Status of the IXS Beamline and Scientific Capabilities

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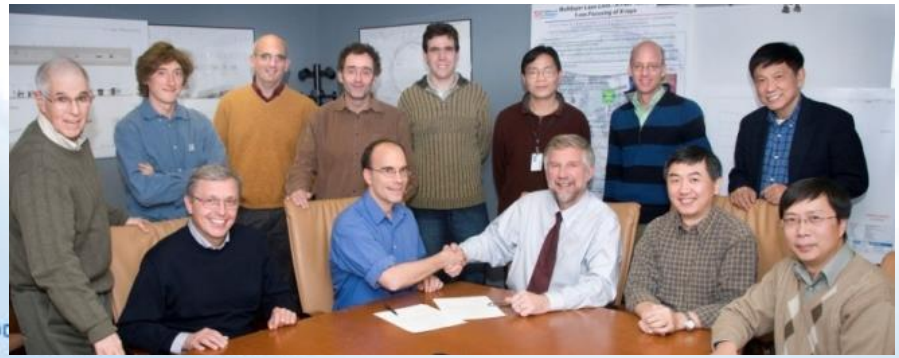
BROOKHAVEN NATIONAL LABORATORY
a passion for discovery

Office of Science

Acknowledgements

- **NSLS-II IXS Team Members**
  - Alessandro Cunsolo, *IXS Beamline Scientist*
  - Alexey Suvorov, *X-ray Optics Scientist*
  - Jeff Keister, *R&D Beamline Scientist*
  - Scott Coburn, *Senior Engineer*
  - Stephen Antonelli, *Engineer*
  - Leo Reffi, *Designer*
  - Gary Whitbeck, *Designer*
  - David Levy, *Technician (BL Support)*
  - Bill Struble, *Technician (Crystal Fabrication)*
  - Nalaka Kodituwakku, *Crystal Fabrication*
  - Yuriy Stetsko, *X-ray Optics*
  - Xianrong Huang, *X-ray Optics (APS)*
  - Marcelo Honnicke, *Multilayer Mirror (Goias, Jatai, Brazil)*
  - Zhong Zhong, *X-ray Optics*

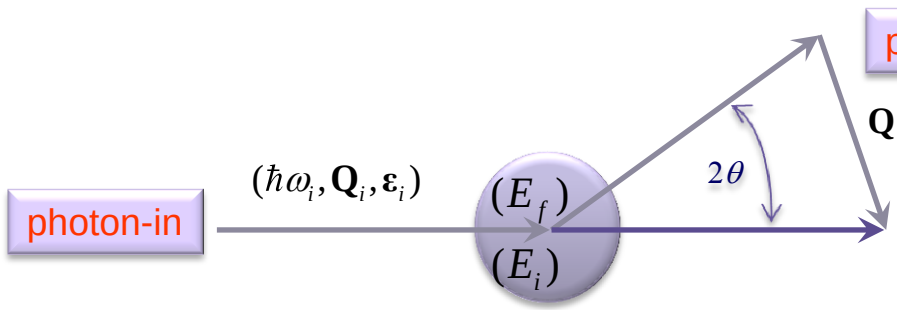


- **Beamline Advisory Team (BAT)**
  - Clement Burn (Spokesperson), *WMU*
  - Alfred Baron, *RIKEN/SPring-8*
  - Sow-Hsin Chen, *MIT*
  - John Hill, *BNL*
  - Michael Krisch, *ESRF*
  - Ho-kwang (David) Mao, *Carnegie*
  - Tullio Scopigno, *Univ. Roma*
  - Stephen Shapiro, *BNL*
  - Yuri Shvyd'ko, *APS*

Inelastic X-ray Scattering

- A photon-in photon-out probe with a rather weak scattering cross section

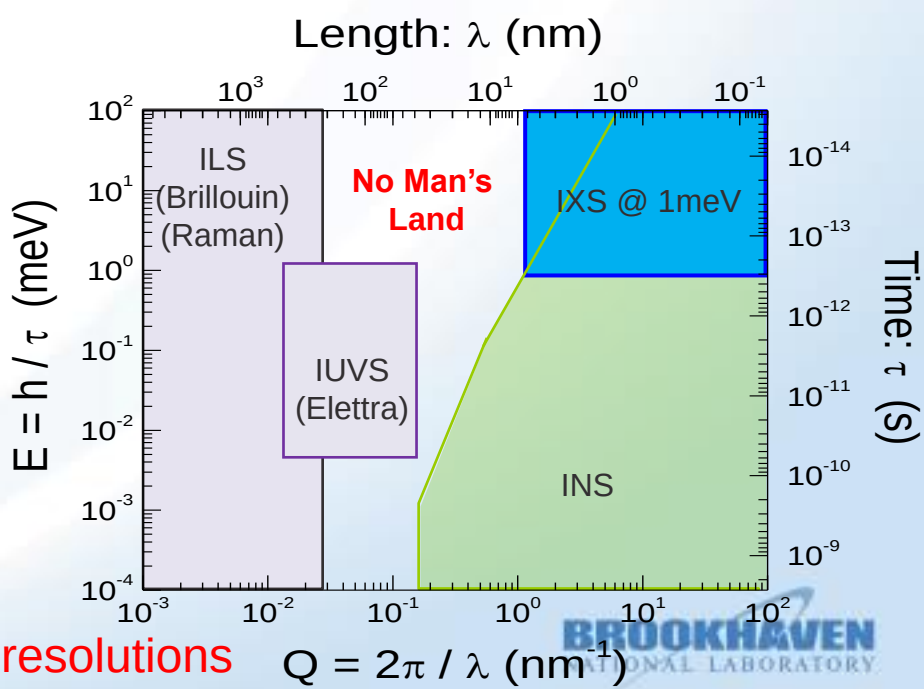
$$\frac{d^2\sigma}{d\Omega d\omega}(\mathbf{Q},\omega) = Nr_e^2(\boldsymbol{\varepsilon}_i\cdot\boldsymbol{\varepsilon}_j)^2\frac{E_f}{E_i}\left[f^2(Q)S_{ion}^{coh}(\mathbf{Q},\omega)+zS_{val}^{inc}(\mathbf{Q},\omega)+(Z-z)S_{ion}^{inc}(\mathbf{Q},\omega)\right]$$



$$\hbar\omega = E_i - E_f = \hbar\omega_i - \hbar\omega_f$$

$$Q = \left|\mathbf{Q}_i - \mathbf{Q}_f\right| = (4\pi/\lambda)\sin(2\theta/2)$$

- Coupling to matter
  - Coupled directly to the electronic charge
  - Lattice excitations via coherent scattering (equivalent to INS)
  - High penetration, truly bulk-sensitive
  - Element, charge and spin specific
  - Applicable to systems under extreme environments, and systems that are not compatible with vacuum (e.g., liquids)



Accessible (E,Q) range limited by achievable resolutions

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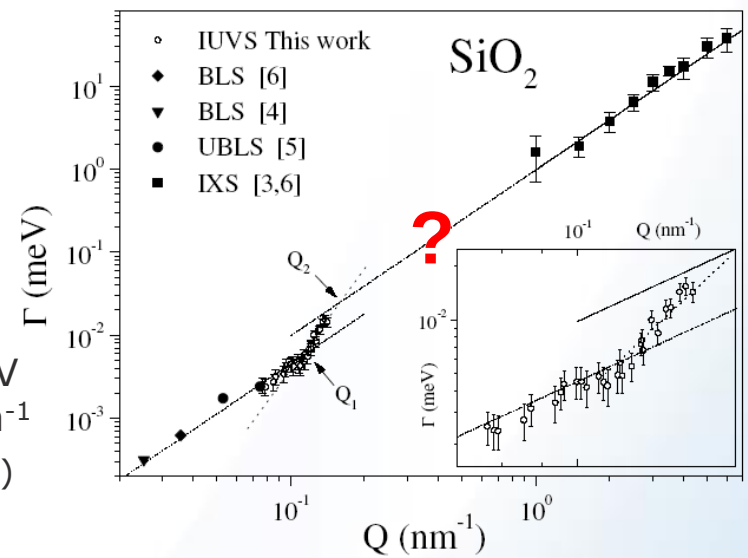
The Need for Higher Resolution in E, Q

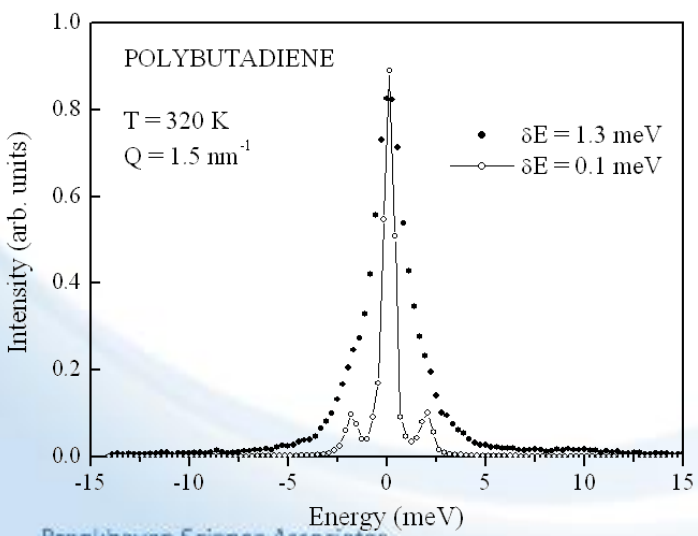
- Better defined energy position
  - Viscoelastic transitions in liquids/glasses
  - Phonon dispersion curves in crystals
- Better defined line width
  - Dynamical heterogeneities in glasses
  - Phonon lifetime

SiO_2: Change in acoustic damping @ 0.01meV < E < 1meV
0.1nm^{-1}< Q < 1nm^{-1}

Masciovecchio et al., Phys. Rev. Lett. 97, 035501 (2006)

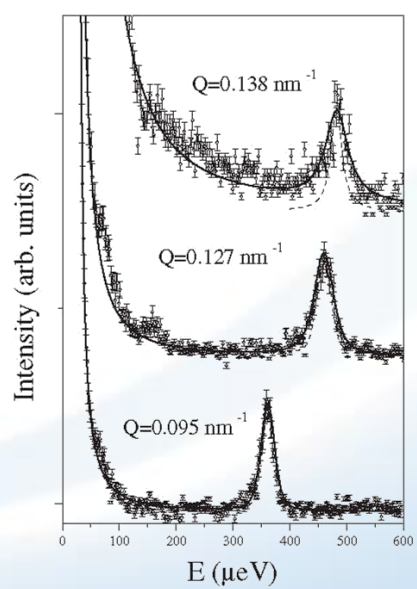


- 1 meV resolution often not sufficient to resolve 1 meV excitations due to strong quasi-elastic tails

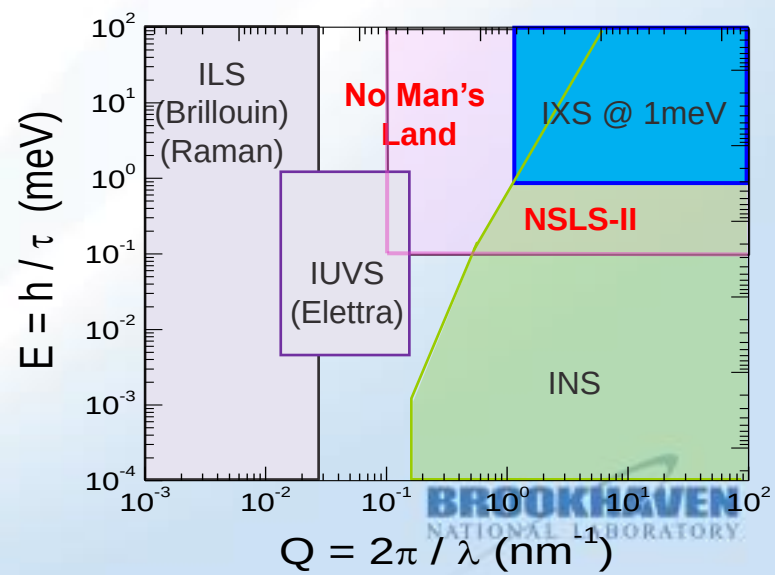


Fioretto et al., Phys. Rev. E (1999)

IUVS: ΔE~ 0.014 meV



"Filling in the Gap"

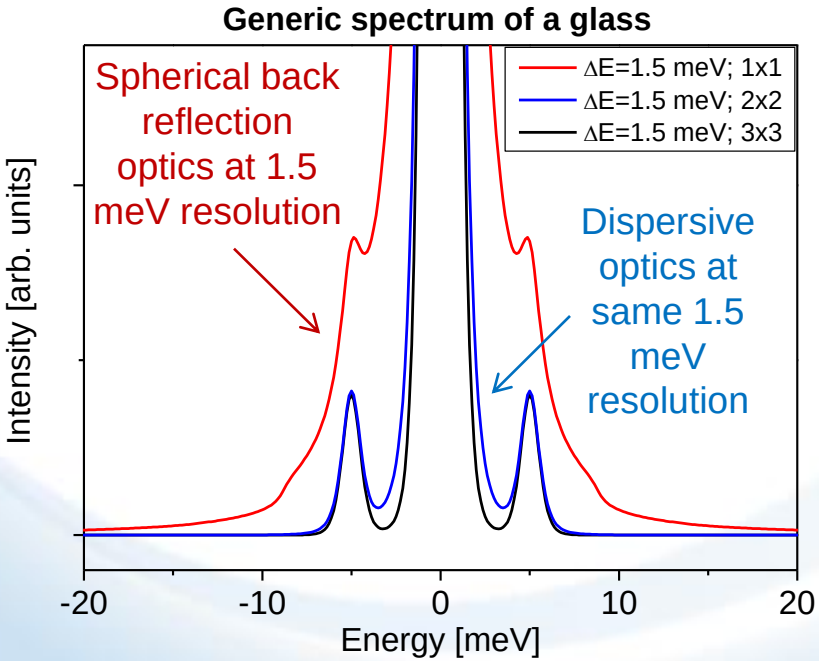


Spectral Contrast Matters

- Better defined line shape
  - Biological systems (membranes)

