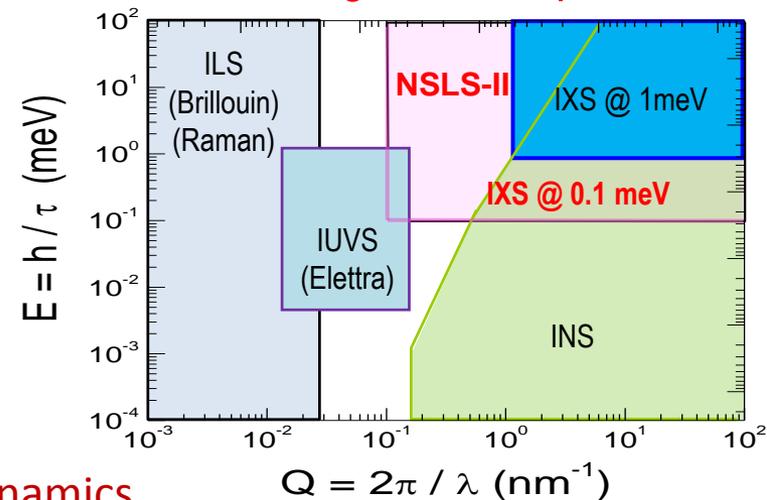


Lipid membrane

High pressure materials



"Filling in the Gap"

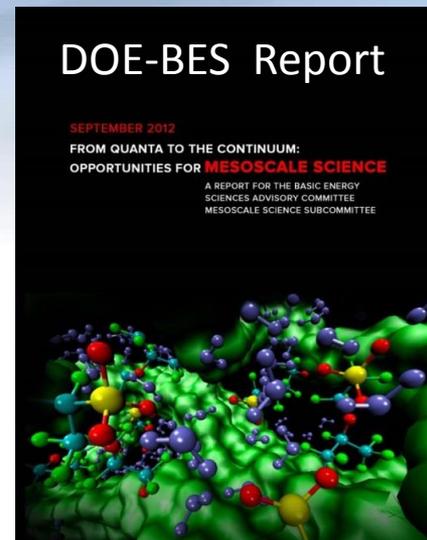


**Ultimate Goal:**

World-leading 0.1 meV energy resolution for studying dynamics

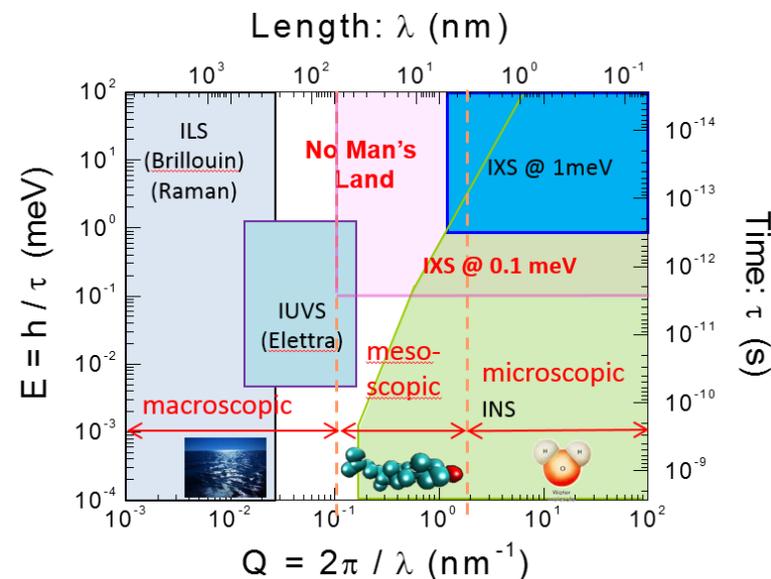
# Science at the Mesoscales

- Addressing scientific challenges at the mesoscopic length scale (5 ~ 50 nm, part of “no-man’s land”)
  - Phononics in functional nanoparticle assemblies - optimizing transport and response properties by design and control of mesoscale structure
  - Fast dynamics of bio-molecular systems and their biological functions - bio-inspired mesoscale inorganic materials.
  - Intermediate regime in disordered systems.



- Recent examples: Tomorrow’s talks

- **Giulio Monaco:** “High-frequency dynamics in liquids and glasses at the mesoscopic scale”
- **Alessandro Cunsolo:** “High resolution inelastic x-ray measurements on soft matter systems: current results and future perspectives”
- **Mikhail Zhernenkov:** “Application of inelastic scattering to study biomembranes: latest results and challenges”



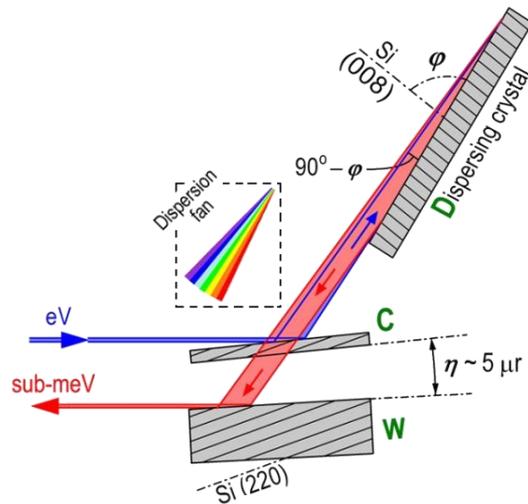
# Our Approach: Angular Dispersive Optics

- Inline 4B mono for ease and range in energy scanning
- Analyzer optics based on CDW scheme proposed by Shvyd'ko (2004, PRL 2006)

## CDW - Analyzer

$$\frac{\Delta E}{E} \approx \frac{\Delta \theta_e}{2 \tan \phi} \approx \frac{\theta_e \Delta \theta_e}{2}$$

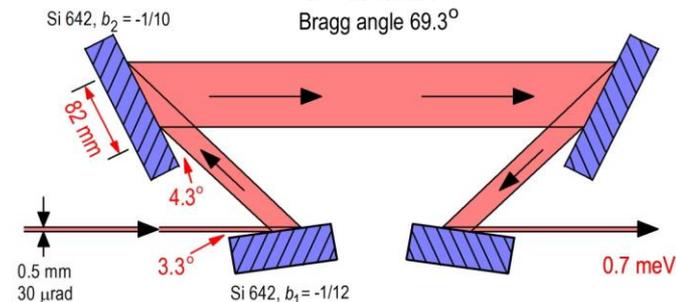
- Angular acceptance  $\sim 100 \mu\text{rad}$
- High peak reflectivity  $\sim 38\%$
- Sharp tails (multiple reflections and anomalous transmission)
- Sub-meV resolution at  $\sim 10 \text{ keV}$



## 4B - Mono

Huang, JSR (2011)

$E = 9.13 \text{ keV}$   
Bragg angle  $69.3^\circ$

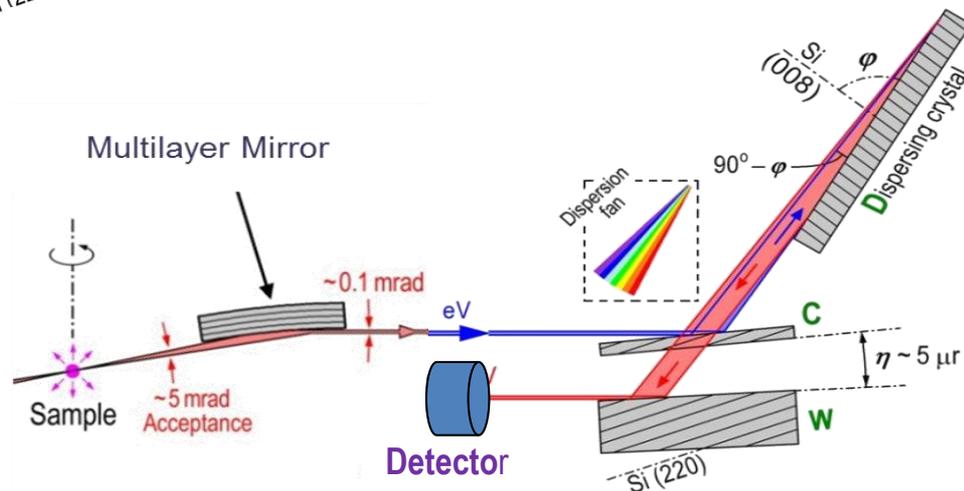


## Major technical challenges

- Lattice homogeneity:  $\Delta d/d = \Delta E/E \sim 10^{-8}$
- Mirror-like strain-free surface quality (SE:  $< 10 \mu\text{rad}$ )
- Precision and stable motion control

## Collimating optics (50-100:1) for large (5-10 mrad) acceptance

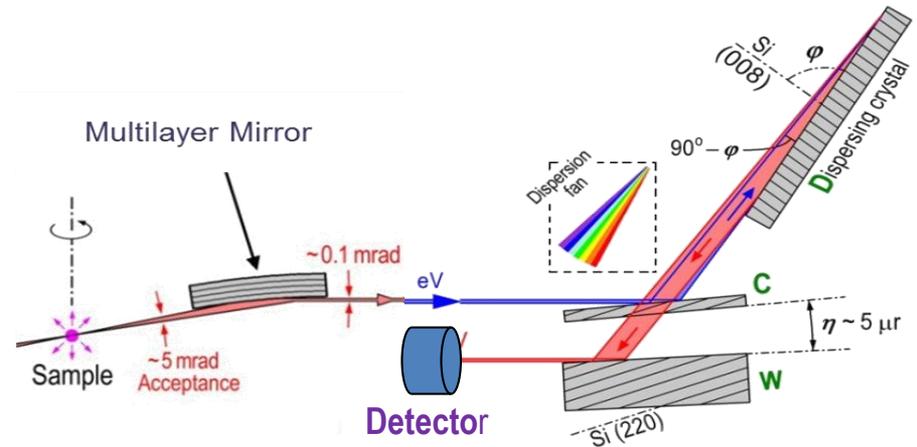
- Long dispersive crystal!!!