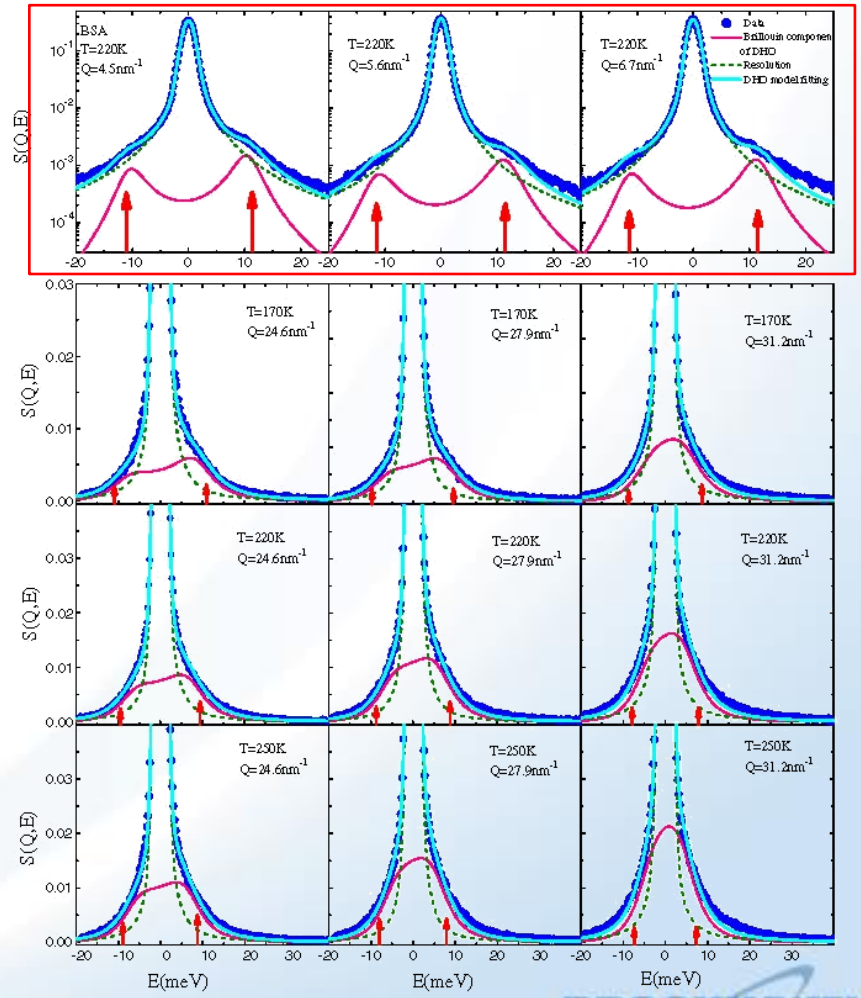
Phonon modes @ E ~ 10 meV
Q ~ 10 nm^{-1}

- Improving contrast is also important!



Phonon-like low-energy excitations

PRL **101**, 135501 (2008) ***Liu and Chen, et al.***



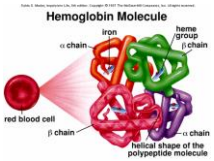
APS 30-ID, E = 23.724 keV, ΔE = 1.5 meV

The Relevant Length Scales

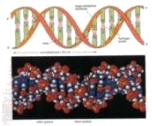
- Better Q resolution allows access to the mesoscopic length scale (5 ~ 50 nm, part of "no-man's land")
  - Fast dynamics of bio-molecular systems
  - Phonons in functional nanoparticle assemblies
  - Intermediate regime in disordered systems

Size (nm)

10^0 10^1 10^2

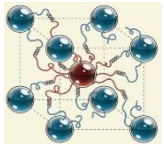


Hemoglobin

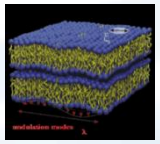


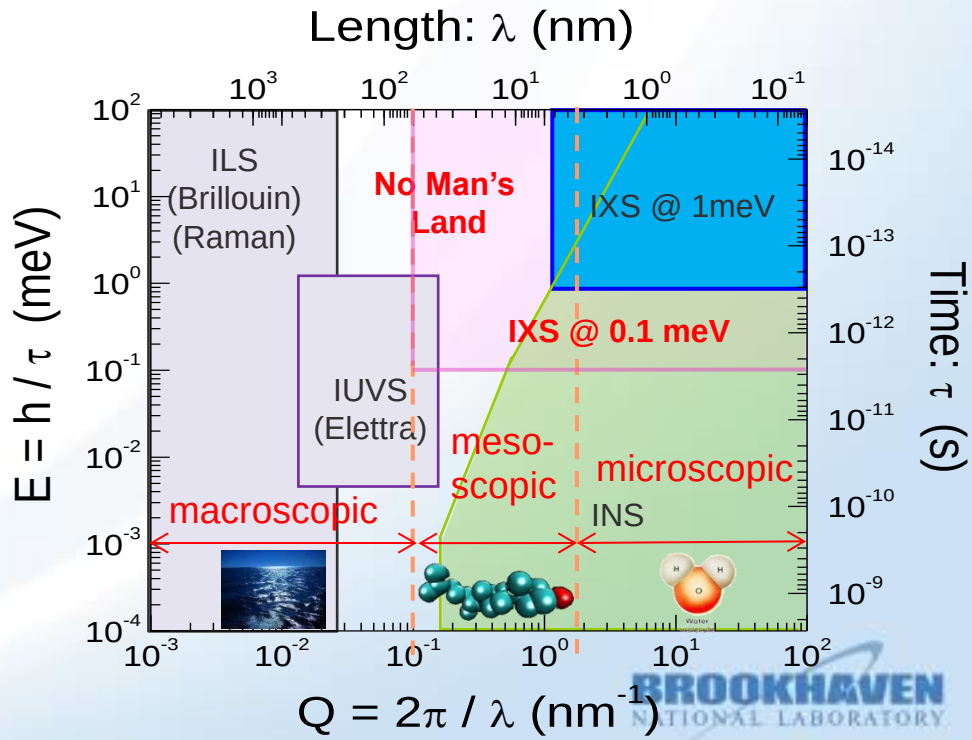
DNA

Super-lattices of nanoparticles



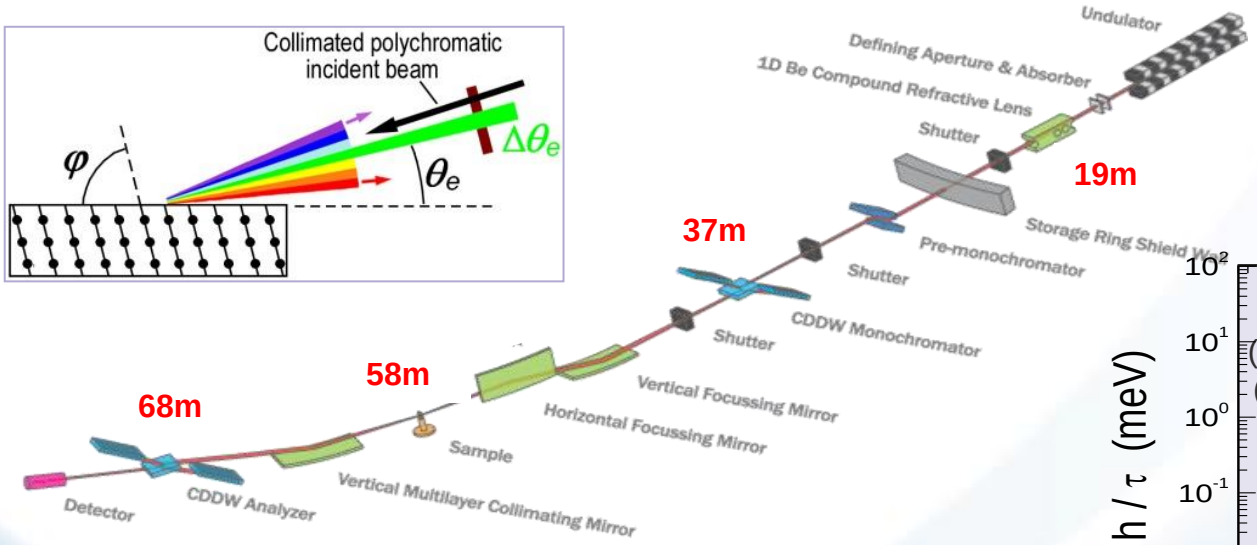
Lipid membrane





NSLS-II IXS Beamline Overview

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



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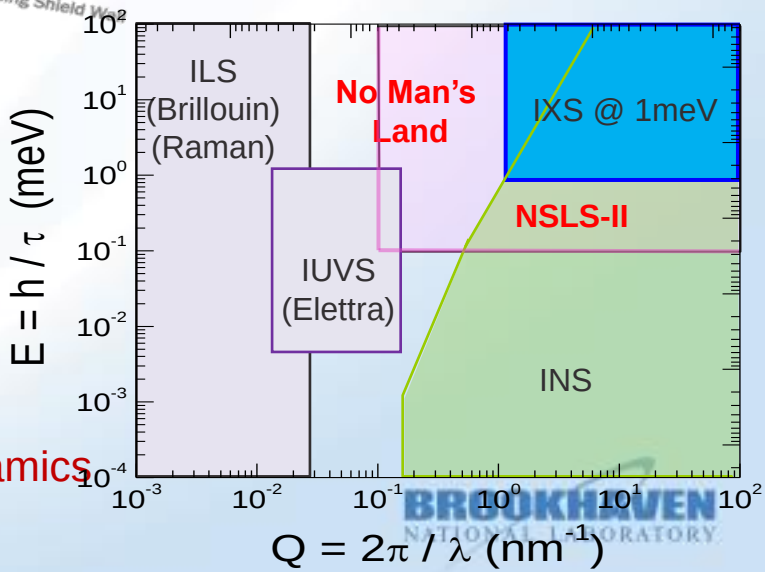
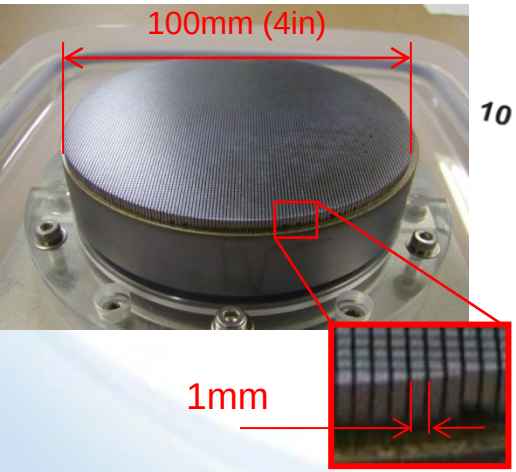


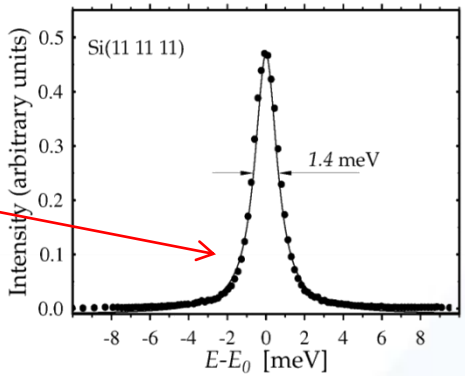
Ultimate Goal:

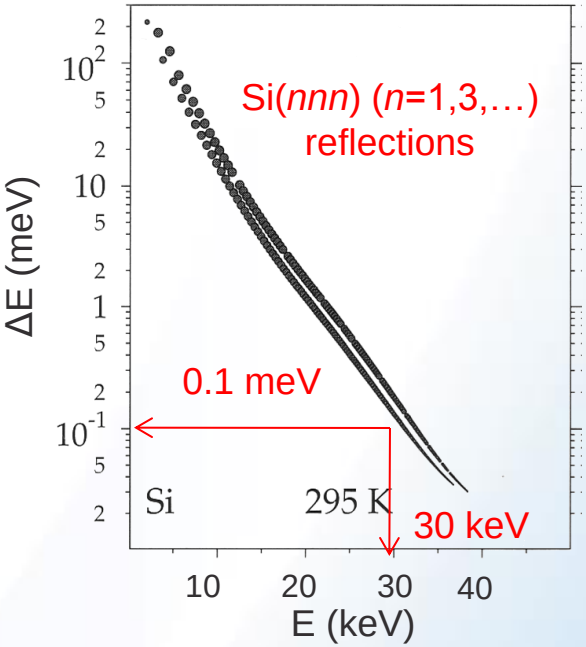
World-leading 0.1 meV energy resolution for studying dynamics

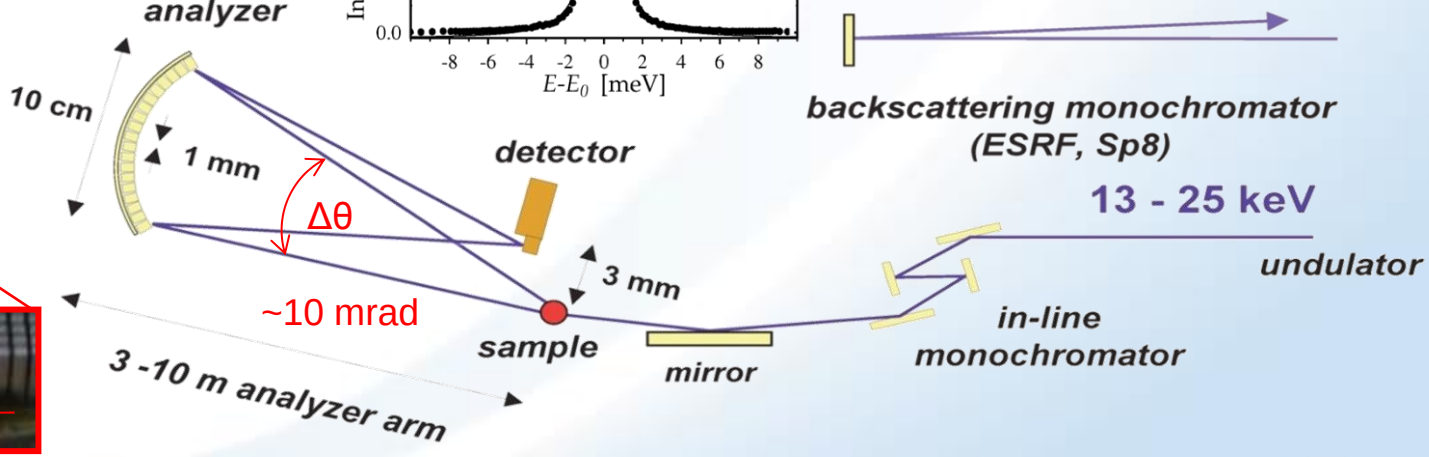
meV IXS: Current Status

- HR optics based on high-order symmetric Bragg back reflections of Si(nnn) (n = 7 - 13)
- Practical E,Q resolutions are flux limited to ~1.5 meV and ~ 0.5 nm^{-1} (i.e., 5 mrad acceptance @ 21.7 keV)
- Spherical diced analyzer to achieve large angular acceptance (~10 mrad)
  - Individual Si blocks (~0.8x0.8x3 mm^3)
  - Lorentzian tails







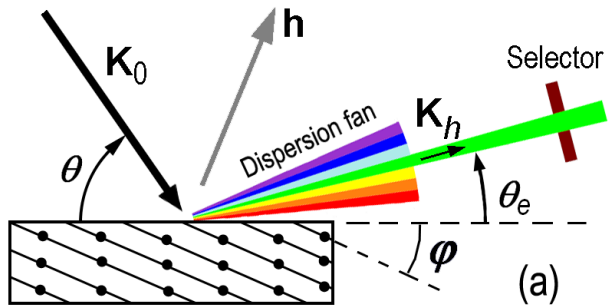


Higher energy resolution requires higher incident energy
→ Incompatible with undulator performance

Principles of Angular Dispersion Optics

Polychromatic

$$\mathbf{K}_{h\|} = \mathbf{K}_{0\|} + \mathbf{h}_{\|}$$



$$\cos\theta_e = \cos\theta + \frac{\sin\varphi}{d}\lambda$$

$\theta = \text{const}$

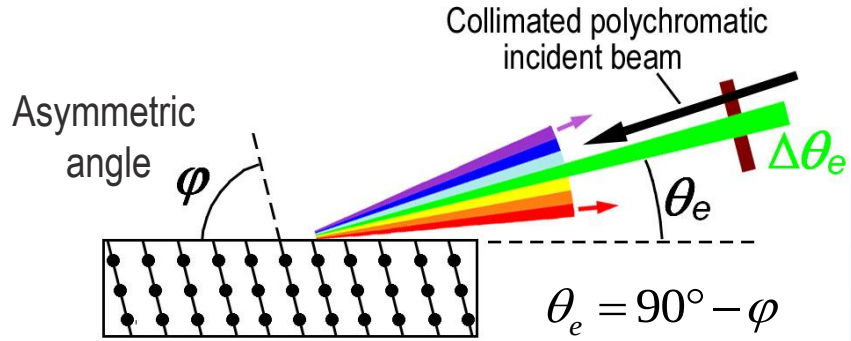
$$\frac{\Delta\theta_e}{\Delta\lambda} = -\frac{\sin\varphi}{d\sin\theta_e}$$

Rigorous !

- Different wavelengths λ diffracted along different directions

(Y. Shvyd'ko, 2006; X. Huang, 2008)

Dispersion maximized in **Grazing Backscattering:**



$$\theta_e = 90° - \varphi$$

$$\frac{\Delta\theta_e}{\Delta\lambda} = -\frac{\sin\varphi}{d\sin(90° - \varphi)} = -\frac{\tan\varphi}{d}$$

$$\frac{\Delta E}{E_H} = \frac{\Delta\theta_e}{2\tan\varphi} \quad \text{where} \quad E_H = \frac{hc}{2d}$$

Si (008), $E_H \approx 9.1$ keV

$\Delta\theta_e = 5$ μrad, $\varphi = 89.6°$

$\Rightarrow$ **ΔE = 0.2 meV**

- Resolution determined by φ and $\Delta\theta_e$, Independent of spectral Darwin width

→ Sub-meV resolution at ~10 keV

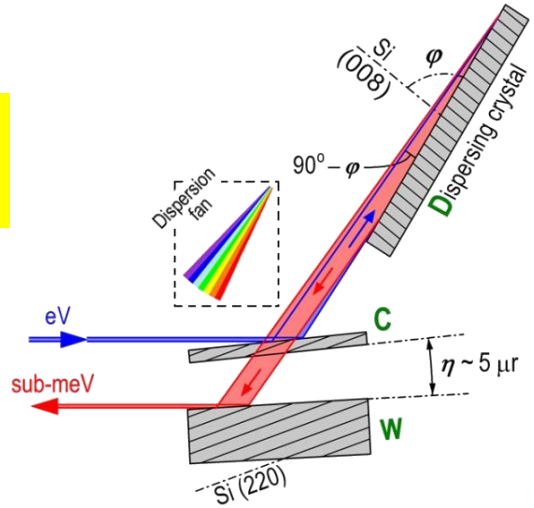
→ Higher Q resolution (~0.2 nm^{-1} @ 5mrad)

CDW & CDDW Schemes

- Proposed by Shvyd'ko (2004, PRL 2006)
- Based on angular dispersion effect in asymmetric Bragg reflections.

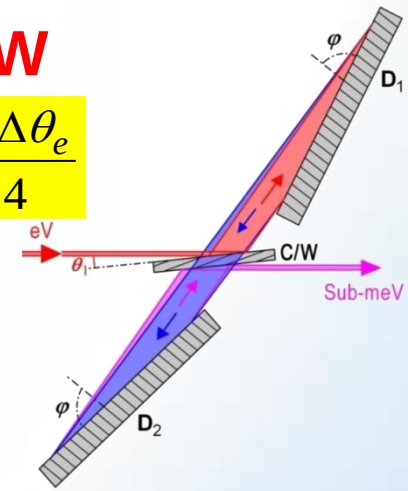
CDW

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



CDDW

$$\frac{\Delta E}{E} \approx \frac{\theta_e \Delta\theta_e}{4}$$



→ Operate at E = 9.13 keV

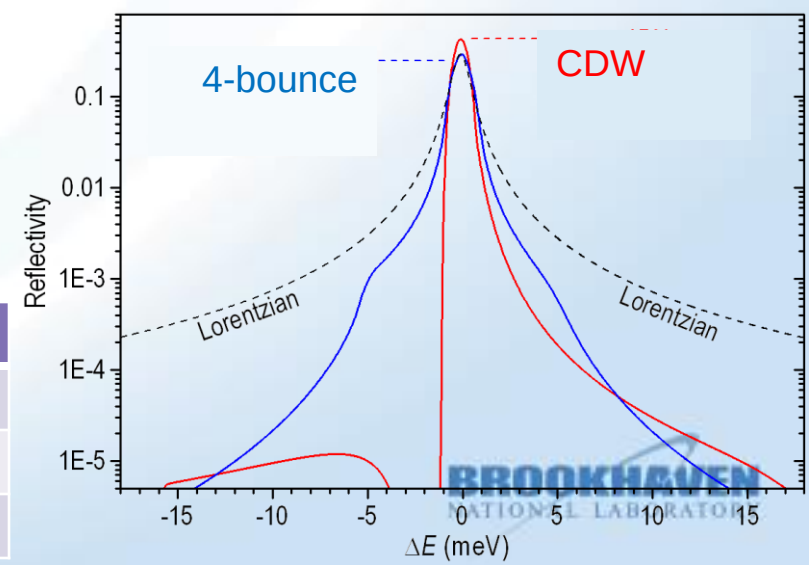
→ Angular acceptance ~100 μrad

→ High peak reflectivity ~40%

→ Sharp tails (multiple reflections and anomalous transmission)

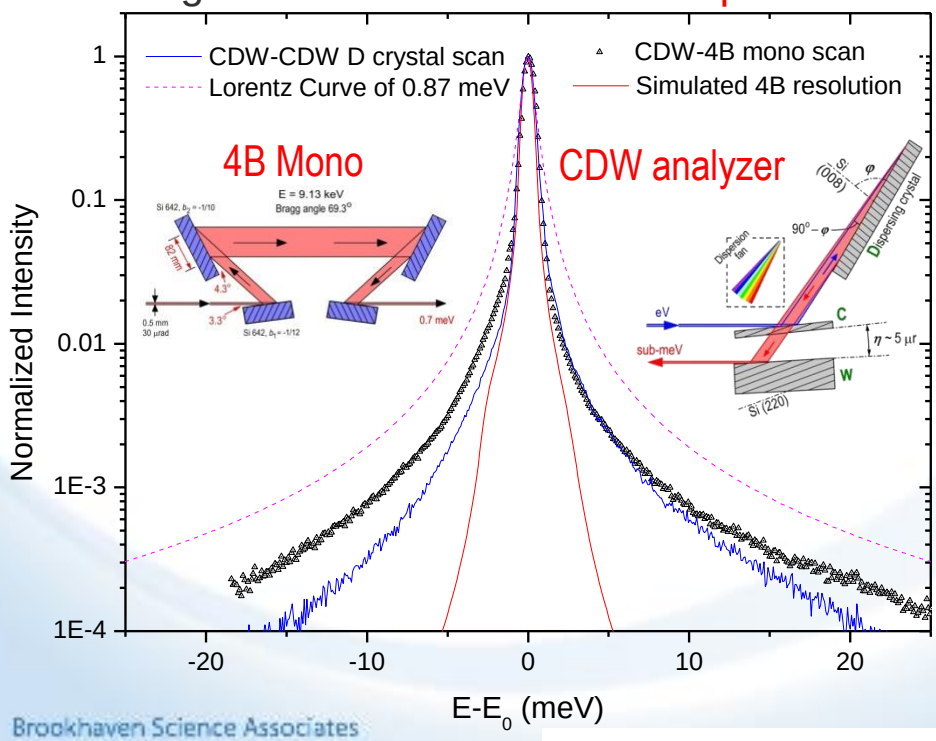
- Major parameters for $\Delta\theta_e$ = 5 μrad, and vertical beam h = 0.5 mm

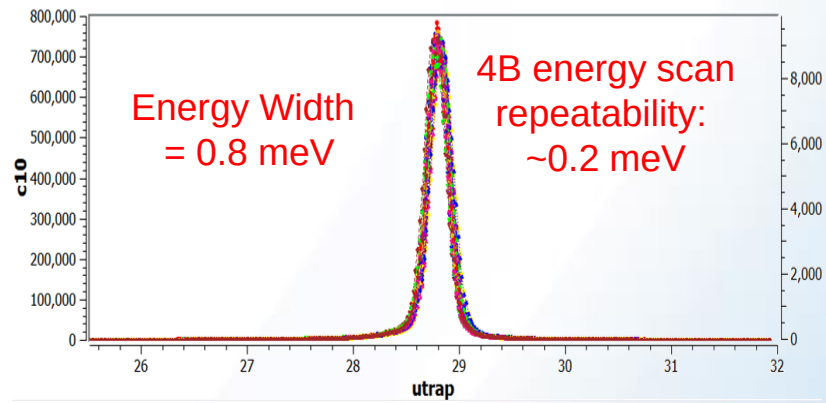
ΔE of CDW	ΔE of CDDW	Θ_e (= 90° – φ)	Length of D
2 meV	1 meV	4.5°	120 mm
0.7 meV	**0.3 meV**	**1.5°**	**380 mm**
0.2 meV	**0.1 meV**	**0.4°**	**1400 mm!**

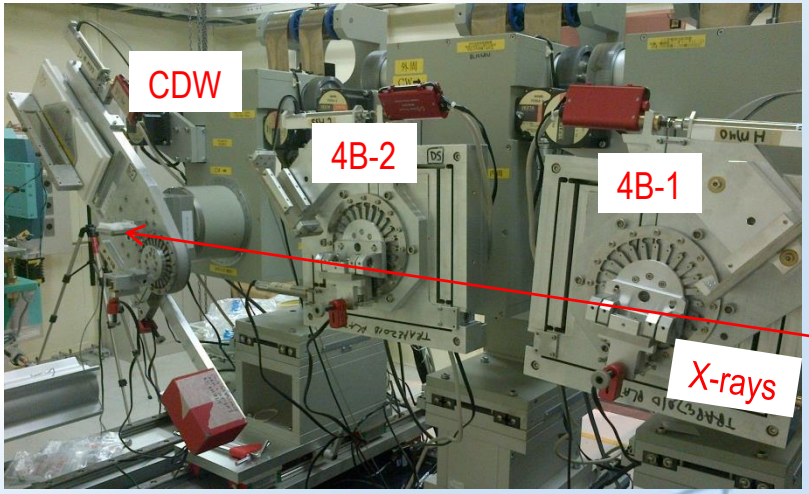


High-Resolution Crystal Optics R&D

- 2008 – 2013: Achieved the initial goal of sub 1 meV resolution.
- Key performance parameters demonstrated include:
  - CDW analyzer (de-convoluted) resolution < 0.7 meV,
  - 4B-CDW combined resolution 0.8 meV,
  - 4B-HRM efficiency ~30% (Theory: ~35%), CDW analyzer efficiency ~20% (Theory: ~38%)
  - Sharp Gaussian-like tails to ~2 orders of magnitude – room for further improvement!