# High-Resolution Optics for IXS

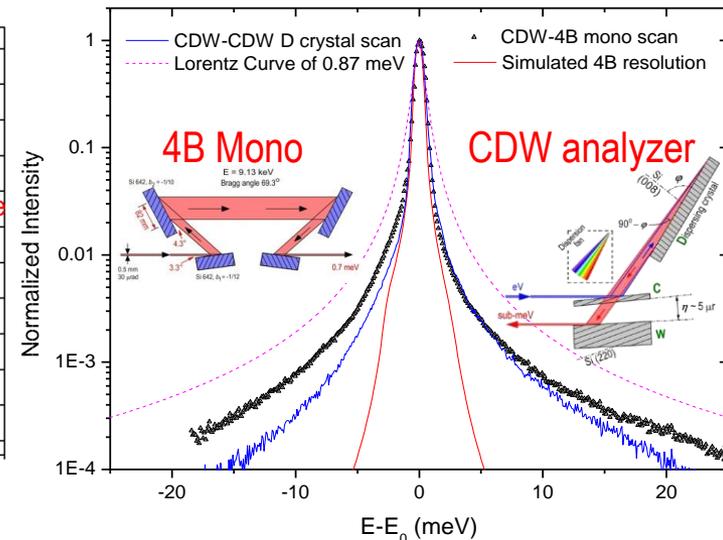
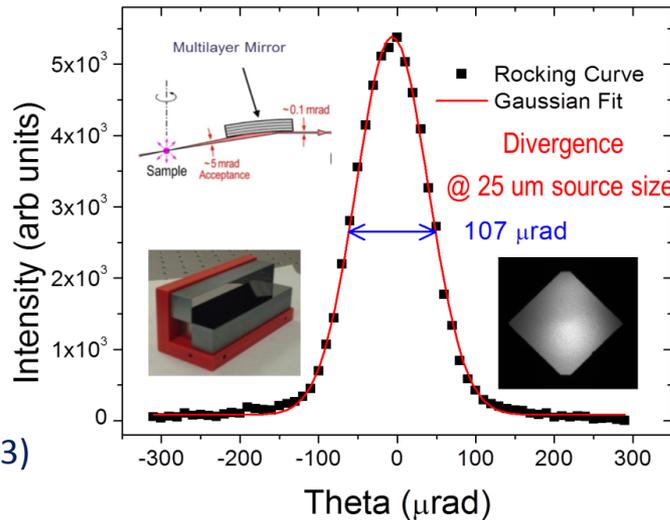
## ■ Demonstrated the initial goal of sub 1 meV resolution:

- CDW analyzer (de-convoluted) resolution:  
 $\Delta E = 0.7 \text{ meV}$ ,
- CDW analyzer efficiency  $\sim 20\%$  (theory:  $\sim 38\%$ )
- 4B mono and CDW analyzer combined resolution  $\Delta E = 0.8 \text{ meV}$ ,
- 4B-HRM efficiency  $\sim 30\%$  (theory:  $\sim 35\%$ )
- Sharp Gaussian-like tails



## ■ Montel collimating mirror performance verified.

- Angular acceptance :  
> 10 mrad
- Volume acceptance:  
 $\sim 20 \mu\text{m}$ , divergence  
< 100  $\mu\text{rad}$ ;
- Efficiency measured:  
 $\sim 47\%$  (theory: 49%)

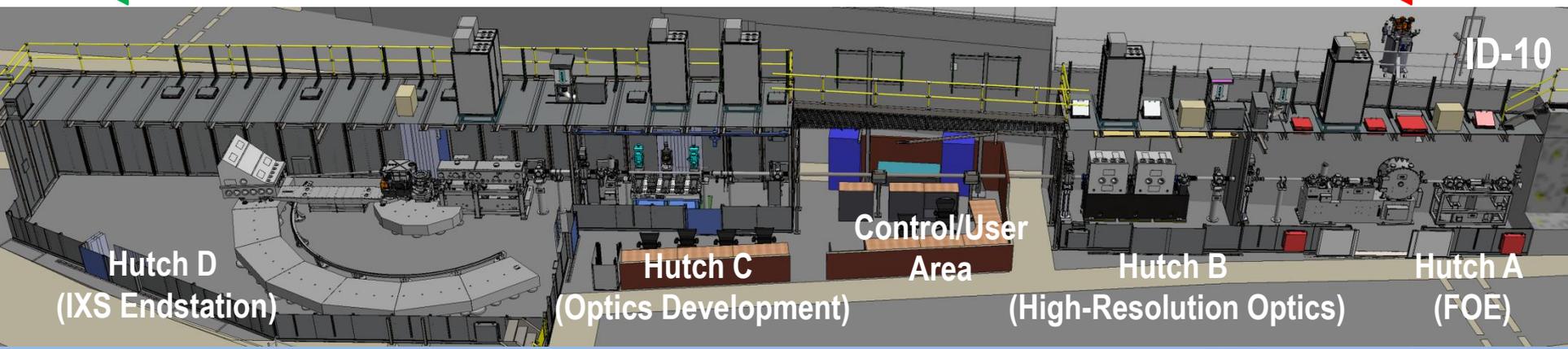
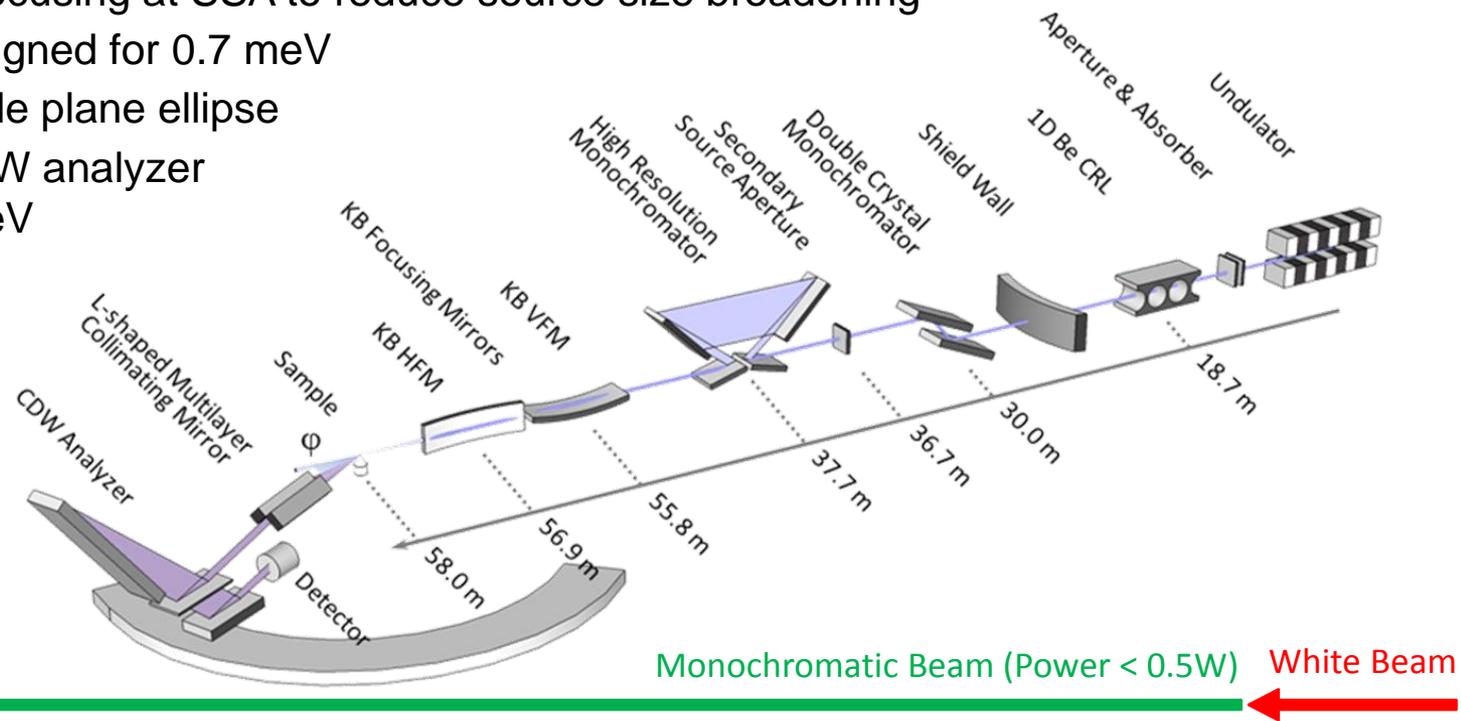


(Cai et al, J. Phys.: Conf. Ser. 2013)

(Suvorov et al, JSR, 2014)

# IXS Optics Layout & Beamline Design

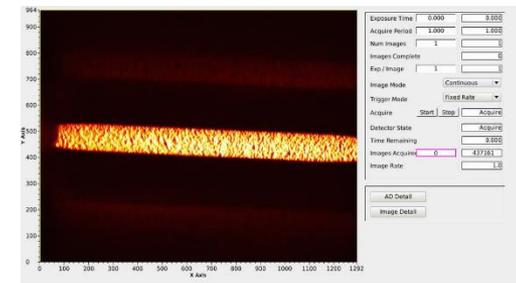
- Insertion device: IVU22-3m, optimized for 9.1 keV (max flux:  $8 \times 10^{14}$  phs/sec/0.1%bw @500mA).
- Be-CRLs for  $\sim 1:1$  focusing at SSA to reduce source size broadening
- HRM: inline 4B designed for 0.7 meV
- KB Mirrors: bendable plane ellipse
- Montel mirror + CDW analyzer designed for 0.7 meV



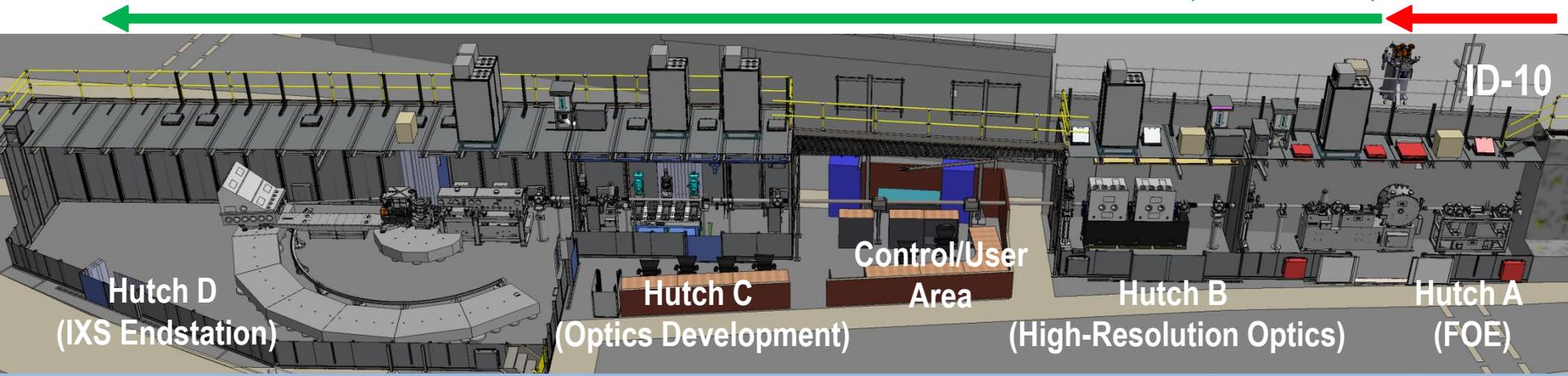
# IXS Commissioning Timeline & Milestones

- **Nov 24, 2014:** First light – Beam delivered to white beam stop in FOE
- **Feb 7, 2015:** Beam delivered to Hutch D; all slits, SSA and BPMs commissioned.
- **March 22, 2015:** KB Mirrors aligned. Beam focus measured optimized.
- **April 25, 2015:** HRM aligned, initial performance characterized.
- **May 2015 shutdown:** Be-CRL assembly installed.
- **June 2015:** Entire beamline optics system aligned, initial performance characterized.
- **July 1, 2015:** Beamline operation at 150 mA begins
- **Oct 4, 2015:** DCM Beam Stability Feedback Control Established.
- **Oct 30, 2015:** Montel mirror & CDW analyzer optics aligned.
- **Feb 10, 2016:** Tagma detector installed.
- **Feb 11, 2016:** First User Experiment (HP H2 – Dave Mao).
- **Apr 14, 2016:** Beamline operation at 250 mA begins
- **July 12, 2016:** Beamline begins general user operation

Nov 24, 2014: First Light

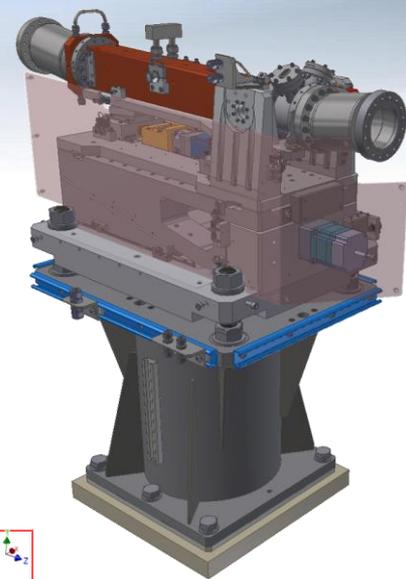
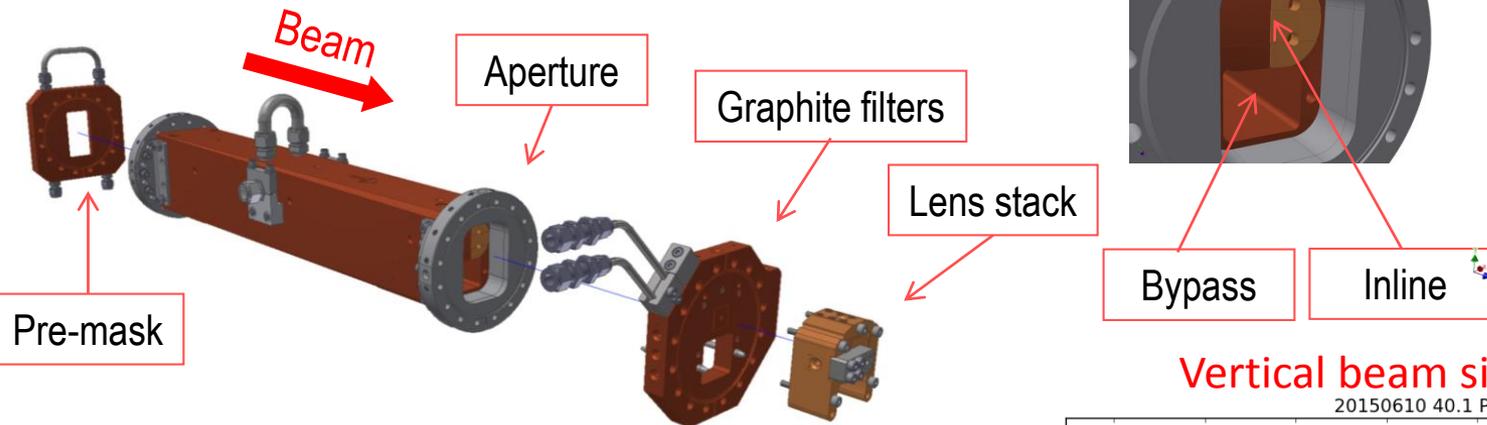


Monochromatic Beam (Power < 0.5W) ← White Beam



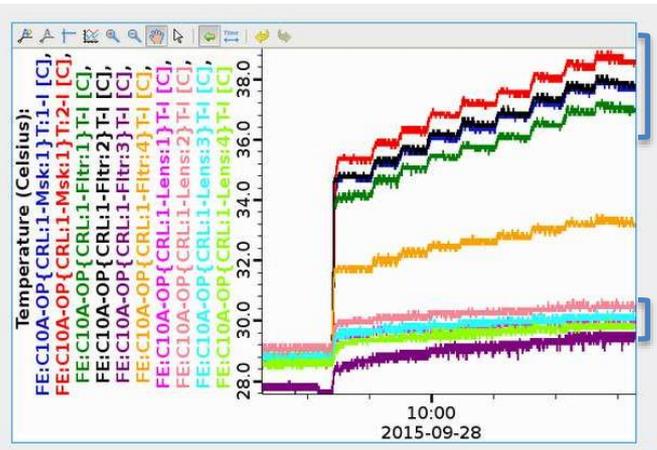
# Be-CRL Assembly Performance

- Very first component in the front end
- Integrated fixed mask; dual mode (inline & bypass) operation
- Lens assembly with integrated graphite filters

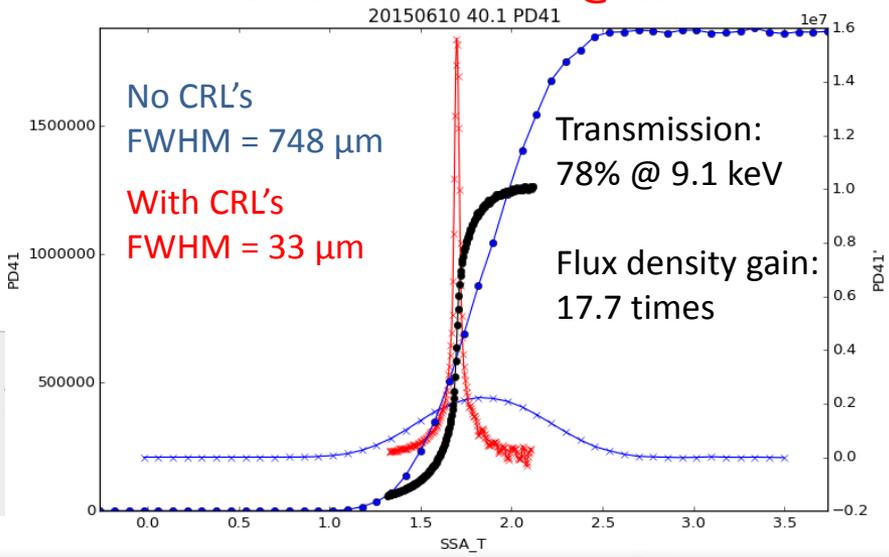
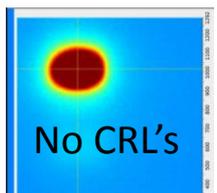