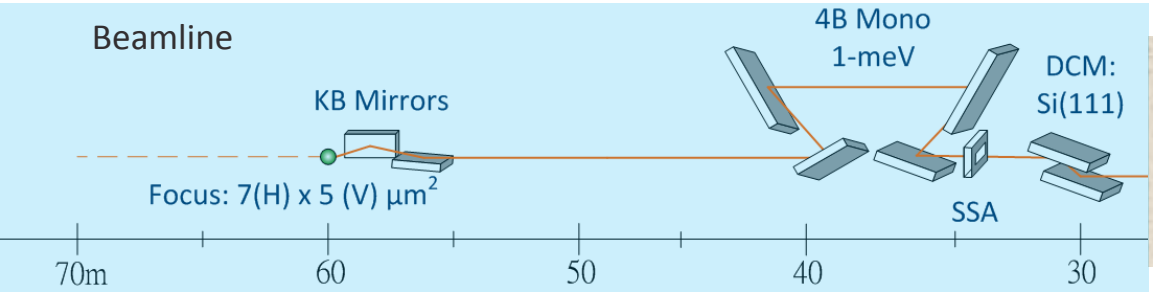


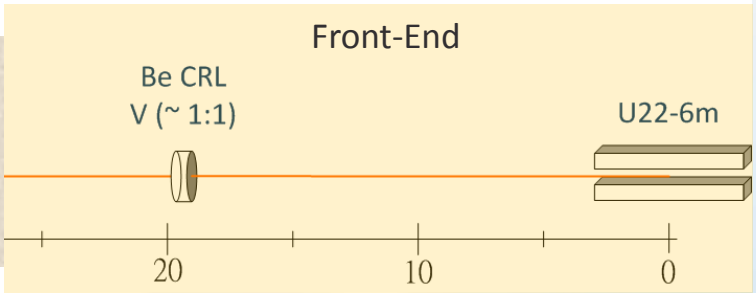
4B-CDW setup

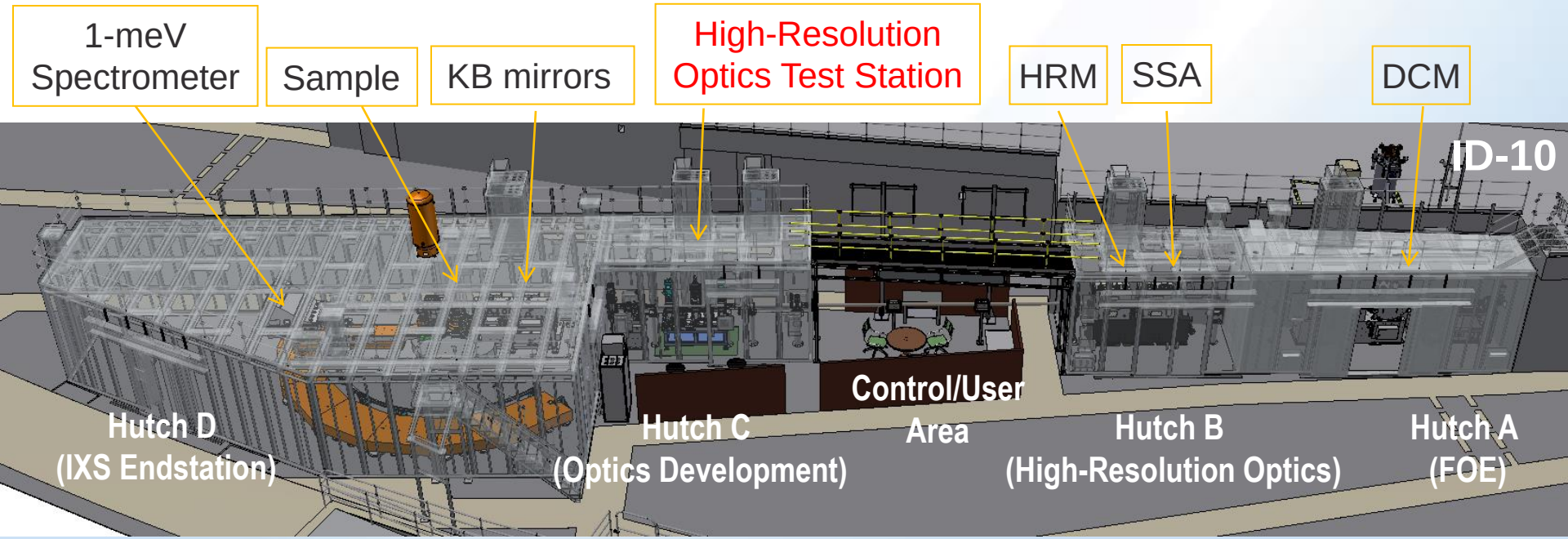
(Cai et al, J. Phys.: Conf. Ser. 425, 202001; Keister et al, J. Phys.: Conf. Ser. 425, 052032)

Beamline Design

- Be-CRLs for ~1:1 focusing at SSA (Vertical beam size ~30 µm FWHM, critical for 0.1 meV with CDDW scheme)
- HRM: inline 4B design (base line scope) for 1 meV.
- KB Mirrors: large demagnification with bendable plane ellipse figure for fine focus on sample
- High-resolution optics test station: support continuing development towards 0.1 meV.

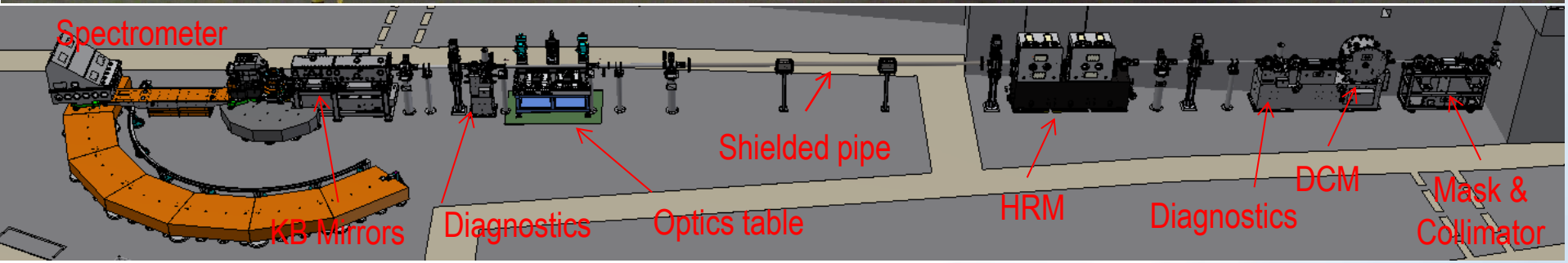






Beamline Development Status

- All hutches now completed, utilities installation in progress



- Components installation to be completed and ready for beam May 2014.
- Total technical commissioning time estimated: ~ 9 months (150 beam days)

NSLS-II Project Beamlines	2014												2015												2016											
	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D
Inelastic X-ray Scattering (IXS)																																				
IXS 1 meV instrument																																				

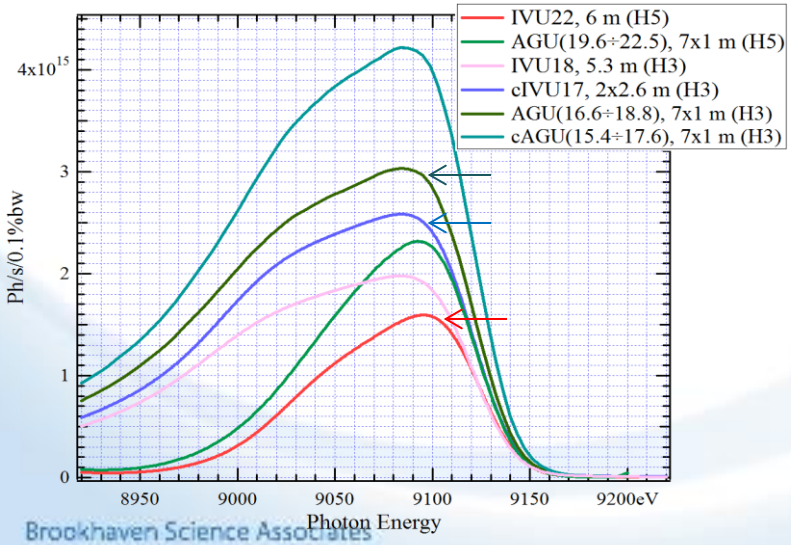
- Science Commissioning / User Experiments expected by April 2015

IXS Insertion Device

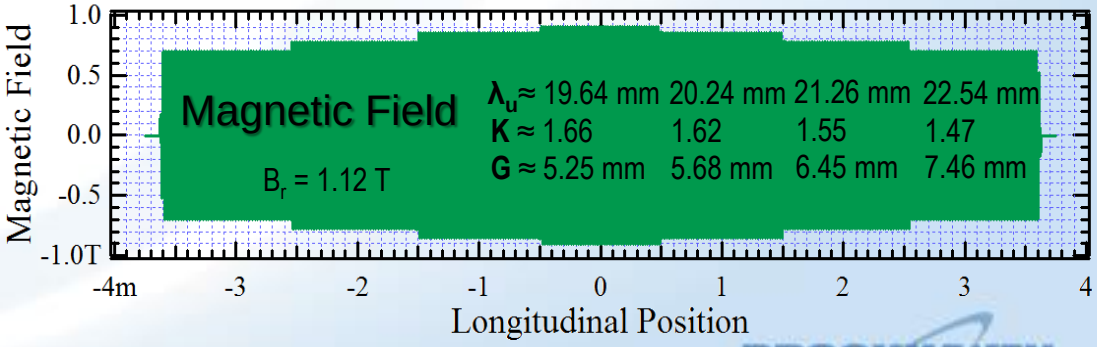
- IVU22-6m: fully optimized RT device to produce maximum flux at 9.1 keV: ~1.6×10^{15} photons/sec/0.1%bw
- Baseline: IVU22-**3m**, installation scheduled for May 2014.
- Upgrade options

  Possibilities includes(from Oleg Chubar)
  - cIVU17, 2x2.6m (3rd Harmonic), ~ 3X more than IVU22-3m
  - AGU (16.6~18.8mm), 7x1m (3rd Harmonic), ~ 4X more than IVU22-3m

Name	IVU22-6m
Type	PMU (NdFeB@300K)
Period (mm)	22
Length (m)	6
Minimum Gap (mm)	6.95
Maximum Field Bmax (T)	0.74
Maximum Deflection Kmax	1.52
Total power (kW)	9.4
Power Density (kW/mrad^2)	7.45
Flux (ph/sec/0.1%BW)	1.6E+15

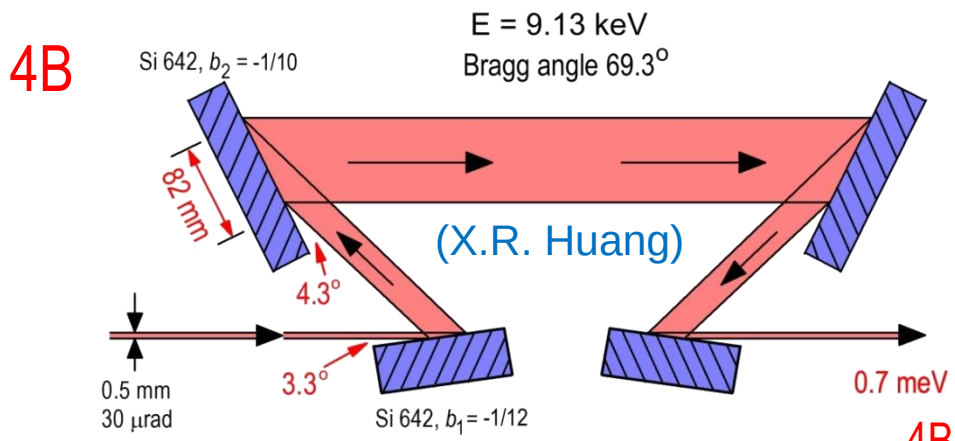


AGU: Adaptive Gap Undulator

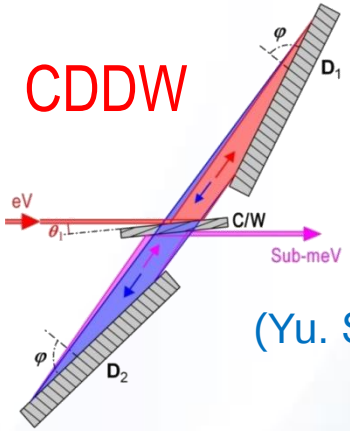


High Resolution Monochromator

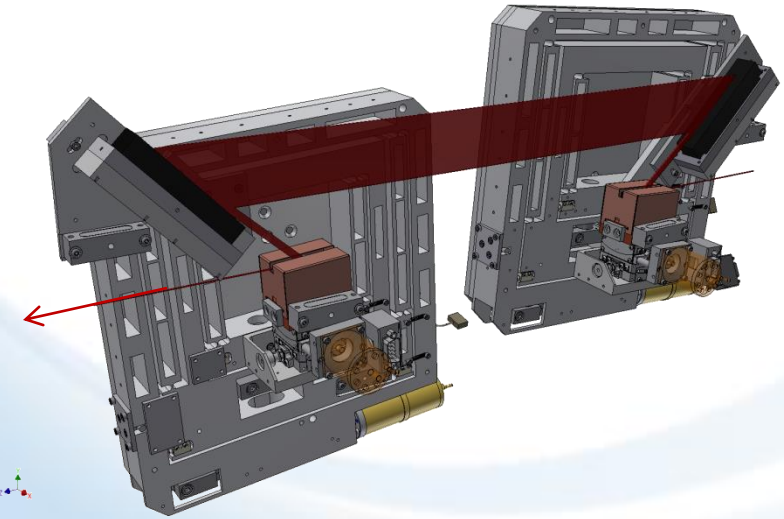
- Base line scope: 4B for 1 meV, including provision for 0.1 meV (CDDW)
- Expected flux ≥ 1.6 x 10^{10} photons/sec (IVU22-3m, 500 mA, with 4B)

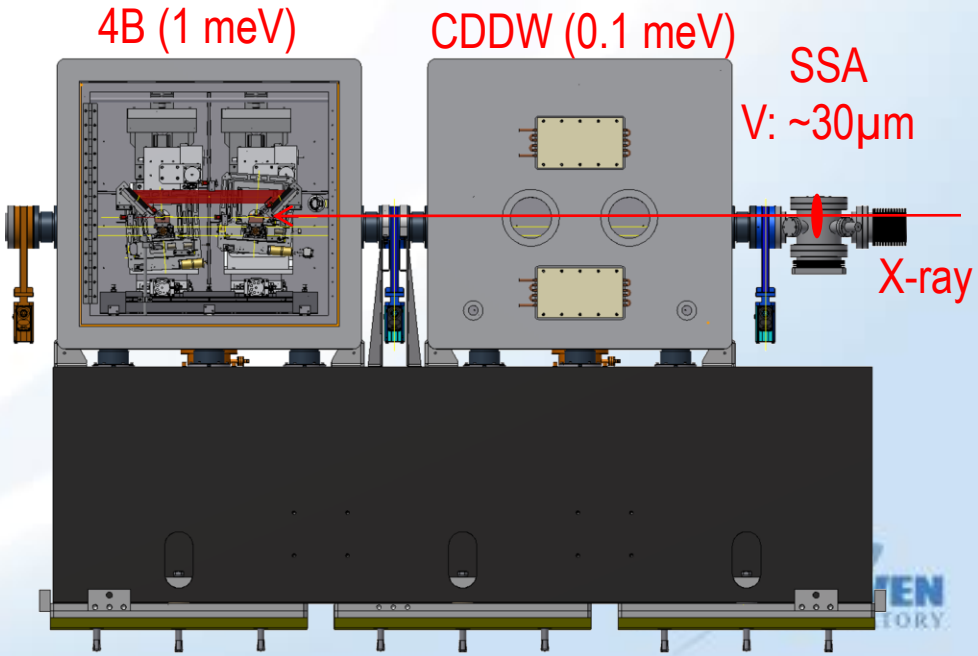


(X.R. Huang)



(Yu. Shvyd'ko)

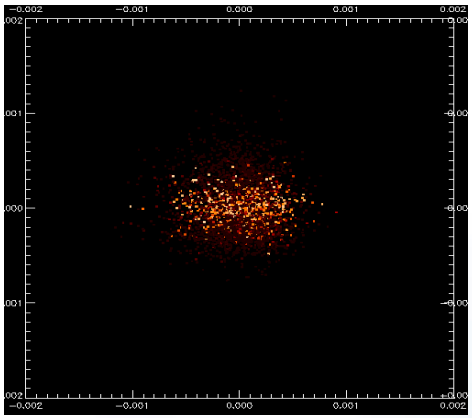


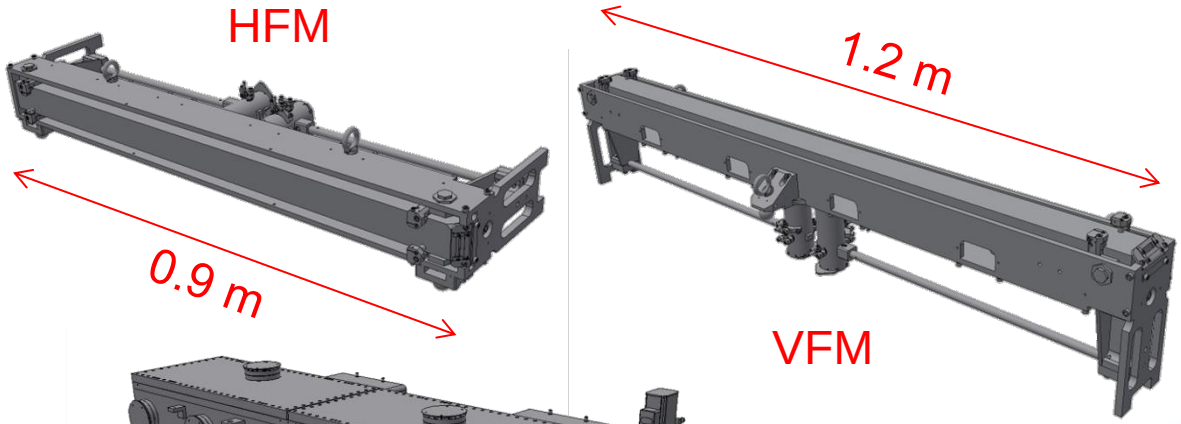


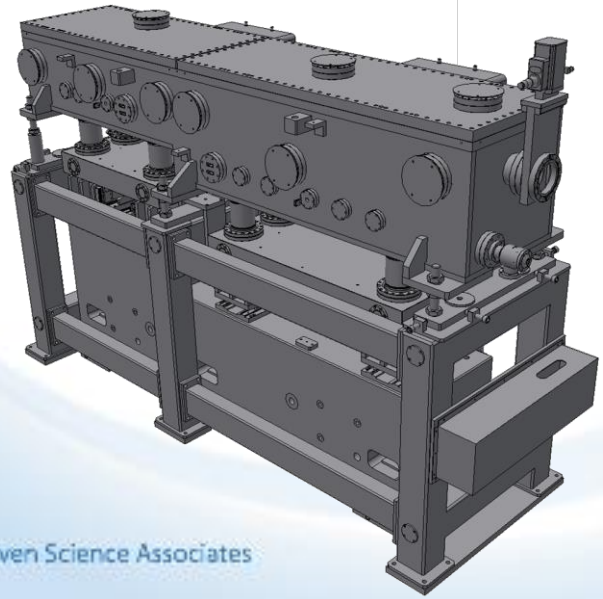
KB Mirrors

- Large, prefigured, bendable, to achieve slope error < 0.3 µrad
- Focal size at sample: ~ 5(V) x 7(H) µm^2