RC: 150mA ..... 225 mA

Vertical beam size @ SSA

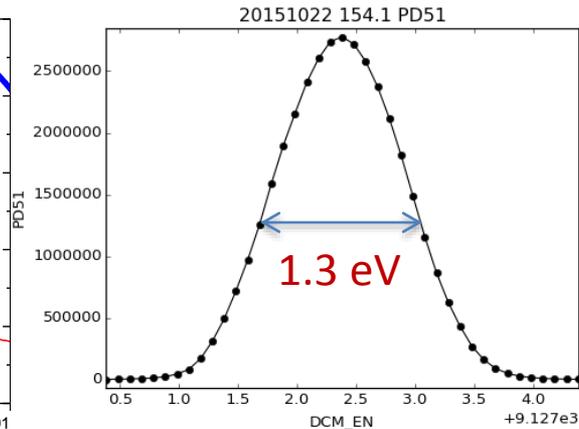
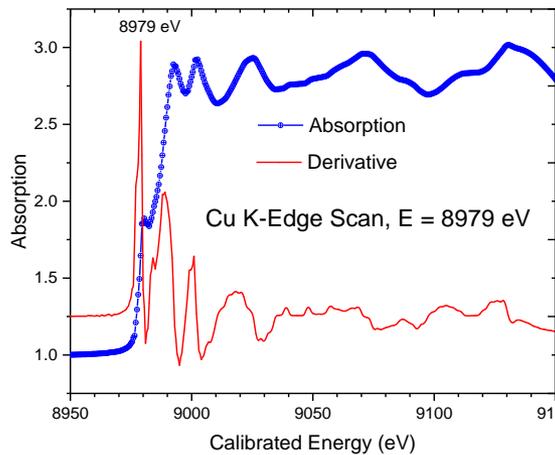


@ BPM1

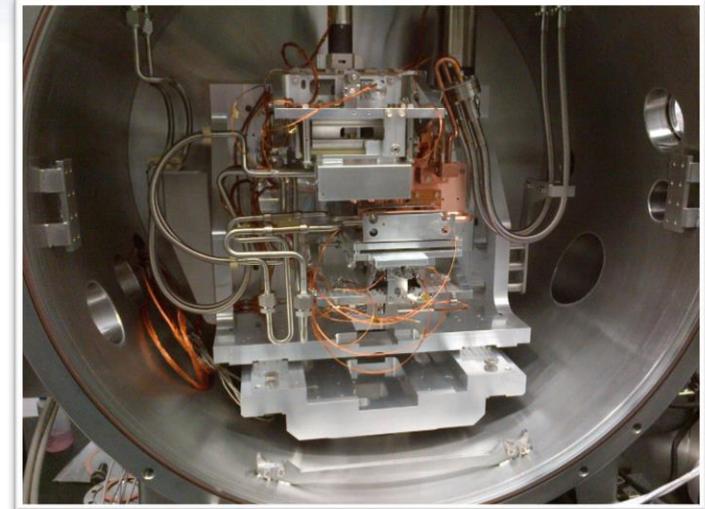
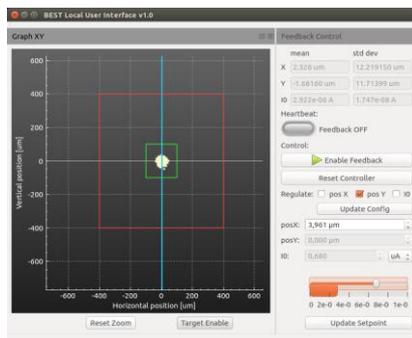


# Double Crystal Monochromator Performance

- Bruker DCM with LN2 cooled Si(111) or Si(220)
- Gravity-fed water jacket to maintain temperature stability
- Fixed exit or pseudo channel-cut mode
- Energy (lattice constant) calibrated for energy scan

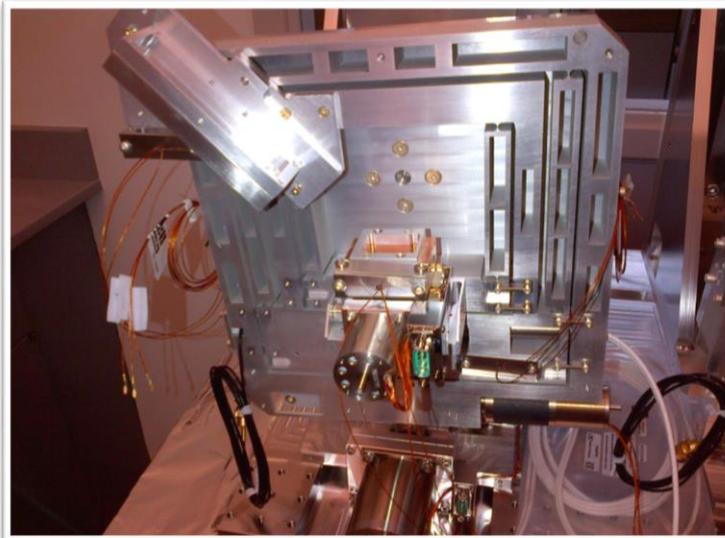
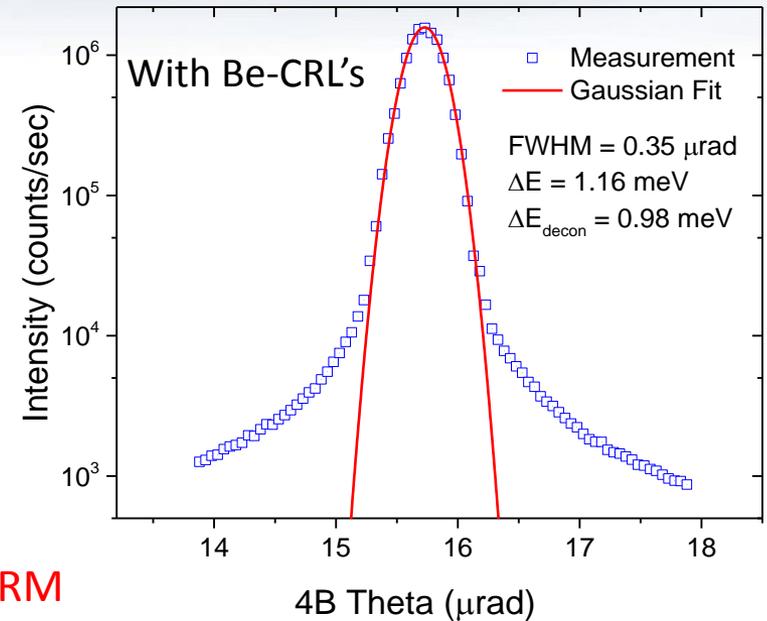


- CAENels BEST system for monitoring and feedback control

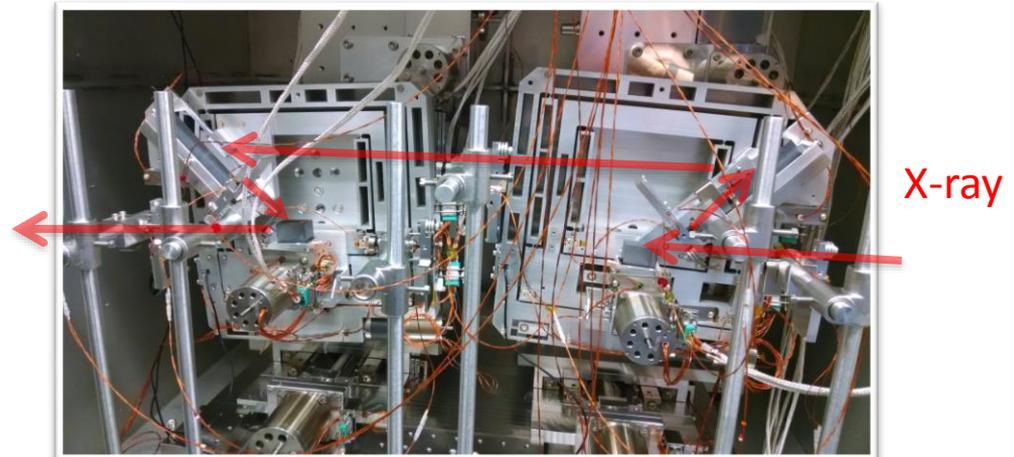


# High Resolution Mono Performance

- Mechanical design based on in-house developed trapezoid flexure with 10 nrad angular resolution
- Energy resolution results
  - Measured energy resolution:  $\Delta E \sim 1 \text{ meV}$
  - Characterized using the same CDW setup in R&D with a known  $\Delta E \sim 0.65 \text{ meV}$
  - Sharp tails down to 2 orders of magnitude



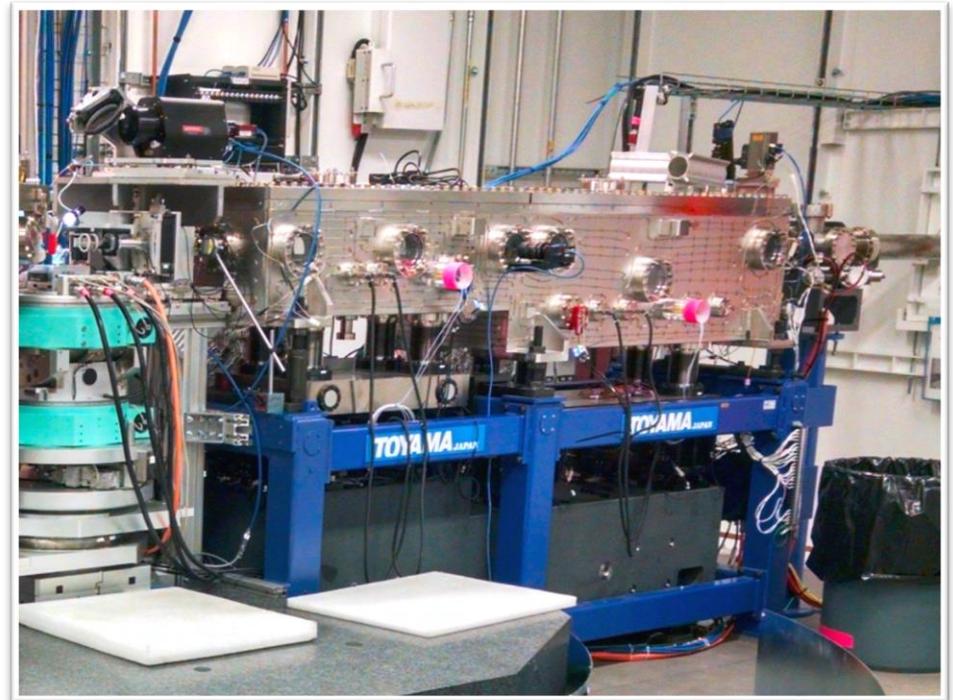
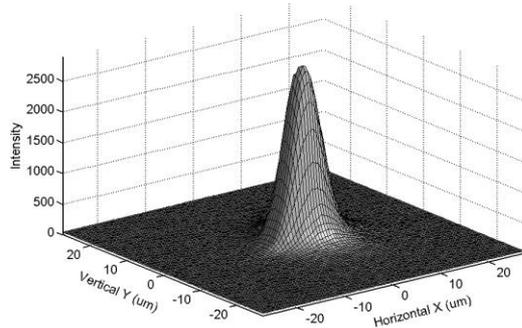
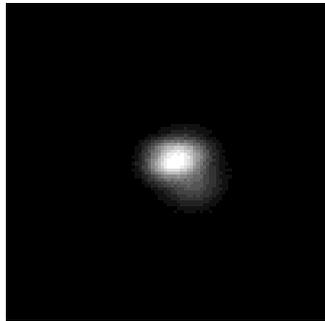
4B - HRM



X-ray

# KB Mirror Performance

- VFM: 1200 (L) x 55 (W) x 47 (H) mm<sup>3</sup>, slope error 0.29 μrad
- HFM: 900 (L) x 50 (W) x 37 (H) mm<sup>3</sup>, slope error 0.71 μrad.
- Measured focal size at sample compare well with designed value of 5 (V) x 7 (H) μm<sup>2</sup>

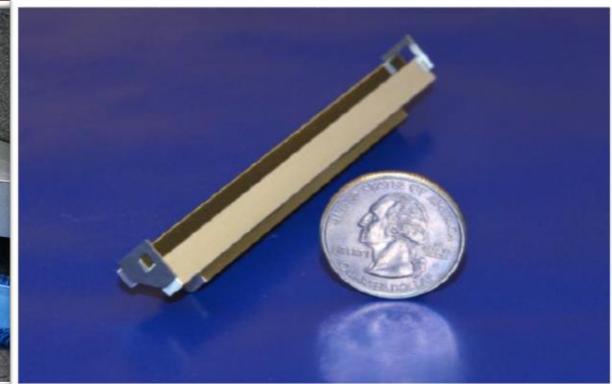


Without CRL's: FWHM = 5.9 (V) x 7.8 (H) μm<sup>2</sup>

With CRL's, beam focus slightly broadened to ~10 x 10 μm<sup>2</sup>

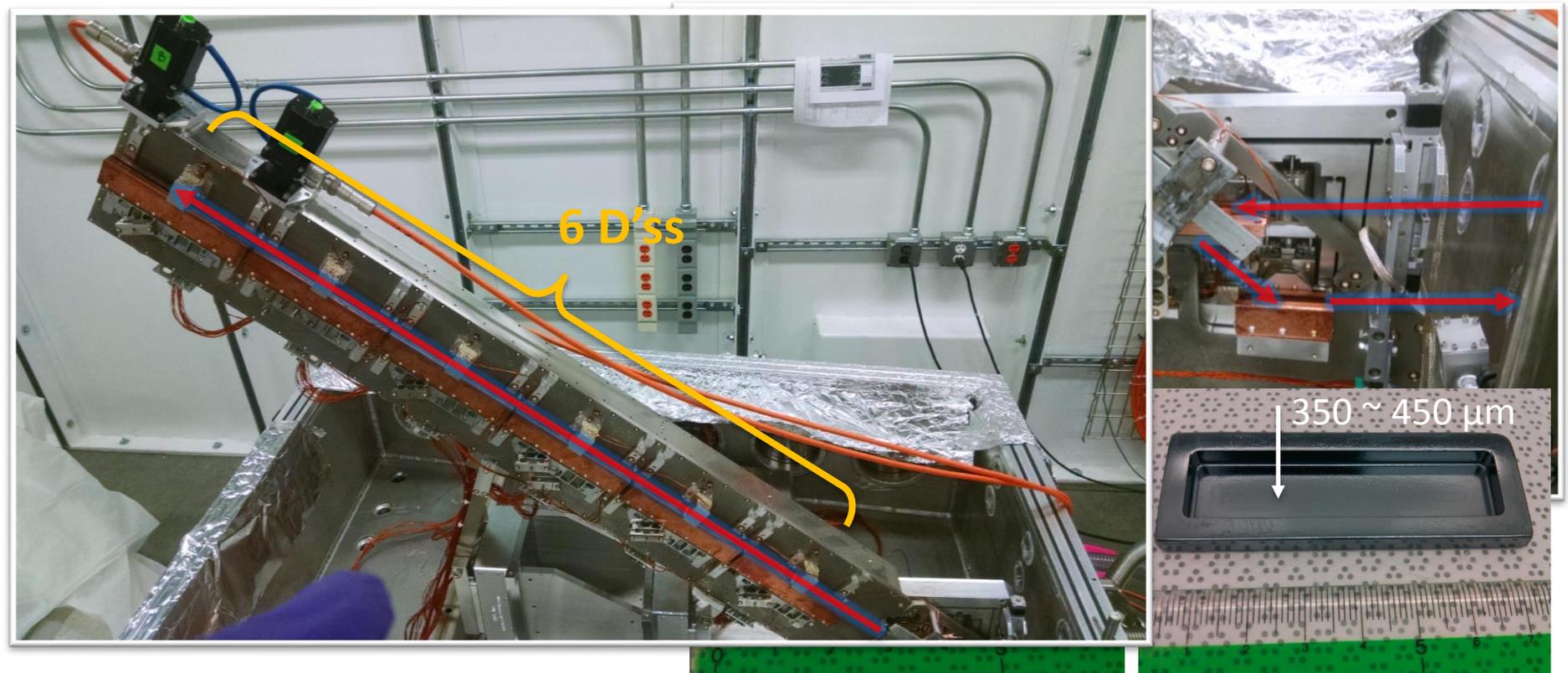
# IXS Spectrometer System

- Montel mirror to provide comparable angular acceptance to spherical diced analyzers @ full illumination:  $\geq 10 \times 10 \text{ mrad}^2$



# CDW Analyzer

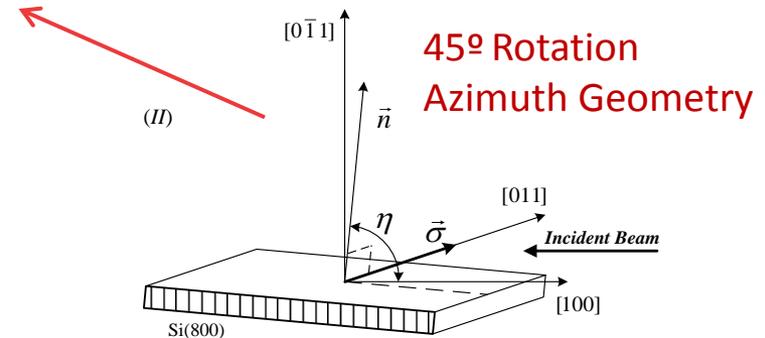
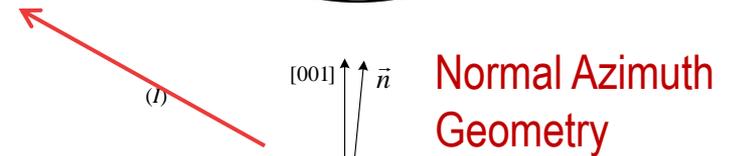
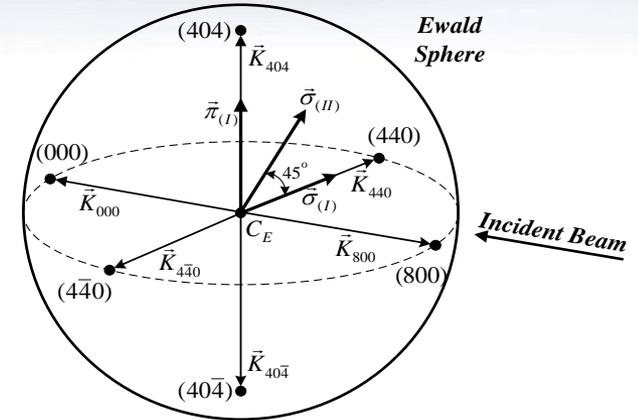
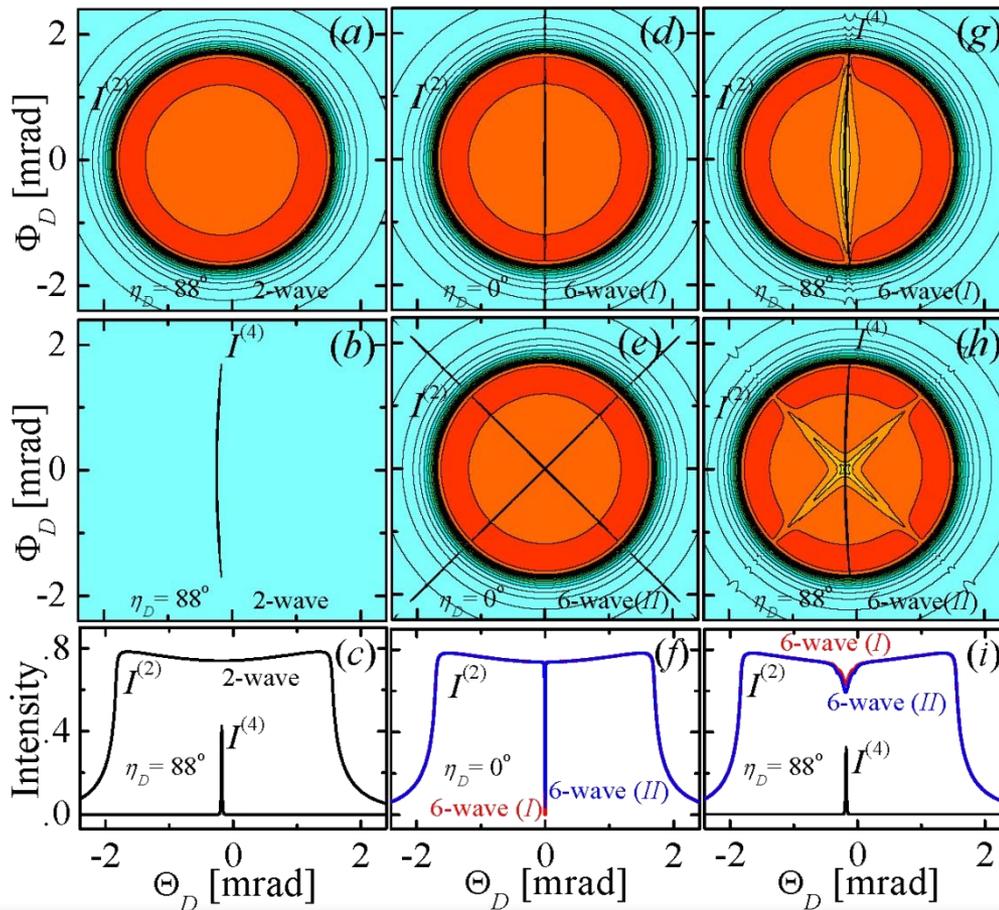
- 6 D crystals, each 200mm long with full position control based on trapezoid flexure, make up a total length of 1.2 m to match the angular acceptance of the Montel mirror.