Ray Trace Results

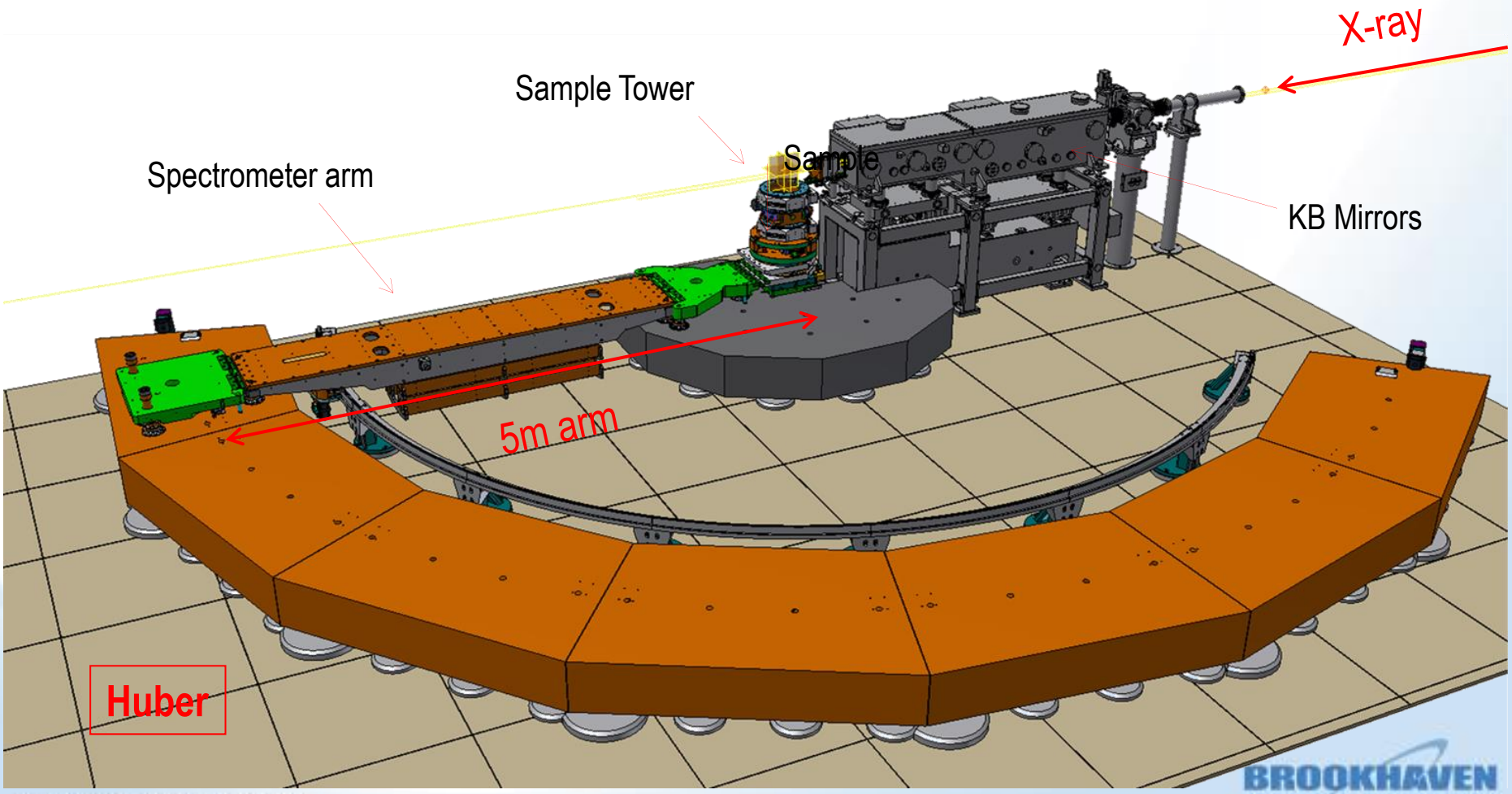






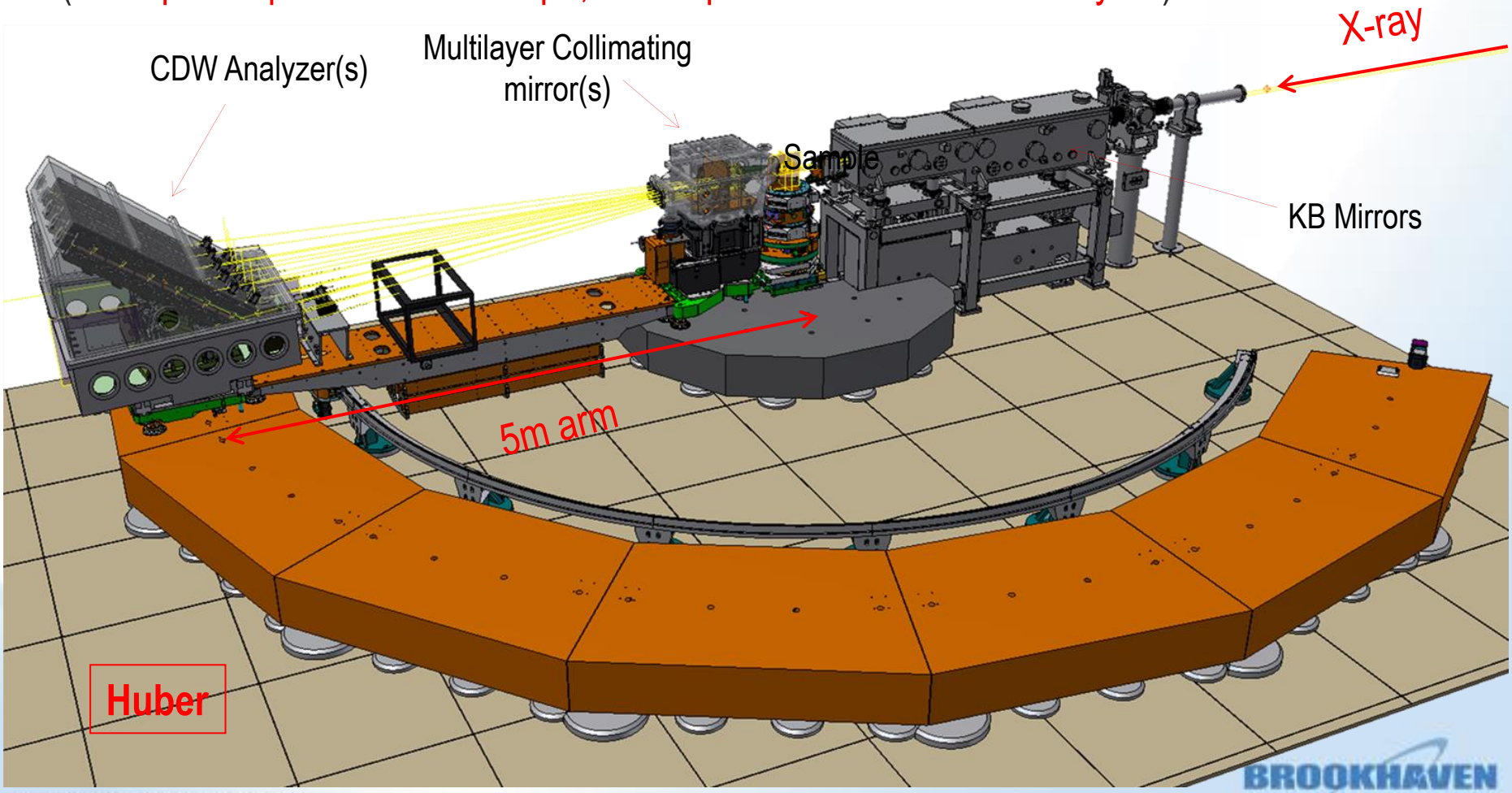
1-meV Spectrometer

- Spectrometer base mechanism design complete, components in production (Huber)
- Spectrometer arm scattering angle range: -7 to ~130 deg (Q_{MAX} ~ 80 nm^{-1})



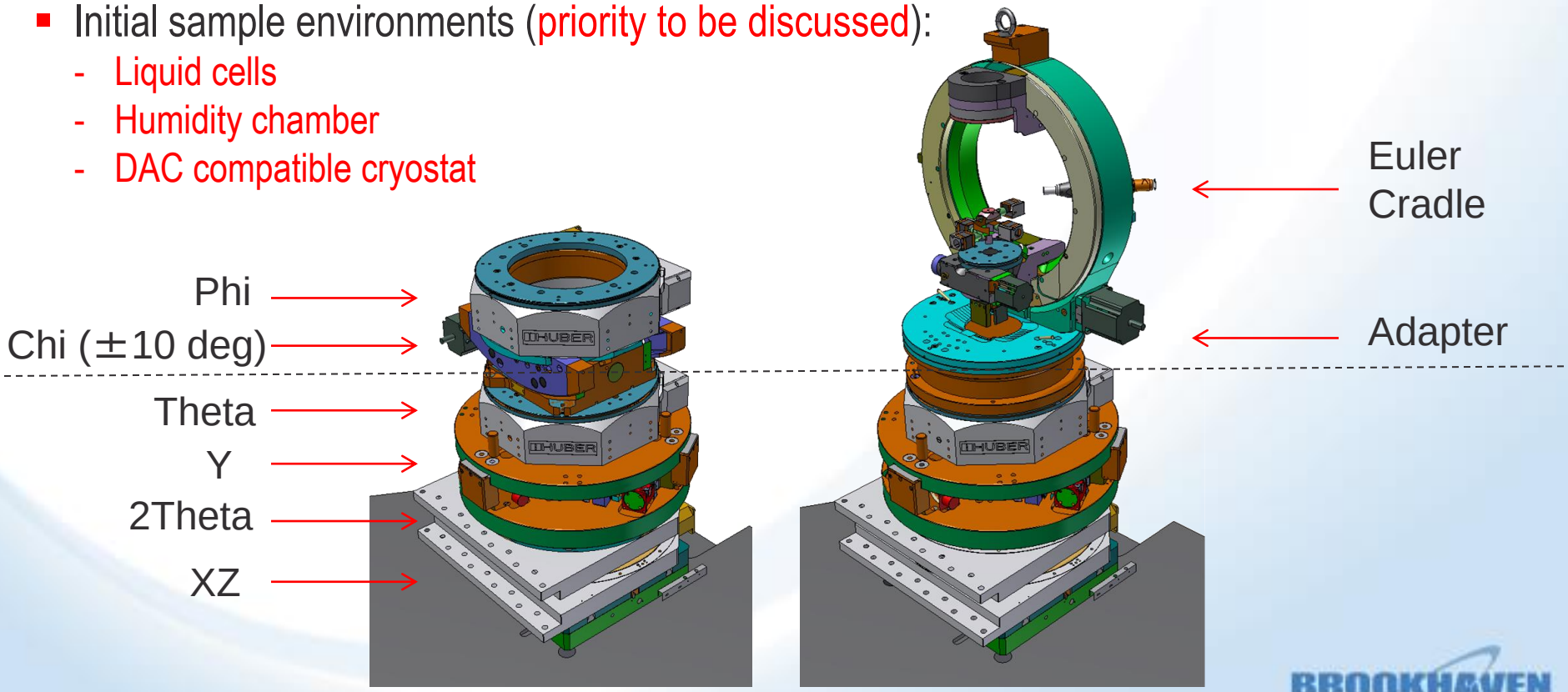
1-meV Spectrometer

- Support up to five analyzers, but only one analyzer will be built initially (base scope).
- Q range limited to ~40 nm^{-1} initially for scattering angle < 60 deg due to polarization effects (need phase plate – future scope, and improvement on CDW analyzer)



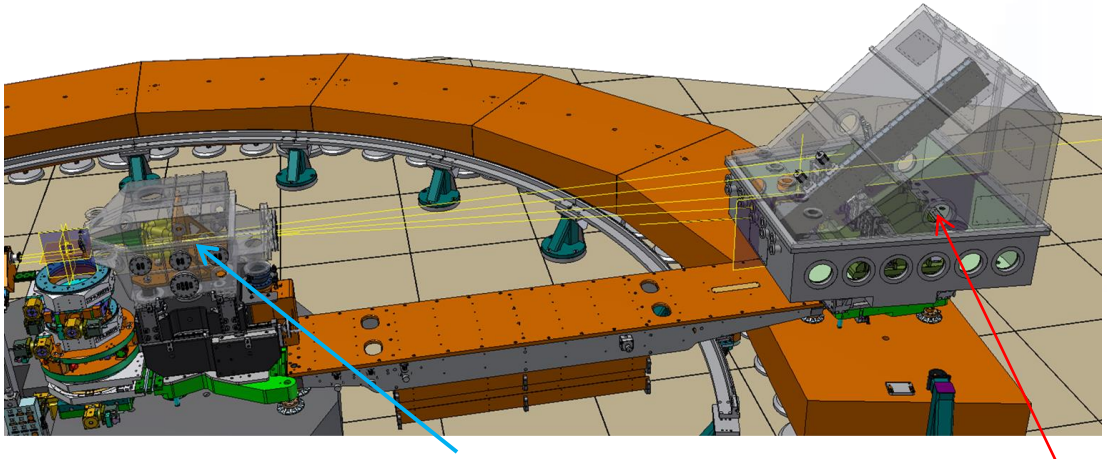
Sample Tower: Two Configurations

- Common XYZ, Theta and 2Theta motions
- Configuration A uses Chi tilt and Phi rotation stages: heavy sample environments (e.g., DAC compatible cryostat, large volume pressure cells)
- Configuration B uses Huber Euler cradle (Model 512.1): alignment capability for single crystals, Displex cryocooler, humidity chamber, etc.
- Initial sample environments (priority to be discussed):
  - Liquid cells
  - Humidity chamber
  - DAC compatible cryostat

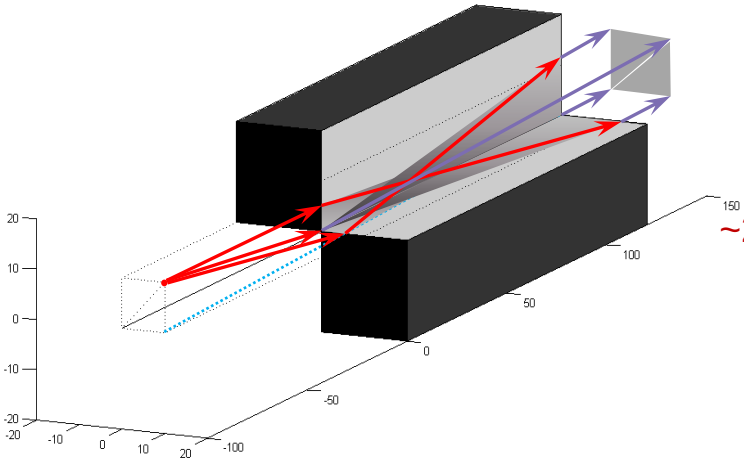


CDW Analyzer – Montel Mirror

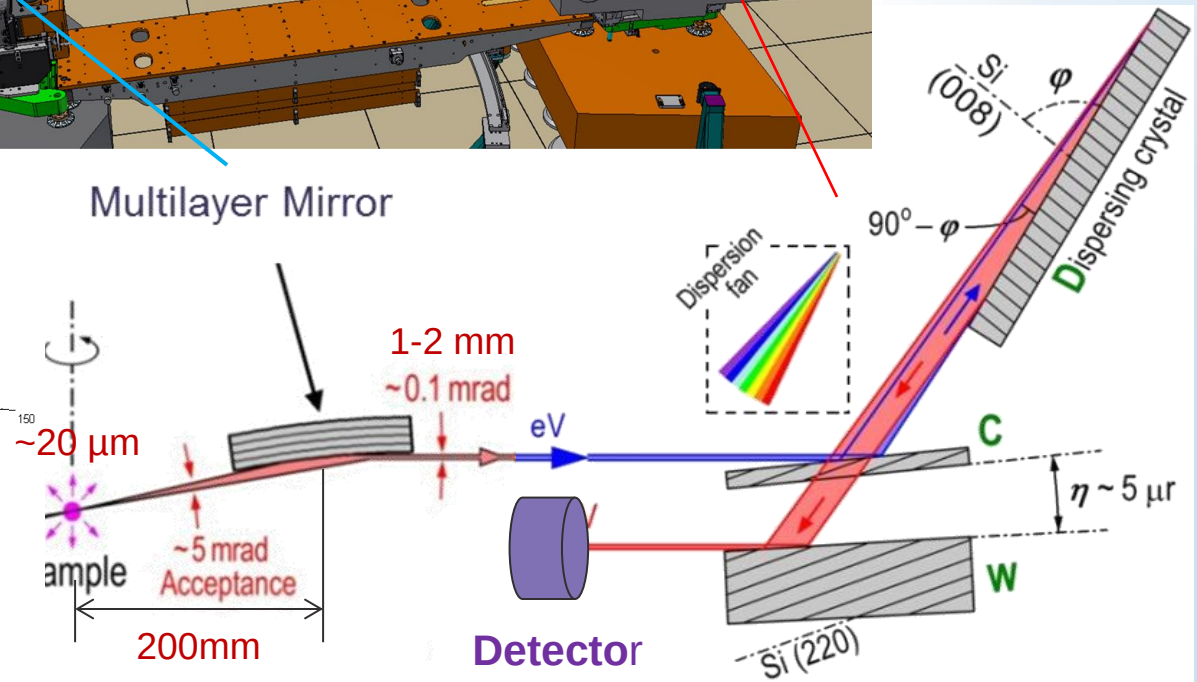
- The use of CDW optics for analyzer requires collimation: ≤ 0.1x0.1 mrad^2
- Montel mirror designed to achieve comparable acceptance to spherical diced analyzers: Angular acceptance @ full illumination: ≥ 10x10 mrad^2



Montel mirror



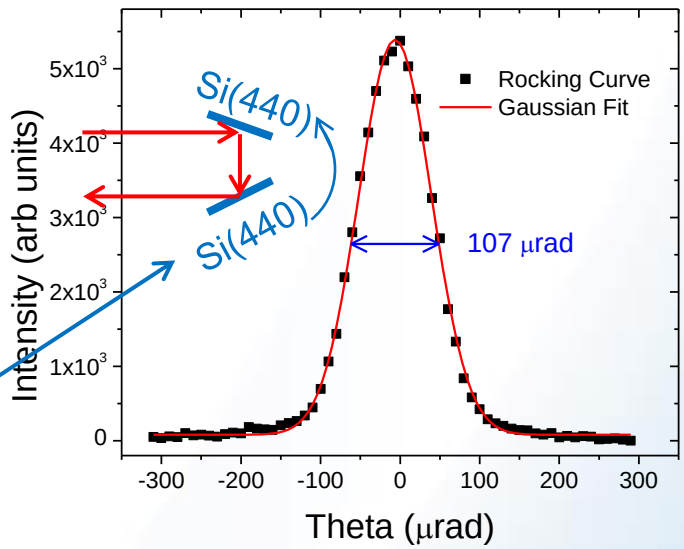
Multilayer Mirror



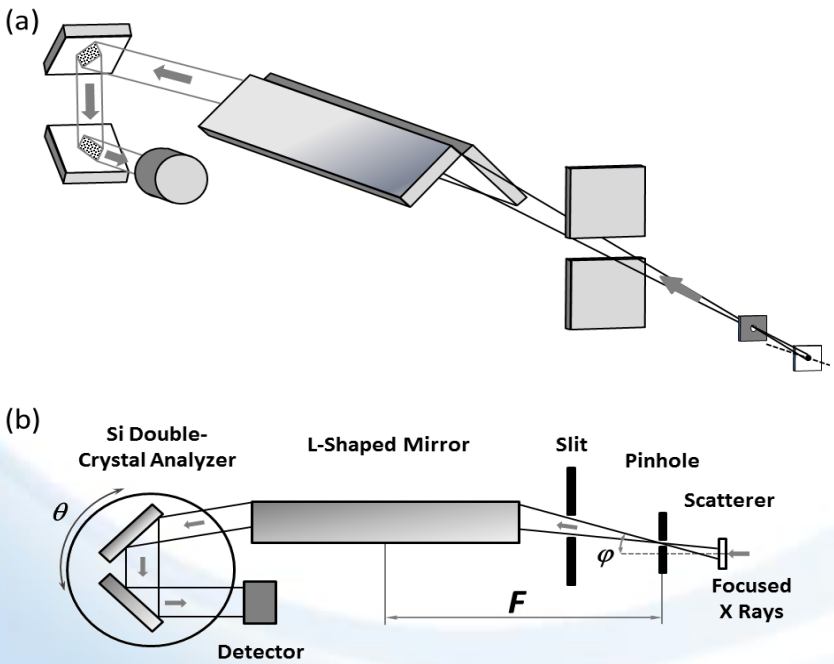
Montel Multilayer Mirror Test

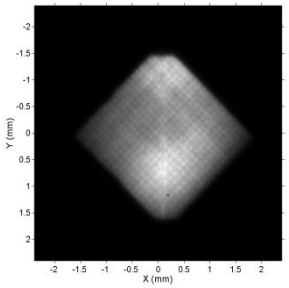
- **Performance**
  - Focal length: ~195 mm
  - Angular acceptance @ full illumination: > 10x10 mrad^2
  - Collimated beam divergence depends on pin hole size
  - Below ~ 20 µm, divergence < 100 µrad.
    - At 25 µm pin hole, divergence = 107 µrad.
  - Efficiency measured: ~ 47% (theory: 49%)

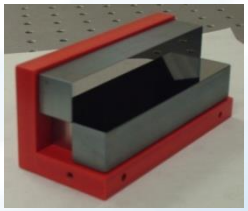
(Suvorov et al, submitted)

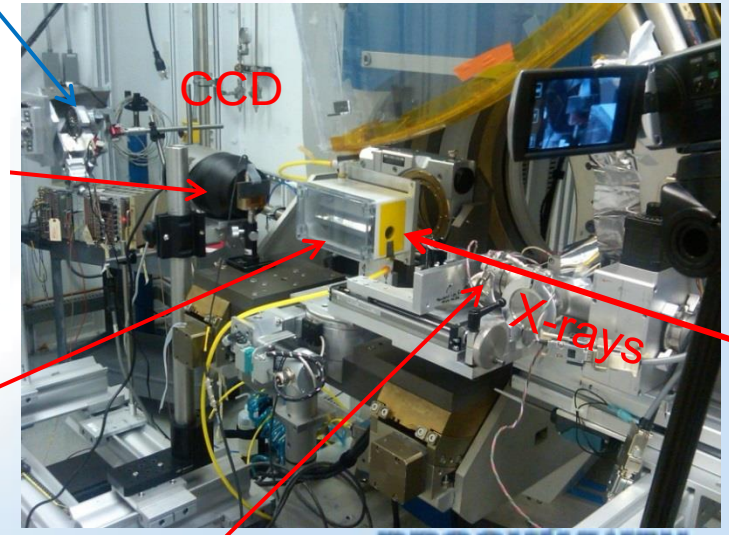


Divergence Analyzer







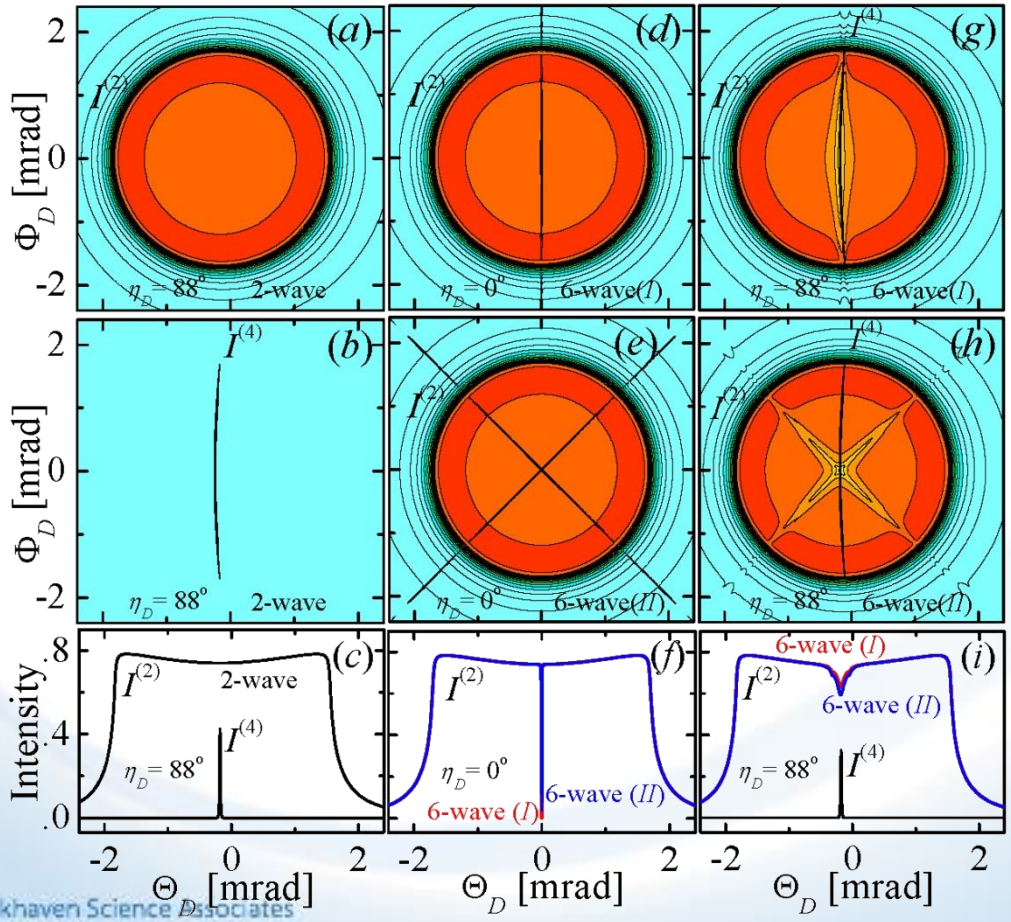


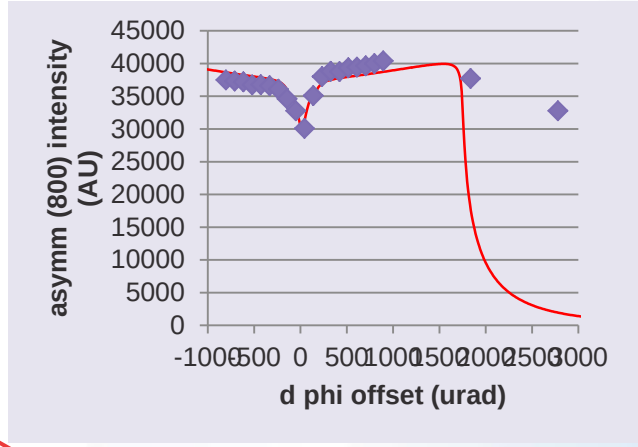
Scatter Source & Pin Hole

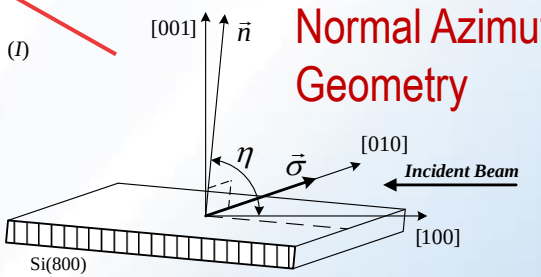
Multiple Beam Diffraction Effect

Stetsko *et al*, PRL (2011)

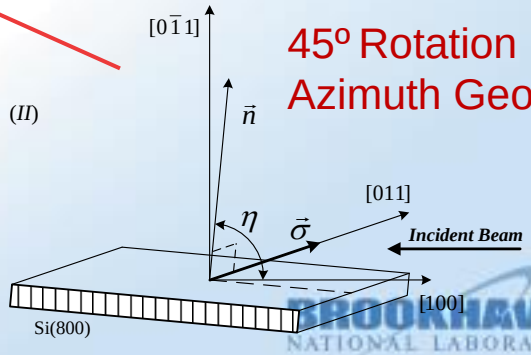
- MBD in CDW/CDDW causes 10-30% loss of spectral efficiency, but can be removed by introducing Φ angle offset with the 45º rotation azimuth geometry







Normal Azimuth Geometry

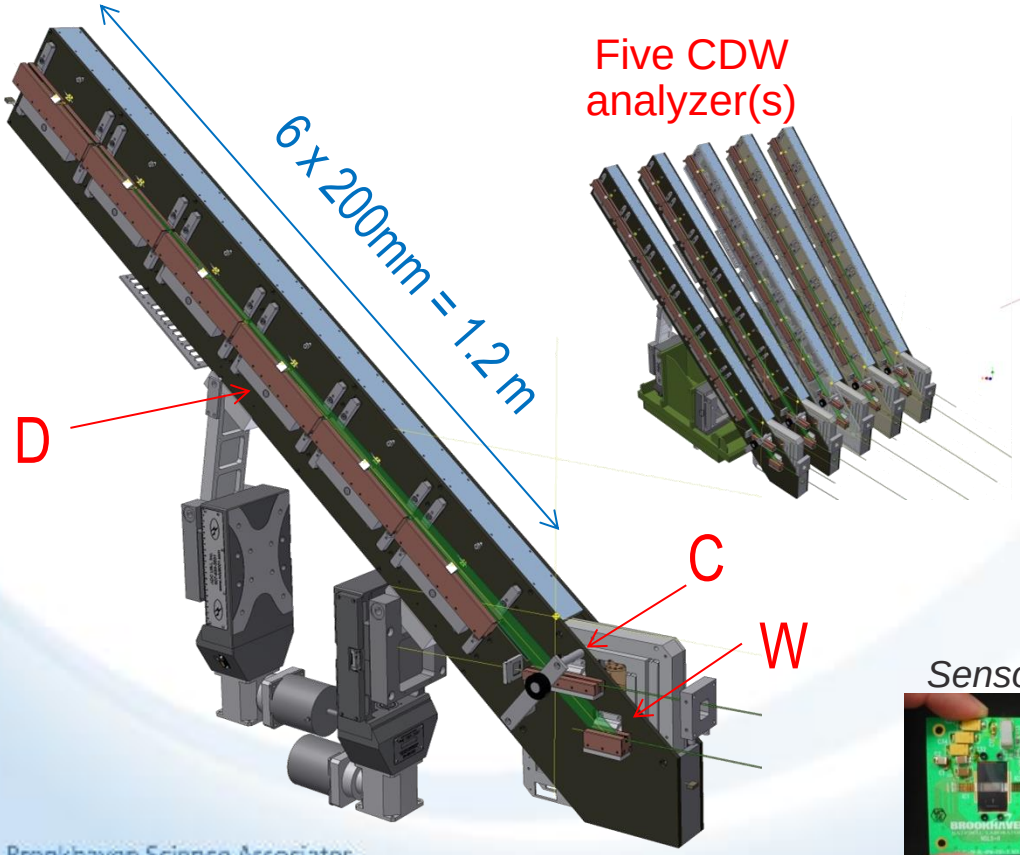


45º Rotation Azimuth Geometry

Analyzer Mechanism Final Design

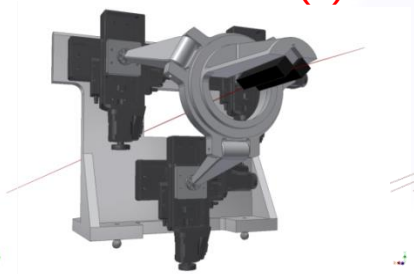
S. Coburn, S. Antonelli, *et al*

- CDW configuration with six D crystals, 200 mm length each, individual adjustment and detection, accepting total of 1.5 mm vertical incident beam size.
- Pseudo 2D strip detector to distinguish reflections from individual D crystal & utilizing Φ de-tuning to remove MBD loss (cf, *Stetsko et al, PRL 2011*).
- Support up to 5 CDW analyzers using single-reflection toroid mirrors (Future scope)