# Multiple Beam Diffraction Effect

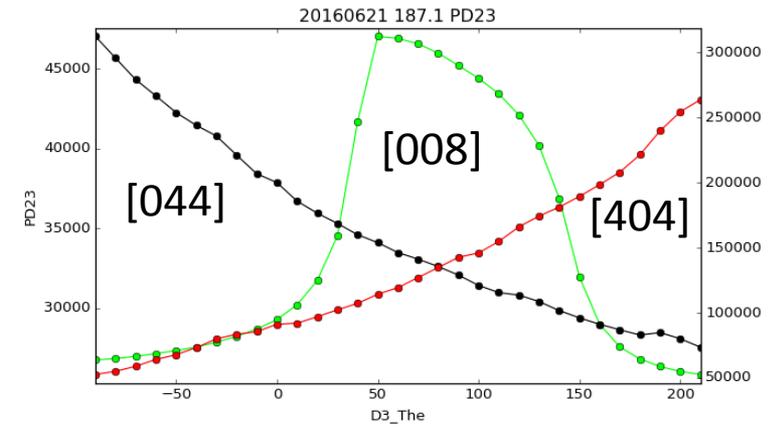
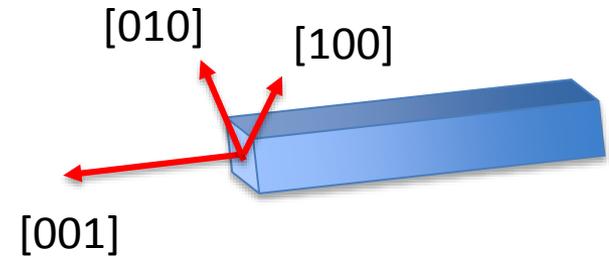
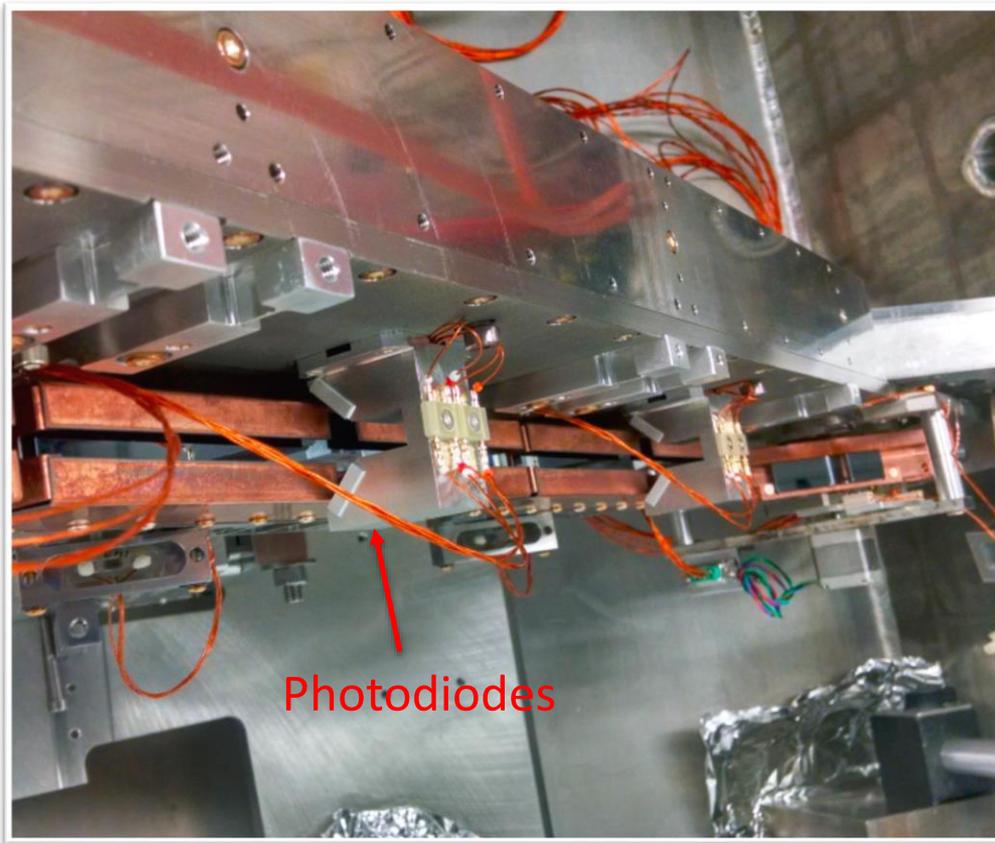
Stetsko *et al*, PRL (2011)

- MBD in CDW/CDDW causes 10-30% loss of spectral efficiency, but can be removed by introducing  $\Phi$  angle offset with the  $45^\circ$  rotation azimuth geometry



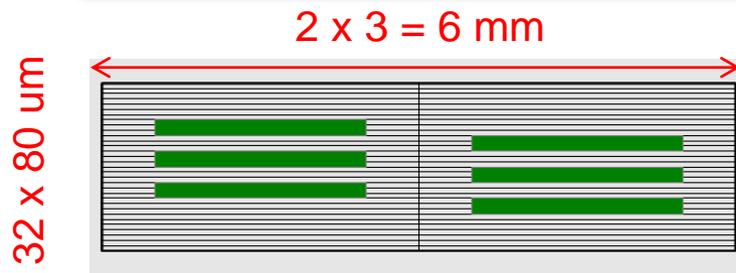
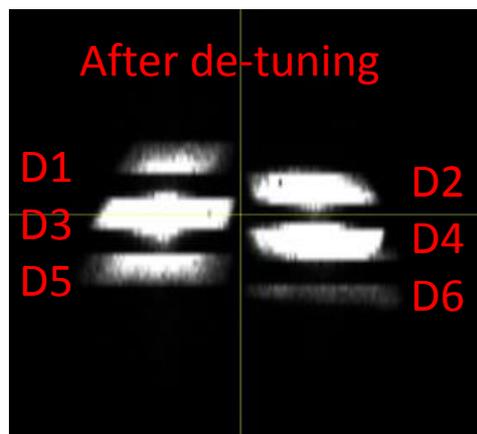
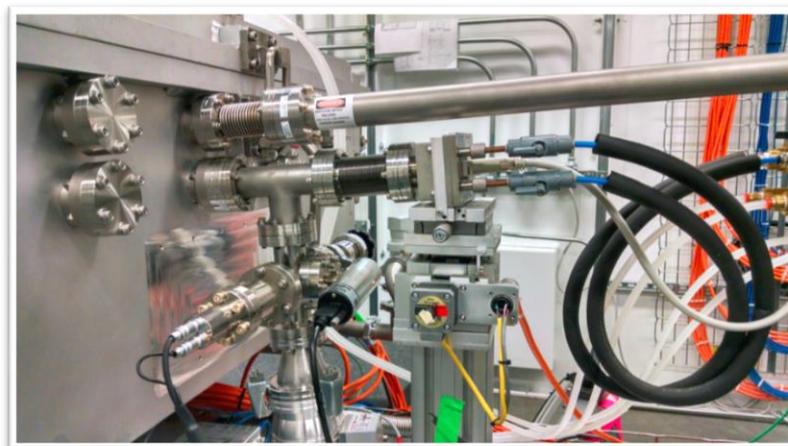
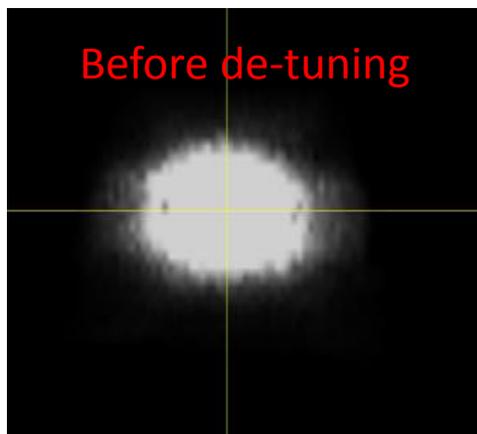
# D Crystal Orientation and De-tuning

- MBD provides the most convenient diagnostic for D crystal alignment.
- Azimuthal de-tuning removes MBD and recovers ~20% of intensity.