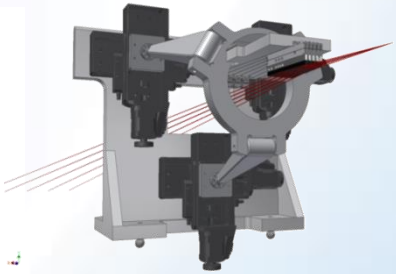


Five CDW analyzer(s)

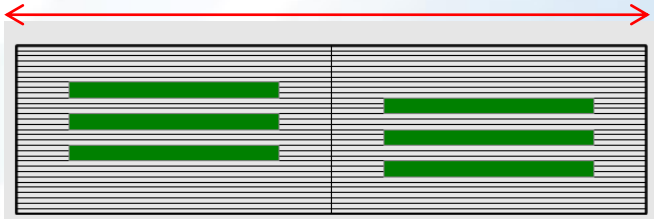
One to Three Montel mirror(s)



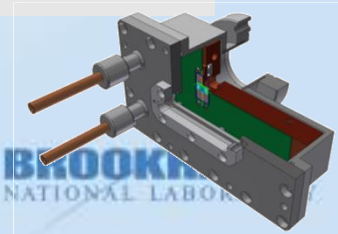
Five single-reflection toroid mirrors



2 x 3 = 6 mm



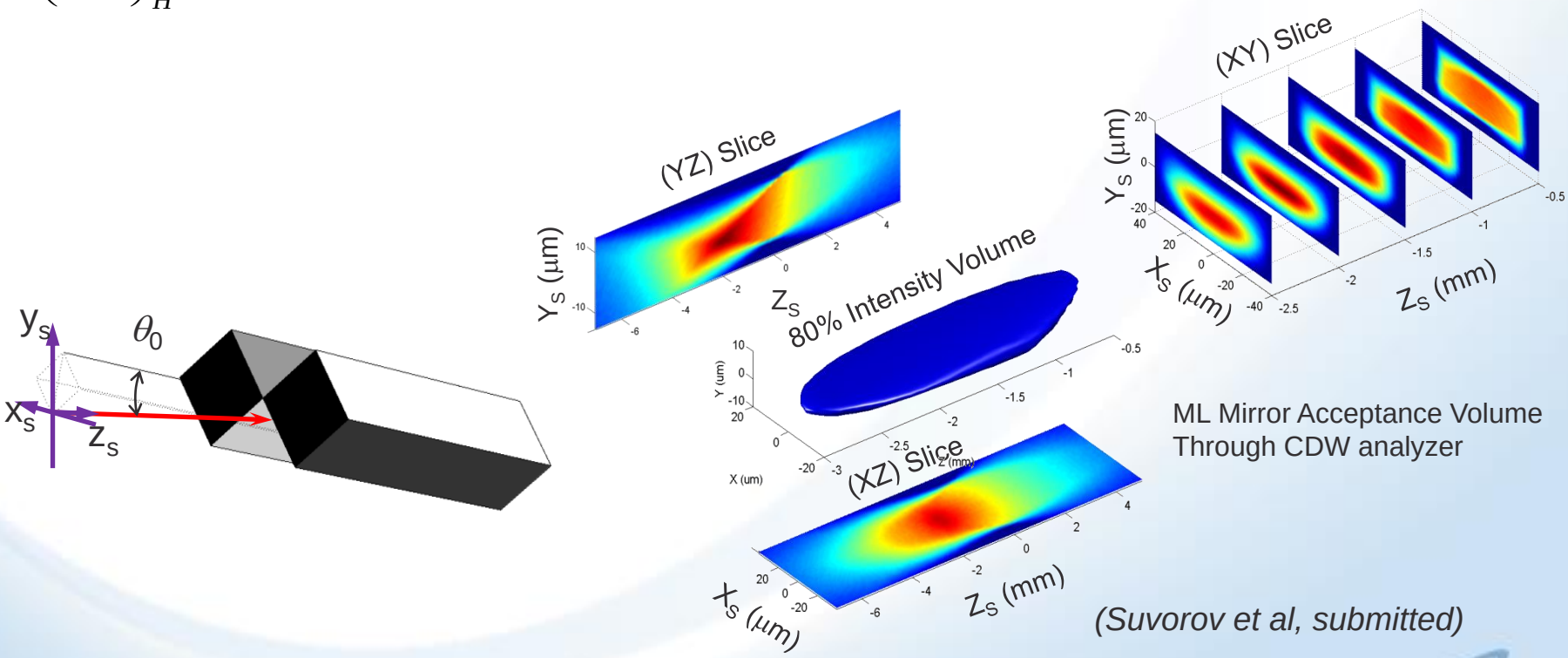
Sensor Board



Sample Acceptance Volume

- Acceptance volume in forward scattering: ~20µm (X) x 20µm (Y) x **2mm** (Z)
- Vertical divergence of collimating beam: No effect on energy resolution
- Horizontal divergence of collimating beam can be relaxed: larger acceptance volume

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

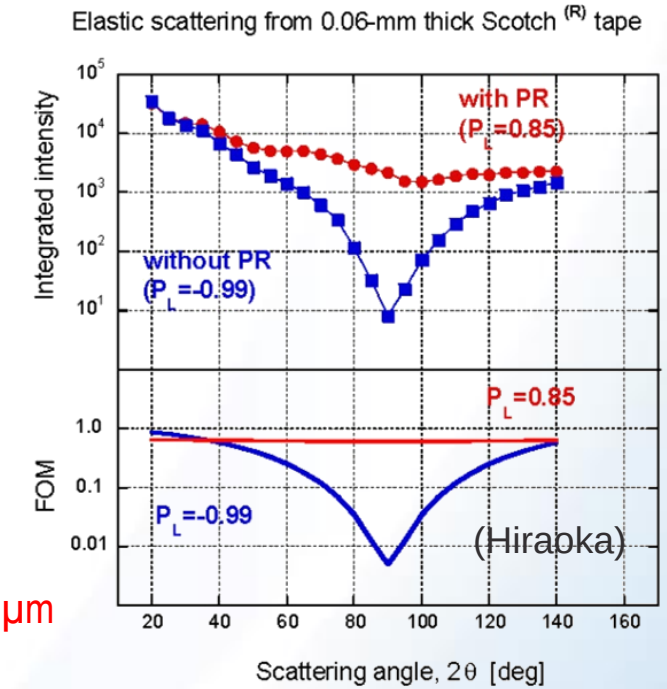


ML Mirror Acceptance Volume Through CDW analyzer

(Suvorov et al, submitted)

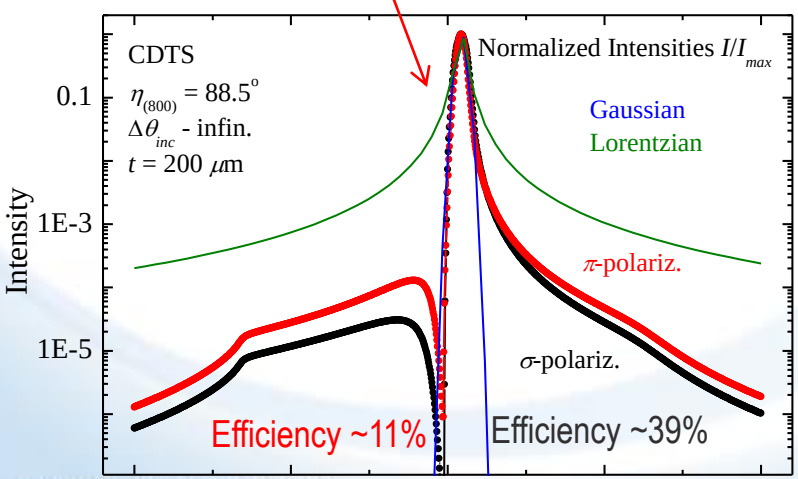
Analyzer Optics for large Q (> ~40 nm^{-1})

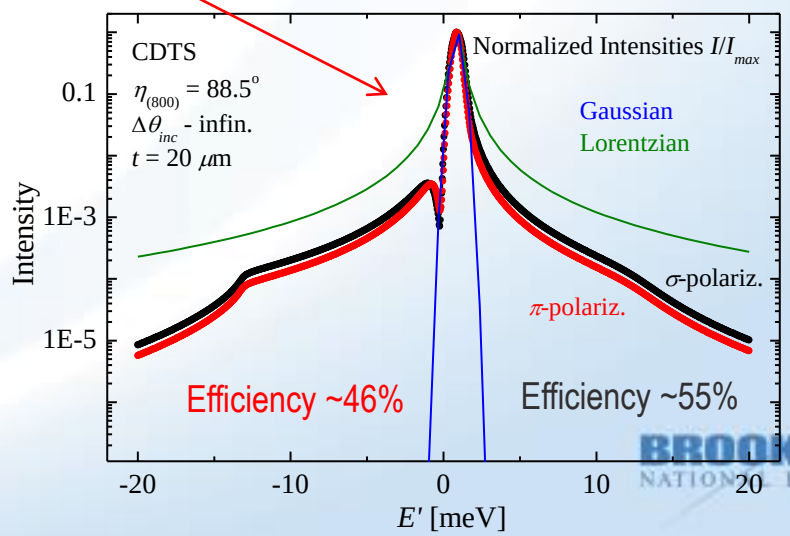
- Incident beam requires phase plate (future scope)
- CDW analyzer efficient reduced by a factor of ~4 for π polarization (cause: reduced anomalous transmission in C crystal).
- Solution: develop ultrathin (~20μm) C crystals. Minimum impact on resolution (Yuriy Stetsko)



Resolution function for t = 200μm

Resolution function for t = 20μm





Initial Performance & Capabilities

Performance Comparison :

Facility (Beamline)	ΔE (meV)	ΔQ** (nm^{-1})	E (keV)	$I_{inc.}$ @ ΔE (photons/sec)	Beam Size (V × H μm²)	Flux Density (photons/sec/μm²)	Sharp Res. Tails
ESRF (ID28)	1.6	0.5	21.7	6×10^9	7 × 12	7.1×10^7	--
APS (30-ID-C)	1.5	0.6	23.8	2×10^9	15 × 35	3.8×10^6	--
SPring-8 (43LXU)	1.5	0.5	21.7	$\sim 5 \times 10^{10}$	20 × 35	$\sim 7.1 \times 10^7$	--
NSLS-II (IXS)	1.0	0.2	9.1	$\sim 1.6 \times 10^{10}$ (4B HRM)*	5 × 7	**$\sim 5 \times 10^8$**	yes

* Performance for a IVU22-3m at 500 mA (flux 8×10^{14} phs/sec/0.1% bw) and 30% spectral efficiency for the 4B monochromator.
** Assuming 5 mrad acceptance angle.

$$\frac{I}{I_0} = \frac{r_e^2 \hbar^2 c^2 (\delta q)^2}{2eE_i^2} Z^2 \rho l_{abs} \frac{k_B T}{M \upsilon^2}$$

$$\frac{I}{I_0} \propto \left(\frac{\delta q}{E_i}\right)^2 l_{abs} = \left(\frac{2}{\hbar}\delta\vartheta\right)^2 l_{abs}$$

H. Sinn, J. Phys. Cond. Mat. (2001)

Count Rate Estimates (single analyzer):

Sample	Thickness (μm)	ESRF ID28 (cnts/sec)	NSLS-II IXS (cnts/sec)
v-SiO_2	2100/190	~0.2	**~0.2**
H_2O (HP)	1000/1000	~1.0	**~8**
La_2CuO_4	75.3/7.13	~0.5	~0.04
Solid O_2	10/10	~1.5	**~2**

(ESRF data courtesy of M. Krisch)

- Unique research strength for low-Z materials and high-pressure DAC systems (small beam size, highest flux density)
- Initial performance may be lower by a factor of 5 due to lower operation current (~100mA)

Summary

- The new angular dispersive optics offers NSLS-II a unique opportunity to build a fundamentally new IXS spectrometer with unprecedented performance.
- Latest CDW-CDW and CDW-4B tests results validate the baseline performance goal for the IXS beamline.
- Count rate estimate for 1 meV resolution indicates better performance for low-Z materials in general, and for HP systems in particular, with substantial signal gain compared to state-of-the-art optics operating at 1 meV, and much enhanced contrast due to sharp resolution tails.

Look forward to an exciting workshop discussing possible experiments

&

Thank you for your attention!