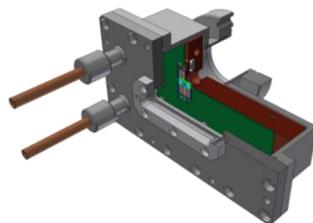


# Azimuthal De-tuning and Tagma Detector

- D crystal azimuthal de-tuning allows separation of individual D reflections.



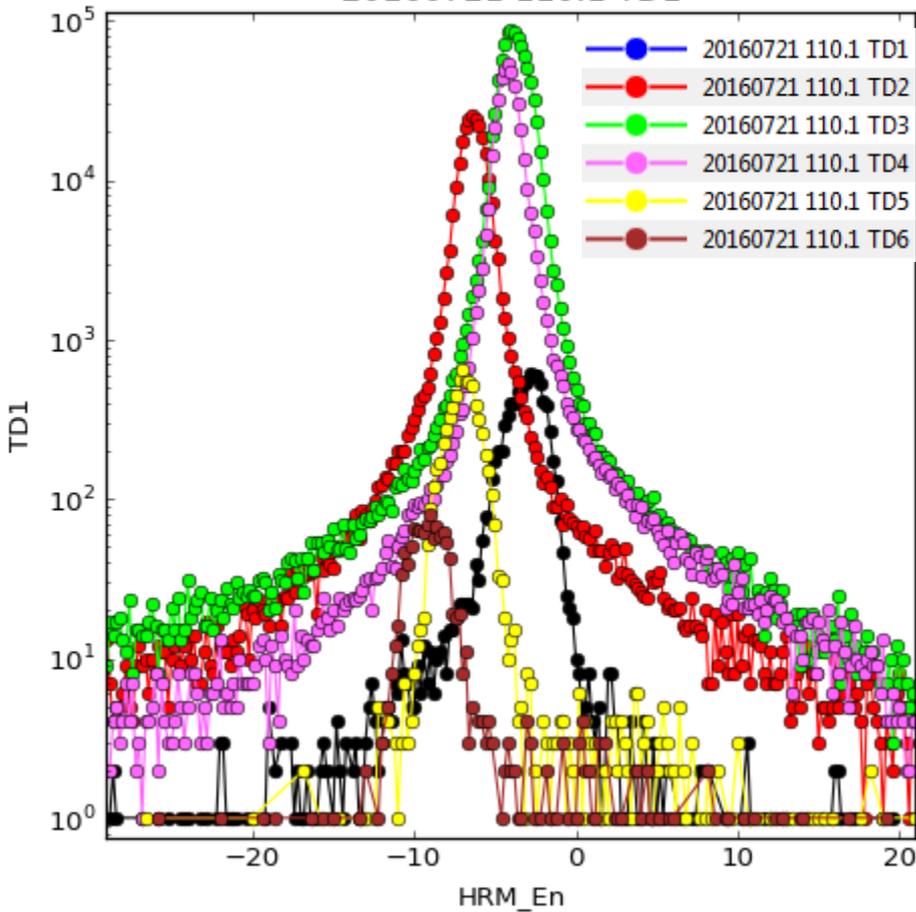
Sensor Board



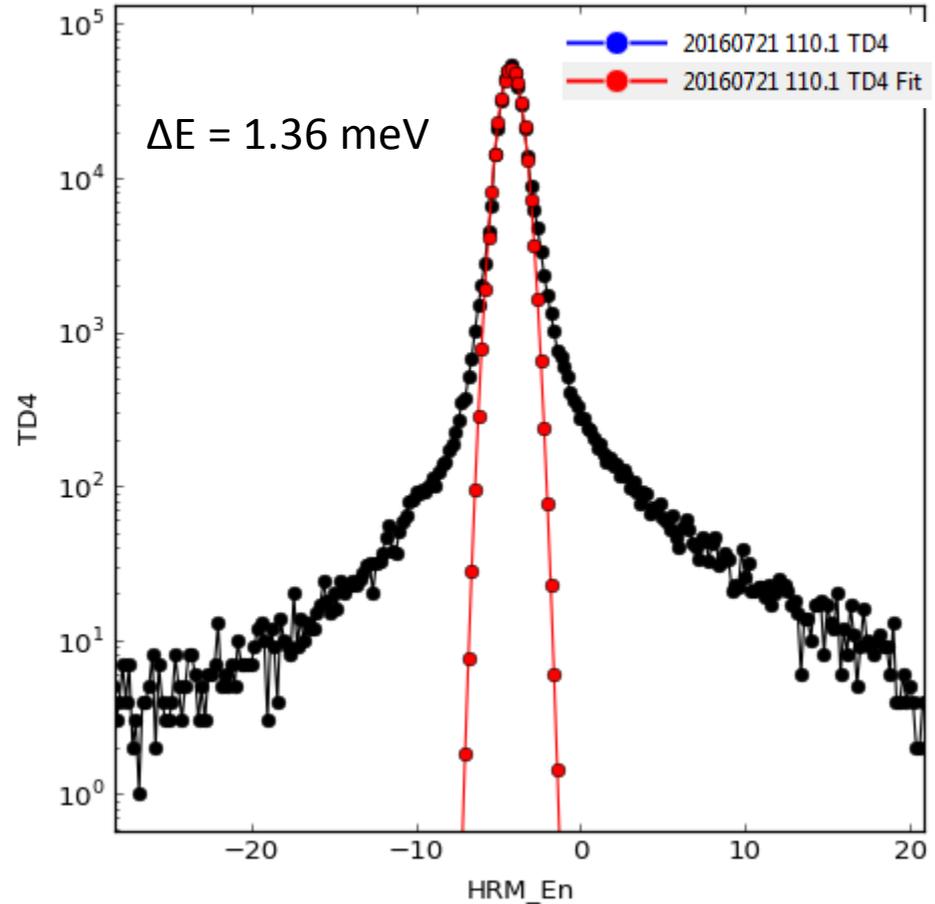
(Keister, et al, J. Phys.: Conf Ser. 2014)

# Resolution Function

20160721 110.1 TD1

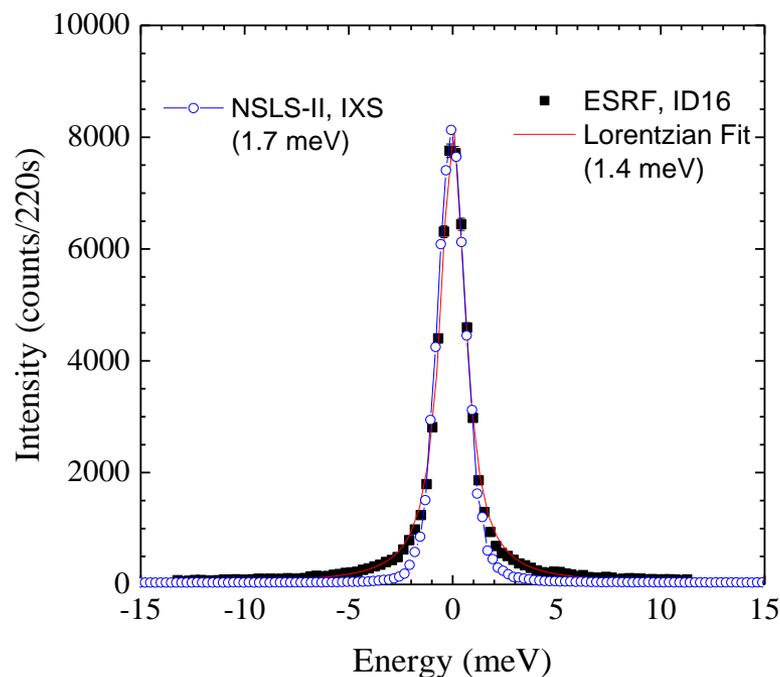
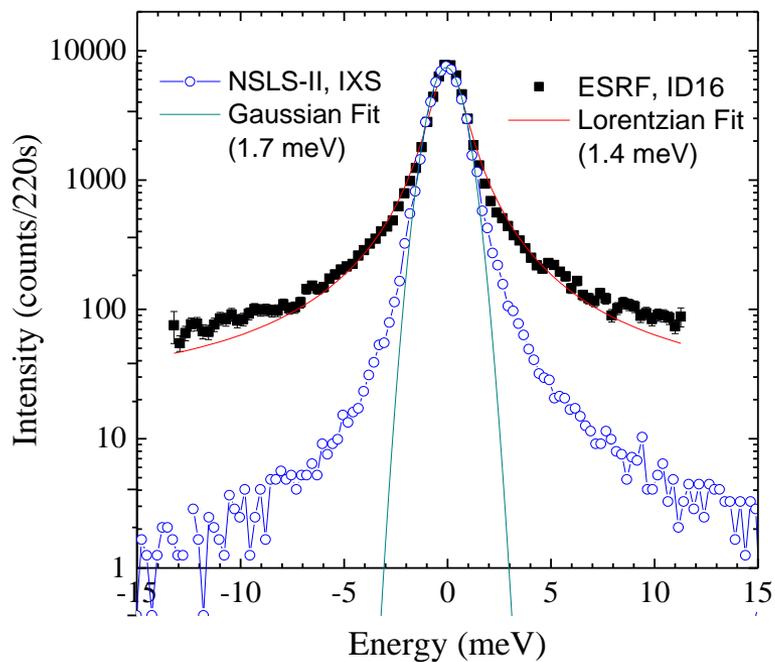


20160721 110.1 TD4



# Resolution Function

- Resolution functions compared to ESRF show significantly sharper tails of the new spectrometer.

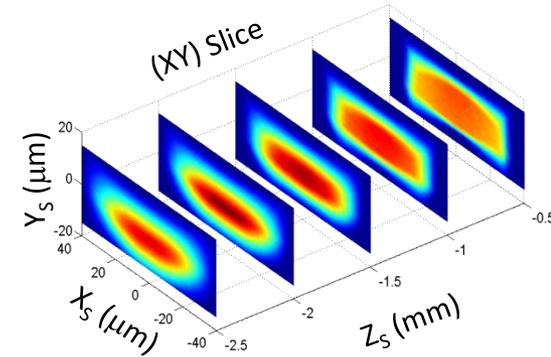
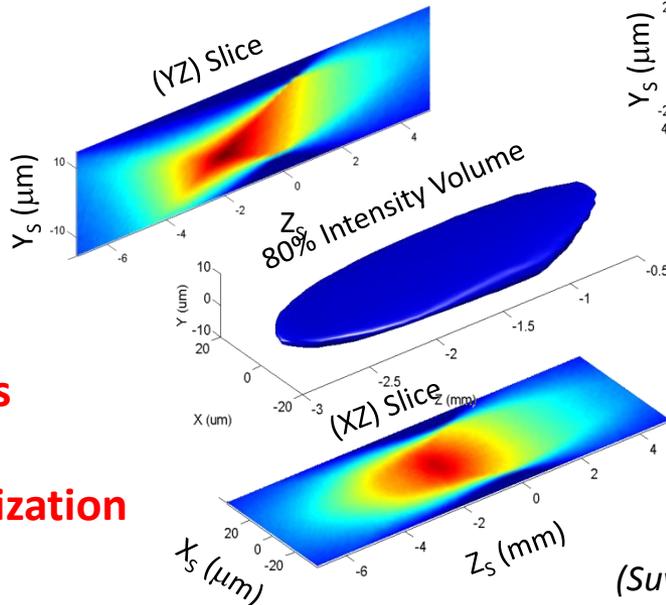
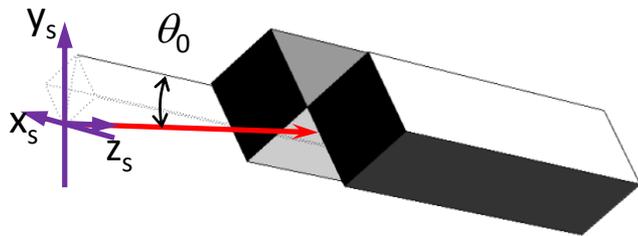


# Slides on Science Commissioning Experiments were removed

# Analyzer Optics: Montel Mirror

- Design (to achieve comparable acceptance to spherical diced analyzers)
  - Angular acceptance @ full illumination:  $\geq 10 \times 10 \text{ mrad}^2$
  - Collimation:  $\leq 0.1 \times 0.1 \text{ mrad}^2$
- Acceptance volume in forward scattering:  $\sim 20 \mu\text{m}$  (X)  $\times 20 \mu\text{m}$  (Y)  $\times 2 \text{mm}$  (Z)
- Vertical divergence of collimating beam: **No effect on energy resolution**
- Horizontal divergence of collimating beam contributes to energy resolution

$$\left( \frac{\Delta E}{E} \right)_H = \frac{\phi^2}{2} \quad : \quad \phi \leq 0.15 \text{ mrad for } 0.1 \text{ meV}; \leq 0.5 \text{ mrad for } 1 \text{ meV}$$



ML Mirror Acceptance Volume Through CDW analyzer

(Suvorov et al, JSR 2014)

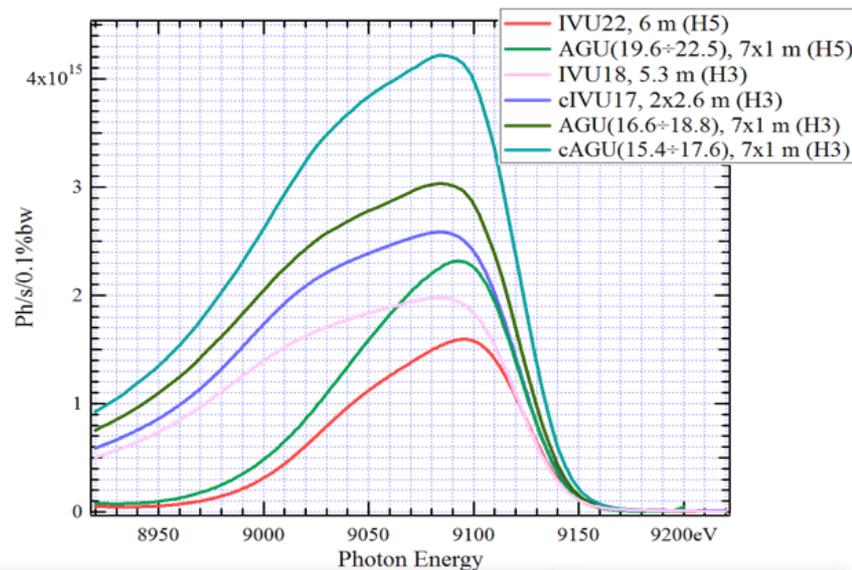
- **Projection of the scatter volume is expected to lead to faster drop of scattered intensity than the polarization factor.**

# Performance Comparisons (current & outlook)

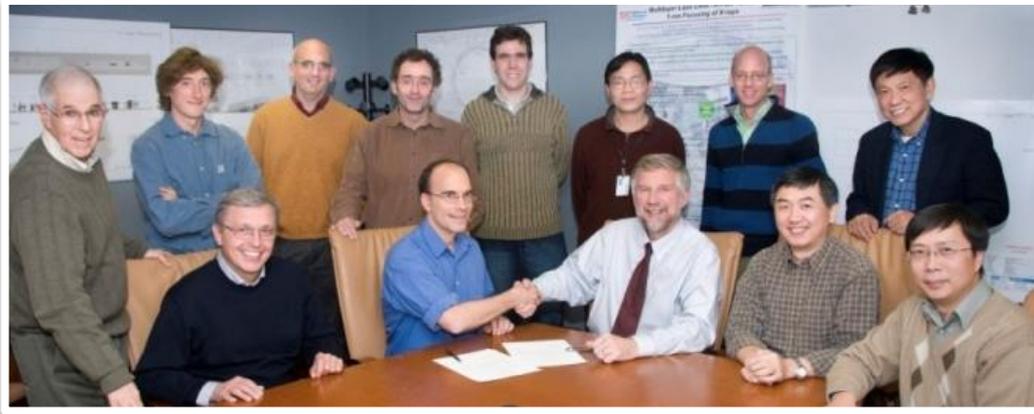
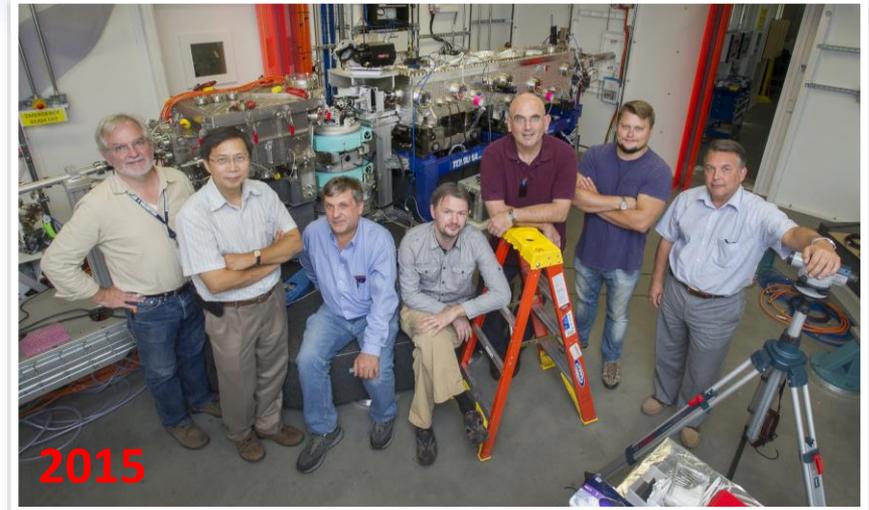
Facility (Beamline)	$\Delta E / E$ (meV) / (keV)	$\Delta Q^{**}$ (nm <sup>-1</sup> )	Flux@sample (photons/sec)	Beam Size (V×H μm <sup>2</sup> )	F.Density@sample (photons/sec/μm <sup>2</sup> )	Analyzer Setup array/MaxSA[mrad <sup>2</sup> ]	Sharp Res. Tails
ESRF (ID28)	1.5 / 21.7	0.5	3.6×10 <sup>9</sup>	13×6	4.6×10 <sup>7</sup>	9x1 array / [Φ14] ea.	--
APS (30-ID-C)	1.5 / 23.7	0.6	5×10 <sup>9</sup>	20×35	7.1×10 <sup>6</sup>	9x1 array / [Φ11] ea.	--
SPring-8 (43LXU)	1.3 / 21.7	0.5	2.0×10 <sup>10</sup>	50×12	3.3×10 <sup>7</sup>	11x4 – 2 array / [9.4 x 8.9] ea.	--
NSLS-II (IXS)	1.7 / 9.1	0.2	4×10 <sup>9</sup> *	5×7	3.4×10 <sup>7</sup>	Single / [15 x 15]	yes

\*projected flux @ 500mA, 1.2×10<sup>9</sup> measured @ 150mA; \*\* Q resolution @ 5 mrad angular acceptance.

- **Undulator upgrade can achieve a potential flux gain by more than 5 times** (using cAGU-7x1m), providing a total flux @ 9.1 keV of > 2×10<sup>10</sup> photons/sec/meV. **Comparable to SPring-8 43LXU**
- **Factor of ~2 improvement with better crystals**
  - Montel mirror measured reflectivity: 42%
  - Current CDW analyzer efficiency: ~20%
- **More Analyzers**



# Thank You for your attention!



**BAT MOU, Dec 8, 2008**



**EFAC members (2007)**